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OXIDATIVE MODIFICATION OF CELLULOSE

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Abstract

Cellulose, as the most abundant natural polymer, is a promising raw material for the preparation of biocompatible and biodegradable materials via selective oxidation. In our study, we developed and pilot-tested a one-step TEMPO-mediated oxidation method capable of yielding oxidized cellulose with a carboxyl content exceeding 1.0 mmol COOH/g. The process was based on activation of the catalytic system, oxidative treatment of bleached kraft pulp, and subsequent purification steps. The efficiency and selectivity of the method were confirmed by conductometric titration according to SCAN-CM 65:02 and internal protocols. The results demonstrate the potential of this process for the production of high-quality oxidized cellulose suitable for medical and pharmaceutical applications.

Introduction

Cellulose is a naturally abundant, renewable, and biodegradable polysaccharide with a wide range of industrial and biomedical applications. Beyond its conventional use in the paper industry, cellulose serves as a valuable precursor for various functional materials via chemical modification. Among these, oxidative modification is one of the most important strategies for converting cellulose into materials with unique properties, especially due to the introduction of carboxyl groups[1].

Oxidized cellulose has been extensively studied and utilized for its excellent biocompatibility, bioresorbability, and functional versatility. It is widely applied as a haemostatic agent, anti-adhesion barrier, tablet binder, wound dressing, and scaffold material in tissue engineering. Additionally, oxidized cellulose is considered an intermediate[3] in the preparation of nanocellulose and, under deep oxidation, as a feedstock for low molecular weight carboxylic acids such as formic and acetic acid[2].

A particularly efficient and selective method for cellulose oxidation is the TEMPO-mediated process, which primarily targets the primary hydroxyl groups of the anhydroglucose units, transforming them into carboxyl functionalities. This reaction proceeds under mildly alkaline conditions in the presence of NaOCl and a catalytic amount of TEMPO and NaBr, generating nitrosonium ions as active oxidants[4].

In the present work, we describe the development and scale-up of a one-step TEMPO-mediated oxidation process, aimed at producing oxidized cellulose with a high carboxyl group content. The resulting material was characterized using conductometric titration methods, confirming the effectiveness and repeatability of the process.

Experiment

Materials

Bleached birch kraft pulp was used as the cellulose source. Sodium hypochlorite (NaOCl, 174 g Cl_2/L), TEMPO (2,2,6,6-tetramethylpiperidine-N-oxyl), sodium hydroxide (NaOH, 7% solution), and sulfuric acid (5.6% solution) were used for oxidation. All reagents were of technical grade. Deionized water with conductivity <0.1 mS/cm was used throughout.

TEMPO-mediated Oxidation Procedure

The oxidation process consisted of several steps, carried out in a pilot-plant setup:

- **Catalyst activation:**

  8.6 kg of deionized water at 40 °C was introduced into a 12 L stirred plastic tank. To this, 250 g of NaOCl solution was added and pH was adjusted to 7.5 using diluted sulfuric acid. Subsequently, 32 g of TEMPO was added and pH was further lowered to 6.5.

- **Pulp disintegration:**

15 kg of bleached kraft pulp, cut into ~10×10 cm pieces, was soaked in 575 L of deionized water (50–52 °C) in a 1000 L reactor for 15 minutes without agitation, followed by 45 minutes of mixing at 35 rpm.

- **Oxidation:**

  After disintegration, 35 L of activated catalyst solution was added, and stirring was increased to 55 rpm. Then, 22 kg of NaOCl was gradually dosed over 2 hours (¾ in the first hour, ¼ in the second hour), while maintaining pH at 8.5–9.0 with parallel addition of NaOH. After dosing, the suspension was stirred for another 1.5 hours for complete reaction.

- **Washing and separation:**

  The reaction slurry was separated using a horizontal centrifuge and washed with 20 L of deionized water. The pulp was then suspended in 700 L of warm (50 °C) deionized water, stirred for 5 minutes, and centrifuged again to yield the oxidized cellulose.

Determination of Carboxyl Group Content

Carboxyl group content was determined using conductometric titration[5,6] based on SCAN-CM 65:02 and internal method PI-VO 149/2015:

1. **Sample preparation:** The oxidized cellulose was protonated by treatment with 1% HCl, thoroughly washed to remove residual acid (confirmed via $AgNO_3$ or pH titration), and dried to constant weight at 100 °C.
2. **Titration:** 1 g of dried, protonated cellulose was suspended in 400 mL of deionized water. A few drops of bromophenol blue were added as a pH indicator. The suspension was titrated with 0.1 mol/L NaOH while recording conductivity after each addition. The titration curve typically exhibited three phases, with the carboxyl group content calculated from the NaOH volume difference between the start and end of the second phase.
3. **Calculation:** The amount of carboxyl groups $c_{(}COOH_{)}$ in µmol/g was calculated using the formula:

$$c_{(}COOH_{)} = ((V_2 - V_1) \times c_{(}NaOH_{)} \times 1000) / m$$

where:
V_1 and V_2 = start and end volume of titration phase for COOH groups (in mL),
$c_{(}NaOH_{)}$ = concentration of NaOH (mol/L),
m = mass of dry sample (g).

Discussion and Result Analysis

The TEMPO-mediated oxidation process developed and tested in our pilot-plant trials proved to be a robust and reproducible method for introducing carboxyl functionalities into the cellulose backbone. The conductometric titration results, summarized in Table 1, confirm that the method can consistently yield oxidized cellulose with a carboxyl content above 1.0 mmol COOH/g.

Table I
Summary of pilot-scale oxidation trials and analytical results

Trials	Product [kg]	Dry Matter [%]	COOH [µmol/g]	Conductivity [µS/cm]
01	60.1	20.2	1107	575
02	50.54	22.22	1024	435
03	59.08	20.22	993	440
04	51.0	23.73	1045	430
05	50.9	23.65	1006	490
06	54.4	15.10	950	515
07	74.7	15.98	1039	520

The highest carboxyl content was observed in sample 01, reaching 1107 µmol/g (1.107 mmol/g), which exceeds the typical values reported for single-step TEMPO oxidation (usually 0.7–0.9 mmol/g). These results confirm that, under optimized conditions (e.g., precise pH control, effective reagent dosing, and controlled reaction time), it is possible to achieve high degrees of oxidation even without a secondary chlorite oxidation step.

The relatively stable conductivity values in the range of 430–575 µS/cm indicate consistent washing efficiency and a minimal presence of residual salts or acidic byproducts. This is important for applications in biomedicine, where ionic purity of materials is crucial.
Moreover, the process demonstrates scalability, as the trials were carried out using 15 kg batches of cellulose and volumes exceeding 500 L. The use of standard industrial equipment such as a 1000 L plastic reactor, horizontal centrifuge, and standard dosing systems supports the applicability of this method for industrial upscaling.
From a technical point of view, the high carboxyl group content, confirmed via validated conductometric titration (compliant with SCAN-CM 65:02 and internal protocol PI-VO 149/2015), makes the oxidized cellulose suitable for applications requiring strong anionic surface functionalities. These include:

- haemostatic materials (where surface charge aids blood clotting),
- wound dressings (enhancing fluid absorption),
- drug delivery matrices (where –COOH groups can interact with APIs), and
- biodegradable gels and scaffolds.

Conclusion

In this study, a one-step TEMPO-mediated oxidation process of bleached kraft pulp was successfully developed and validated at pilot scale. The optimized procedure enabled the selective oxidation of primary hydroxyl groups to carboxyl groups, resulting in oxidized cellulose with consistently high carboxyl content exceeding 1.0 mmol COOH/g.
The oxidation process demonstrated high reproducibility, operational simplicity, and scalability, making it suitable for future implementation in industrial environments. The resulting oxidized cellulose exhibits properties that are highly relevant for biomedical and pharmaceutical applications, including high anionic functionality, water dispersibility, and biocompatibility.
The process control strategy, particularly pH regulation and reagent dosing, was essential to achieving high yields and selectivity without the need for a secondary chlorite oxidation step. The application of conductometric titration for carboxyl group quantification ensured accurate characterization of the final product.
Future work may focus on further process optimization, evaluation of product performance in specific end-use applications, and long-term stability assessments of the oxidized cellulose material.

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BIOTECHNOLOGY AND BIOREFINERY

COMPARATIVE METHYLATION ANALYSIS OF CALDIMONAS THERMODEPOLYMERANS USING THIRD GENERATION SEQUENCING

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Abstract

DNA methylation in bacteria plays a crucial role in epigenetic regulation, influencing gene expression and environmental adaptation. In this study, we conducted a comparative analysis of methylation patterns in the Gram-negative bacterium *Caldimonas thermopolymerans* DSM 15344^T (CT) cultivated under different conditions and deposited in two microbial collections: CT-DSMZ (Germany) and CT-CCM (Czechia). Using Oxford Nanopore Technologies sequencing, we assessed whether cultivation conditions and phenotypic differences correlate with methylation patterns. To enhance detection, we also integrated data from the Pacific Biosciences Sequel IIe platform. CT-CCM exhibited higher modification counts, with 7,350 6mA, 2,764 5mC, and 732 4mC sites, compared to 6,884, 2,681, and 643 in CT-DSMZ, respectively. Methylation distribution across genomic annotation features reflected similar trends. Our study highlights the potential impact of cultivation conditions and environmental factors on bacterial epigenomes and contributes to a better understanding of how methylation affects physiology and adaptation in prokaryotes.

Introduction

DNA methylation is a fundamental epigenetic modification involving the addition of a methyl group to a nucleotide base within the DNA molecule. This does not alter the DNA sequence itself but can influence how genes are expressed, replicated, or repaired [1]. It is widespread across both prokaryotic and eukaryotic organisms and serves diverse biological functions. In bacteria, methylation typically occurs in the form of N6-methyladenine (6mA), 5-methylcytosine (5mC), and N4-methylcytosine (4mC), each catalysed by specific methyltransferases. It plays critical roles in regulating gene expression, initiating DNA replication, modulating genome stability, mediating host-pathogen interactions, and enabling bacterial adaptation to environmental changes [2, 3]. These modifications are catalysed by specific DNA methyltransferases, often within the context of restriction-modification (RM) systems [4]. While traditionally viewed as defensive barriers against foreign DNA, emerging research has shown that methylation also functions independently of RM systems to regulate transcription, control mobile genetic elements, and influence phenotypic plasticity [5].

Advancements in third-generation sequencing platforms have made it possible to study DNA methylation directly from native DNA without chemical conversion or enrichment. Two of the most widely used long-read sequencing technologies are Pacific Biosciences (PacBio) and Oxford Nanopore Technologies (ONT), offering the ability to detect base modifications at single-nucleotide resolution across entire bacterial genomes [6]. The PacBio platform detects DNA methylation by observing subtle changes in how the DNA polymerase moves along the strand during sequencing, which makes it highly sensitive and accurate [7]. In contrast, ONT sequencer reads DNA directly as it passes through a tiny nanopore, detecting methylation by measuring disruptions in the electrical signal. This approach allows ONT to sequence the genome and identify methylation patterns at the same time, using the raw signal data. The continued development of ONT basecalling models and methylation calling tools has significantly improved the resolution and interpretability of bacterial methylomes.
In this study, we investigate DNA methylation variation in *Caldimonas thermodepolymerans* DSM 15344^T (CT), a thermophilic, Gram-negative bacterium notable for its ability to synthesise polyhydroxyalkanoates (PHAs), which are biodegradable polymers [8, 9]. PHA has attracted interest for their potential role in sustainable bioplastic production, making *C. thermodepolymerans* significant for industrial and environmental biotechnology applications. It was originally isolated from activated sludge in Germany. The type of strain was deposited in two culture collections under the Leibniz Institute DSMZ in Germany (CT-DSMZ) and the Czech Collection of Microorganisms (CT-CCM) in the Czech Republic. Although genetically identical, these two cultures have

undergone independent cultivation and preservation, potentially leading to phenotypic and epigenetic divergence. While phenotypic changes between strains maintained under different conditions are often noted, their underlying molecular mechanisms, especially at the epigenetic level, are rarely characterised.

Here, we aim to determine whether differences in cultivation history are reflected in the methylation landscapes of CT-DSMZ and CT-CCM. We employed ONT sequencing technology to obtain high-coverage, modification-aware reads and complemented this with high-confidence methylation data from the PacBio sequencing platform. This combined approach allowed us to robustly detect 6mA, 5mC, and 4mC modifications across the genome. By comparing the methylomes of the two strains, we explore how environmental and cultivation differences may contribute to epigenetic variation and potentially influence strain physiology and adaptation.

Materials and Methods

2.1 Bacterial Strains and Sequencing

The study focused on *C. thermodepolymerans* DSM 15344^T. Two specific cultures of this strain were compared: one obtained from the Leibniz Institute DSMZ-German Collection of Microorganisms and Cell Cultures (CT-DSMZ) and another from the Czech Collection of Microorganisms (CT-CCM). Whole-genome sequencing was performed using ONT and PacBio sequencers. We used R10.4.1 flow cells with v14 sequencing chemistry for ONT, and for PacBio, the Sequel IIe system was used.

2.2 Methylation Detection

Raw ONT signal data in POD5 format were basecalled using the Dorado basecaller (v0.7.2)[10], which generated BAM files with modified base calls. The reference genome of *C. thermodepolymerans* DSM 15344^T (GenBank accession: CP064338.1) was used for alignment via Dorado's built-in aligner. Methylation calling was then performed using Modkit (v0.4.1)[11], producing a bedMethyl file containing predicted 6mA, 4mC, and 5mC modifications.

For PacBio data, demultiplexing was performed first using the lima tool (v2.13.0)[12]. The ccs-kinetics-bystrandify tool (v3.5.0) from the PacBio BAM toolkit (pbtk) was then applied to the resulting BAM file to extract and organize existing kinetic information, including interpulse duration (IP) tags, by DNA strand[13]. This step allows strand-specific analysis of methylation signals in downstream analysis. Mapping to the reference genome (GenBank accession: CP064338.1) was done using pbmm2 (v1.17.0), which is minimap2 [14] wrapper for PacBio data, and methylation calling was performed using ipdSummary (v3.0) from the kineticsTools package[15]. The output was provided in GFF format, containing 6mA, 5mC, and 4mC modifications.

2.3 Annotation

Genome annotation of the reference genome was obtained from the NCBI database, where it was annotated using PGAP, a NCBI Prokaryotic Genome Annotation Pipeline designed to annotate bacterial and archaeal genomes [16]. It identified various genomic features, including coding sequences (CDS), transfer RNAs (tRNAs), ribosomal RNAs (rRNAs), and other functional elements. The output included a GFF3 annotation file along with corresponding protein, nucleotide, and functional annotation files, which were used for downstream comparative and functional analyses.

2.4 Quantification of Methylation in Genomic Features

Methylation sites identified in the bedMethyl files were mapped to coding sequence (CDS) features defined in the Prokka-generated GFF3 annotation file. This allowed the assignment of each detected methylation site to specific annotated genes. For both CT-DSMZ and CT-CCM samples, the number of modifications was quantified per CDS feature, including separate counts for each methylation type (6mA, 5mC, and 4mC) and the total number of modifications per gene. Thus, enabling a comparative analysis of methylation patterns across annotated genes in both sample conditions.

2.5 COG Functional Category Analysis

The CDS features from the Prokka annotation file were mapped to Clusters of Orthologous Groups (COG) functional categories to provide insights into the functional context of methylation. Each CDS was assigned a corresponding single-letter COG functional category using an external mapping file derived from the NCBI COG database resources (COG2024 release)[17]. This allowed grouping of genes based on shared biological roles such as metabolism, information storage, and cellular processes. Methylation counts, both total and per modification type (6mA, 5mC, 4mC), were then aggregated for all CDSs within each COG category for both CT-DSMZ and CT-CCM samples. This enabled comparative analysis of functional enrichment in methylation patterns across both bacterial strains.

Discussion and result analysis

Our study aims to investigate whether cultivation of a similar strain under different conditions leads to detectable changes in DNA methylation patterns in *C. thermodepolymerans*. Our analysis revealed that the CT-CCM strain consistently showed a higher number of methylation modifications compared to CT-DSMZ. These differences were evident across both whole methylation counts and gene-specific modifications, which suggests a broad epigenetic response associated with environmental adaptation. Whole-genome sequencing of *C. thermodepolymerans* strains CT-DSMZ and CT-CCM using ONT revealed widespread DNA methylation differences. To ensure consistency and confidence, a minimum modification fraction of 0.95 was used as a filter for identifying high-confidence methylation sites. Overall, the CT-CCM strain showed a higher number of methylation sites across the genome compared to CT-DSMZ, indicating possible epigenetic adaptation due to different cultivation environments and metabolic preferences. CT-CCM showed 10,846 methylation sites, with 10,200 of these located in coding sequences (CDS). These included 7,153 6mA, 2,339 5mC, and 708 4mC modifications. On the other hand, the CT-DSMZ strain had 10,208 methylation sites, with 9,590 in CDS regions, consisting of 6,680 6mA, 2,290 5mC, and 620 4mC sites. While the numerical differences may appear very small and subtle, they reflect significant variation in methylation distribution between the two strains, which may correspond to differences in gene regulation linked to the growth environment.

To understand the functional impact of these modifications, we categorised the methylation counts based on COGs. Across nearly all COG categories, CT-CCM consistently showed higher methylation counts, especially for 6mA, followed by 5mC and 4mC (see Figure 1). Functional groups with the highest total methylation in CT-CCM included Signal transduction (T), Amino acid metabolism (E), Cell wall/membrane/envelope biogenesis (M), and Translation (J). These categories showed significant increases compared to CT-DSMZ, suggesting broader epigenetic involvement in regulatory and metabolic processes.

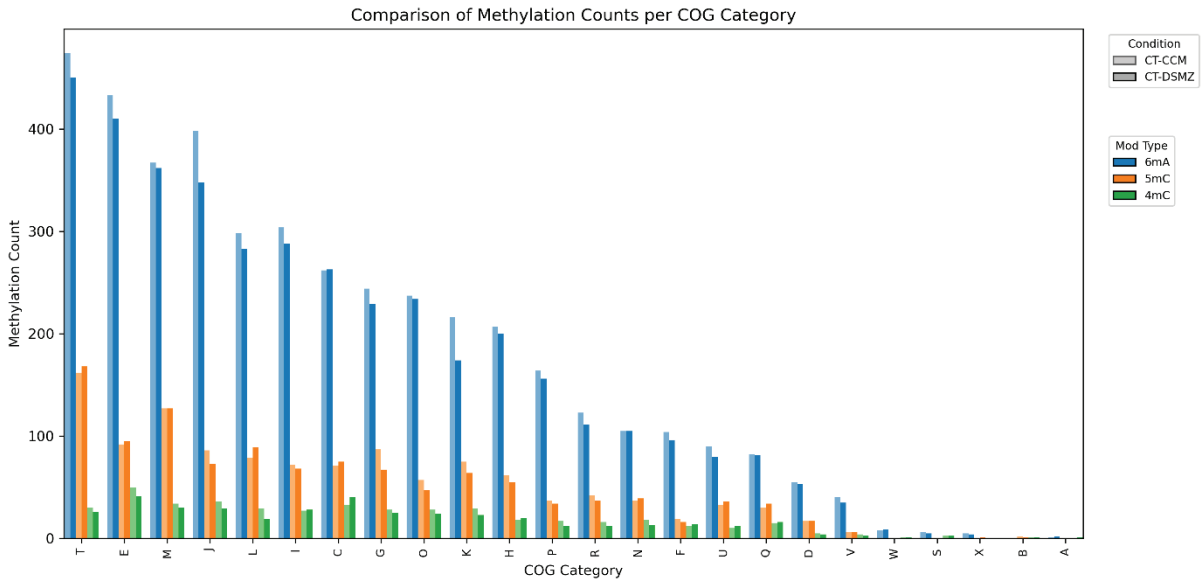

Figure 1. Methylation pattern across COG Functional Categories

In both strains, 6mA remained the most prevalent modification type, particularly in categories T, E, M, and J. The elevated levels of all three methylation types in CT-CCM indicate that adaptation to cultivation conditions may involve complex, gene-specific methylation events across a wide array of functional genes. Further analysis focused on identifying genes with the most pronounced differences in methylation between the two strains (see Figure 2). The patterns observed were not confined to one biological pathway but spread across diverse cellular functions. For example, *entF* (IS481_01739), likely a nonribosomal peptide synthetase, showed the highest total methylation in CT-DSMZ. Similarly, *cheA* (IS481_14430), involved in chemotaxis, and *sps1* (IS481_08830), potentially stress-related, showed substantial changes, implying that methylation may influence environmental sensing and response mechanisms. Other significantly altered genes included *tolC* (a transporter), transcriptional regulators such as *iclR* and *gntR*, and redox-related genes like *mqo*. Interestingly, some genes (e.g., *chvI* and *gntR*) exhibited increased methylation in CT-CCM, while others, like *sps1* and *cheA,* showed higher methylation levels

in CT-DSMZ. These differences highlight how gene-specific methylation patterns are influenced by cultivation history and physiological state.

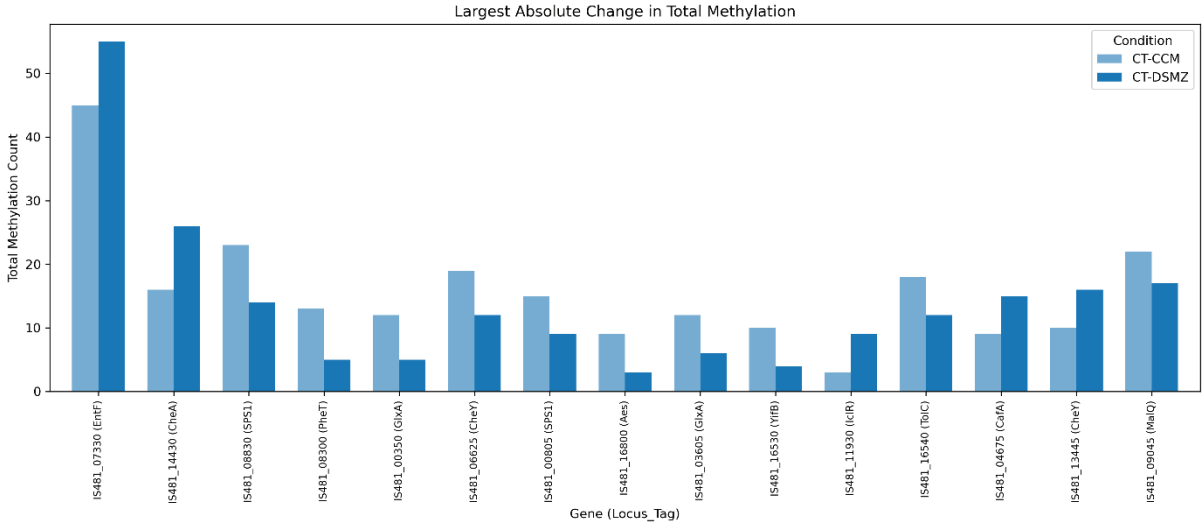

Figure 2. Methylation levels in genes exhibiting the largest change between CT-CCM vs CT-DSMZ

To further improve confidence in the observed methylation profiles, we also compared modification calls detected using ONT and PacBio Sequel IIe sequencing platforms for each strain, again using the same 0.95 minimum modification fraction filter. For CT-CCM, PacBio detected 29,233 unique high-confidence methylation sites, while ONT detected 10,846 sites. Of these, 7,979 were shared between both platforms. Among the shared sites, 6mA modifications were predominant (7,318), followed by 4mC (643), and 5mC (18), as shown in Table I. This high level of overlap between technologies strongly suggests reproducible and stable methylation signals in the CT-CCM sample. In contrast, the CT-DSMZ strain showed far less agreement between platforms. PacBio identified 31,001 high-confidence methylation sites and ONT reported 10,208, but only 14 sites were shared, 13 of which were 5mC and one 6mA, with no shared 4mC detected (see Table II). This striking difference in overlap between CT-CCM and CT-DSMZ points to several possible factors. One explanation could be that methylation marks in CT-DSMZ are more transient or condition-dependent, and therefore not consistently detectable by both platforms. It's also possible that platform-specific detection sensitivities or biases contributed to the mismatch. Technical variables such as differences in DNA quality, library preparation, or input concentration might have influenced the outcome. Lastly, methylation signals in CT-DSMZ may be weaker or more diffuse, resulting in fewer confidently detected modifications passing the stringent filters used.

Table I
Comparison of Common and Platform-Specific Methylation Counts Between ONT and PacBio (CT-CCM)

Modification Type	CT-CCM (PacBio Only)	CT-CCM (ONT Only)	CT-CCM (Common)
6mA	3597	32	7318
5mC	13678	2746	18
4mC	3979	89	643

Table II
Comparison of Common and Platform-Specific Methylation Counts Between ONT and PacBio (CT-DSMZ)

Modification Type	CT-DSMZ (PacBio Only)	CT-DSMZ (ONT Only)	CT-DSMZ (Common)
6mA	12782	6883	1
5mC	11140	2668	13

4mC	7065	643	0

Taken together, our findings show that the physiological adaptation of *C. thermodepolymerans* under different cultivation conditions is closely associated with shifts in DNA methylation. The CT-CCM strain exhibited a more extensive and structured methylation landscape, particularly in genes involved in regulation and metabolism, thus aligning with the observed phenotypic differences. In contrast, the CT-DSMZ strain, despite being genetically identical, showed a lower number of consistent methylation signals and reduced cross-platform concordance, suggesting either a weaker methylation system, more transient modifications, or a lack of strong environmental cues under its original cultivation conditions. These results highlight the importance of long-read sequencing technologies in capturing the complexity of bacterial epigenomes and suggest that DNA methylation plays a key role in microbial adaptation through gene-specific regulation.

Conclusion

This study demonstrates that *C. thermodepolymerans* DSM 15344^T undergoes extensive DNA methylation changes when cultivated under different conditions. By comparing the CT-DSMZ and CT-CCM strains using ONT and PacBio sequencing platforms, we observed consistent differences in the abundance and distribution of 6mA, 5mC, and 4mC modifications across the genome. The CT-CCM strain exhibited more high-confidence methylation sites overall, particularly in COG categories associated with translation, transcription, and amino acid metabolism. At the gene level, several regulatory and stress-response genes displayed significant methylation shifts, indicating gene-specific epigenetic modification. These patterns point to DNA methylation as more than just a passive marker; it likely plays an active role in regulating gene function and shaping how the organism responds to its environment. The changes we observed suggest that methylation helps modify both regulatory and physiological pathways, supporting the organism's flexibility and its ability to adapt under different cultivation conditions. When comparing results from both sequencing platforms, CT-CCM showed an intense match between ONT and PacBio, with thousands of methylation sites detected by both methods. This consistency indicates a robust and stable methylation landscape in the adapted strain. On the other hand, CT-DSMZ showed very little overlap, which might be due to weaker or more variable methylation signals or differences in how the platforms detect modifications. These results also highlight the value of long-read sequencing technologies in capturing the complexity of bacterial epigenomes and how powerful they can be for uncovering small but meaningful epigenetic changes in bacteria, and highlight the vital role of DNA methylation in helping microbes respond and adapt to their environment.

Acknowledgement

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CARBON NEUTRALITY

POSSIBILITIES OF IMPLEMENTING CCS TECHNOLOGY IN SLOVAKIA

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Abstract

Carbon Capture and Storage (CCS) is one of the most promising solutions for reducing CO_2 emissions in industry and energy production. This contribution focuses on the possibilities of CCS implementation in Slovakia by analyzing CO_2 emissions, identifying major producers, and evaluating the suitability of various industrial enterprises for adopting this technology.

The study provides an overview of current CCS projects worldwide and in Slovakia, assessing the technological, economic, and legislative factors influencing their implementation. Various CO_2 capture methods, including post-combustion, pre-combustion, and oxyfuel combustion, are evaluated concerning their technology readiness level (TRL) and commercial viability. Additionally, transport and long-term storage options for CO_2 are analyzed, with particular emphasis on geological formations in Slovakia that could serve as potential storage sites.

The practical part of this contribution focuses on the design of technological processes for flue gas treatment before injection into the storage site. The objective is to remove undesirable components such as CO, HCl, NO_x, and SO_2, which could negatively affect the storage process and the stability of the geological reservoir. The proposed solutions include various separation and purification methods, evaluated in terms of technological feasibility, efficiency, and operational costs.

Introduction

Rise in carbon dioxide emissions over the past decades has become a major concern for the industry. The intention to reduce carbon dioxide emissions is also demonstrated by Paris Agreement, which aims to 50% reduction of these emissions by 2030. As one of the promising approaches appears to be Carbon Capture and Storage Technology (CCS). This technology already has several operational facilities around the world, e.g. projects Sleipner or Northern Lights in Scandinavia. However, wider implementation is limited by economic feasibility as well as by the availability of suitable CO_2 storage options. Generally, three methods are used for carbon dioxide capture – oxy-fuel combustion, pre-combustion and post-combustion capture. Among these, post-combustion capture is the most widely used method. Within this method, the most commonly used CO_2 capture process from flue gas is amine-based absorption, typically MEA (monoethanolamine) and MDEA (methyldiethanolamine) in combination with PZ (piperazine). Another potential option is the use of membranes; however, membranes for efficient CO_2 separation are still under development. Study by J. Kum et al. was aimed to optimize industrial process of capturing CO_2 from methane reforming[1]. As a solvent was used a mixture of MDEA, PZ and water in ratio 35:15:50. Complex economic analysis was carried out, with expenses for capturing one tonne of CO_2 at 47$. Study by S. Mudhasakul et al. was aimed to design kinetic model of MDEA/PZ absorption of CO_2 from industrial gas after natural gas sweetening in ASPEN Plus[2]. For crucial parameters of this study was carried out an analysis with following results - PZ concentration (5 wt.%) and value of CO_2 loading – 0.55 mol absorbed CO_2/mol amine. D. Abooali et al. in their study constructed theoretical formulas to calculate important parameters for correct design of absorption technology[3]. Based on these formulas is possible to predict the most feasible operating conditions in the designed process. In the study by Q. Li et al., various polymeric membrane design options were analyzed, including single-stage and multi-stage systems, with and without retentate recycle. Different pressure ratio conditions were also evaluated, such as 4 bar to vacuum and 10 bar to 1 bar. Based on a detailed analysis, the most economically favorable configuration was a two-stage membrane system with a pressure ratio of 10:1. The estimated cost for capturing one tonne of CO_2 was 30$[4]. On the contrary, recent studies by Turakulov et al. and Kamolov et al. assessed capturing CO_2 from energy sector sources (natural gas-fired power plants) and construction sector (cement production plants) by absorption-based and membrane-based technologies and their combinations, using process simulations in ASPEN Plus software yielded the CO_2 capture costs as high as over 60 $ per ton for optimized technology[5,6]. It can be seen that the CO_2 capture cost range is quite wide leading to uncertainty when considering the economics of CCS projects; the reason for this can partly be seen in the lack of unified approach regarding the required technology complexity and the scope of CO_2 stream treatment and purification. The presented study tries to present a complex view on this problematic, thus, leading to a better understanding of the necessary treatment steps upstream of the CO_2 capture step.

Object of Study

In carbon dioxide capture, the pretreatment of flue gas is a crucial part of the process. Initially, a flue gas pretreatment system was designed, with defined steps to meet the required pollutant limits in the CO_2 stream intended for geological storage. Only after this stage the actual CO_2 capture process can be developed. In this study, two capture methods were considered: absorption using MDEA/PZ amine solvent and a two-stage membrane separation system. To determine which method is more economically and energetically efficient, a comparison of key performance parameters was carried out.

Materials and Methods

The subject of this study is a complex treatment of a flue gas stream with a flow rate of 480 kmol/h, available at a temperature of 165 °C and a pressure of 1 bar. The composition of the gas (in mol%) is as follows: 17.8% CO_2, 56.4% N_2, 7.5% O_2, 18.2% H_2O, 1470 ppm CO, 250 ppm NO_x, 25 ppm SO_2, and 10 ppm HCl.
The entire process was designed using the simulation software Aspen Plus, applying the NRTL-RK thermodynamic model for all process units involving vapor–liquid equilibrium (VLE), and the Peng-Robinson (PENG-ROB) model for heat exchangers, pumps, compressors, and other utility equipment.
After analyzing various options, the following pollutant removal methods were selected for the pretreatment stage of the process (Figure 1). SO_2 and HCl were removed in reactor *R1* through reactions with $NaHCO_3$, followed by an electrostatic precipitator EPS filter to capture the resulting solid particles[7]. In reactor *R2*, CO was oxidized to CO_2 over a Pt/Pd–Al_2O_3 catalyst[8]. To eliminate NO_x, a selective catalytic reduction (SCR) process using NH_3 and a Ni(0.4)–MnO_x catalyst was implemented in reactor *R3*[9]. Any excess NH_3 from the SCR process was removed in a scrubber, ensuring ammonia concentration to remain within the permitted limits. After CO_2 capture and compression part, drying of CO_2 in triethylene glycol (TEG) column with a simplified regeneration unit follows, constituting the last step to obtain CO_2 meeting quality requirements.
In the model of CO_2 capture by absorption, depicted in Figure 1, aqueous amines were used as solvent – MDEA (40 wt%) and PZ (10 wt%), The pressure profile of the absorber column was set to 2.1 bar at the top and 2.5 bar at the bottom. All process parameters were adjusted based on literature data from systems processing similar flue gas. The CO_2 loading of the rich amine stream was set at 0.50 mol CO_2/mol of amine. This stream was directed to the stripper column for regeneration, operated at a pressure of 2.5 bar at the top and 3.0 bar at the bottom. CO_2 loading of regenerated stream was set at 0.025 mol CO_2/mol of amine[1-3,10]. Heat required to operate the solvent regeneration steps was assumed to be produced in a natural gas-fired steam boiler, operated with thermal efficiency of 90 %, based on natural gas lower heating value (LHV) of 48.8 MJ/kg and the CO_2 emission factor considered was 0.202 kg/kWh_{LHV}. For simplicity, heat losses from the equipment were neglected. Carbon footprint of electricity of 0.134 kg CO_2/kWh was assumed.

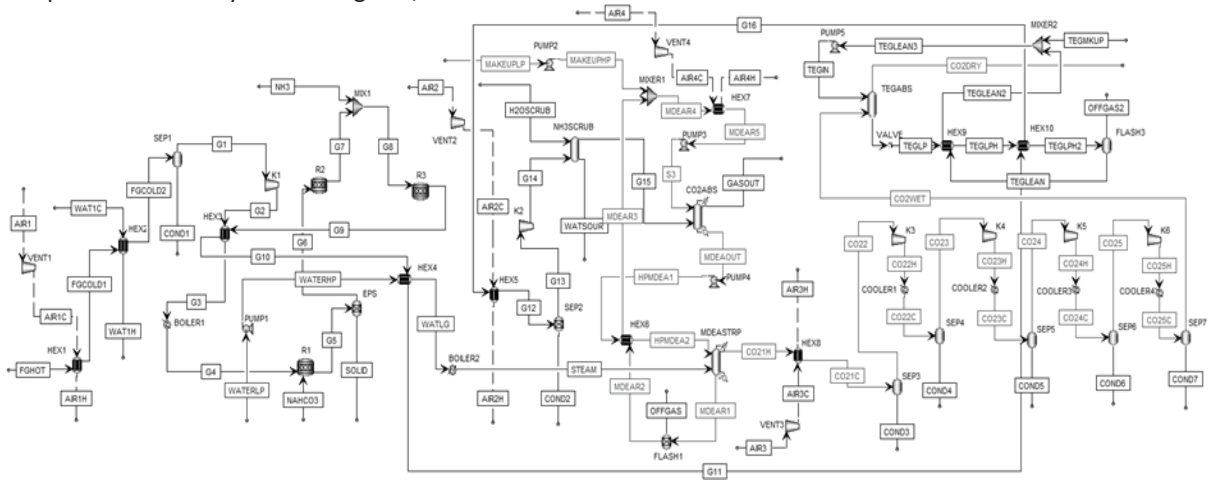

Figure 1. Process scheme of CCS technology with amine absorption of CO_2. ABS – absorber, AIR – cooling air, COND – condensate, FG – flue gas, G – process gas stream, HEX – heat exchanger, K – compressor, MIX – mixer, R – reactor, SEP – (phase) separator, TEG – triethyleneglycol, VENT – fan/blower, WATC – fresh cooling water, WATH – warmed-up cooling water.

CO_2 capture by membranes is still in development, thus, predicting mass transfer without experimental data is challenging. However, literature data under similar conditions allowed us to estimate the performance of the

two-stage membrane separation process. With a pressure ratio of 10 bar/1 bar in both stages, an overall CO_2 recovery of 80% with 95% purity was achieved. Based on this information, we were able to obtain reliable data for comparison with the absorption method.[4]

Results and Discussion

Table I summarizes the comparison of key process parameters for the CO_2 capture technologies. In the absorption variant, electricity consumption was half that of the membrane variant, primarily due to fewer compressors required in the process. On the other hand, the membrane variant had lower heat energy requirements, as there was no need for steam to operate the stripper column, resulting in lower gas consumption. However, since electricity is significantly more expensive than natural gas, the absorption method proves to be the more economically feasible option from energetic perspective.

CO_2 capture efficiency related to amount of CO_2 in processed flue gas is higher for absorption alternative. Expanding the CO_2 balance by accounting for carbon footprint of consumed natural gas and electricity in both alternatives does not change the situation, as the sum of CO_2 produced by heat and electricity production to cover the demand differs by around 0.1 t/h between alternatives. Thus, the sum of residual and process-derived CO_2 emissions is notably higher for membrane technology.

The evaluation of overall economic feasibility, including both CAPEX and OPEX, is the main objective of further investigation. An analysis of the profitability, based on CO_2 emission prices and electricity costs, is visualized in Figure 2. The image shows that the profitability of the amine absorption technology at the current market price of electricity (95€/MWh) and that of emission allowances (65 €/tCO_2) is on the edge of profitability. Considering the expected increase in the price of emission allowances, the profitability of the process may improve. However, as already mentioned, to assess the overall economic efficiency of the technology, it is necessary to determine parameters such as CAPEX and OPEX. The selected flue gas stream originating from an industrial process is of small scale, compared to analogous stream produced in large industrial facilities (tens of t/h vs. up to thousands t/h), meaning that the economic and environmental parameters of both technologies may look better than presented here when applied to large-scale CO_2 sources.

Table I
Comparison of key parameters between Absorption and Membrane CO_2 Capture

Parameter	Absorption	Membrane
CO_2 captured, t/h	3.3	2.8
Electricity consumption, MWh/t	0.42	0.80
Heat energy consumption, MWh/t	0.34	0.068
Natural gas consumption, Nm^3/t	39	7.7
Amine emissions MDEA/PZ, kg/year	15.8/30.8	-
CO_2 residual and process emissions, t/h	0.90	1.30

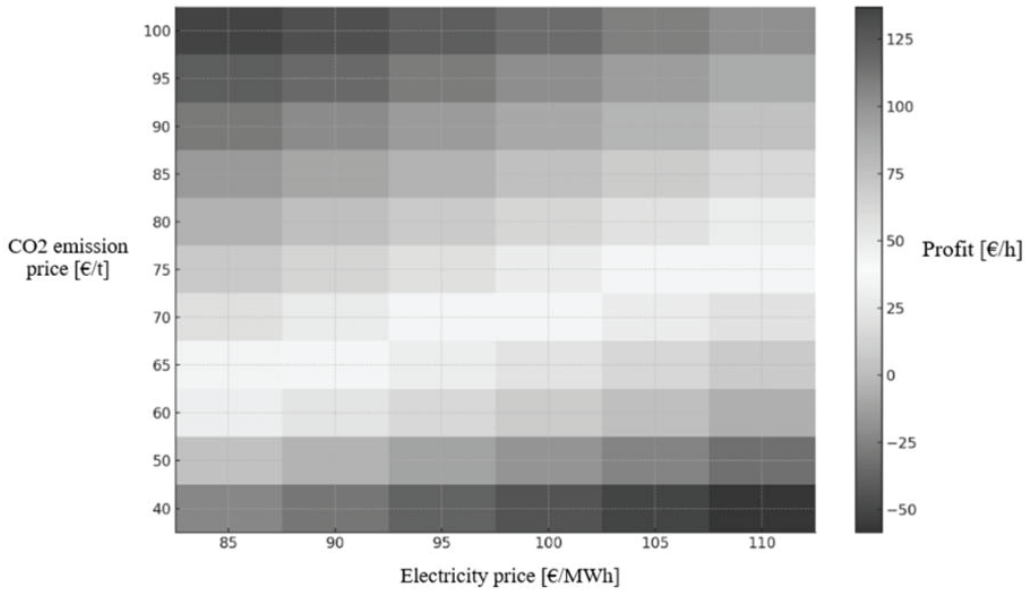

Figure 2. Profitability of absorption technology based on prices of CO_2 emission and electricity.

Conclusions

After designing and comparing the amine absorption and membrane separation technologies as methods for CO_2 capture, absorption appears to be the more advantageous option. At the current prices of electricity and emission allowances, its profitability—based on these two factors—stands at the edge of economic feasibility. However, profitability alone does not reflect the overall economic efficiency of the technology, as payback period also depends on the determination of CAPEX. Given the currently low profitability of the process, we can assume that, once all costs are taken into account, the technology is unlikely to be economically viable in terms of payback period.

Acknowledgement

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INTEGRATION OF SEA WATER DESALINATION INTO AMMONIUM THIOSULPHATE PRODUCTION

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Abstract

Ammonium thiosulphate (ATS) is an inorganic compound than among other applications is being used as a fertilizer. Its production process produces a significant amount of heat that can be used for sea water desalination, especially in countries that rely on desalination for drinking water production. Demineralized water is also required for the production unit operation, and being self-reliant in water supply in water-scarce regions can be a great advantage. This contribution investigates how the heat produced during ATS production can be used for sea water desalination. There are two approaches to this problem: desalination by using steam from ATS production for direct evaporation and electricity generation from steam turbines to power reverse osmosis systems. The study evaluates thermal efficiency and energy consumption along with water recovery performance for each method while comparing the advantages and disadvantages of direct heat use and conversion of heat into electric energy. The evaporative desalination method uses steam to boil water in an evaporator whereas the RO system depends on steam turbines to generate electricity for operating high-pressure pumps. The goal of this study is to find the most efficient desalination method that achieves minimal energy waste. The research results deliver an assessment of how ATS production byproducts can enhance desalination efficiency and support environmental sustainability.

Introduction

The rising global demand for freshwater and sustainable energy has led to intensified research into the integration of industrial processes to improve energy efficiency and environmental performance[1]. One of the most pressing challenges remains the desalination of seawater, which is essential for securing potable water in water-stressed regions but is also known for its significant energy consumption. Depending on the technology used, desalination processes can be thermally or electrically driven, with reverse osmosis (RO) being the most energy-efficient and widely deployed membrane process today. Nevertheless, even RO systems require high-pressure pumps and consume electric power, typically in the range of 3–5 kWh/m³ of freshwater produced[2]. Thermal desalination technologies, such as multi-stage flash distillation (MSF), demand even more energy in the form of heat, typically in the range of 50-80 kWh/m^3, making them well-suited for integration with processes generating waste heat[3]. Industrial waste heat recovery represents a promising avenue for increasing overall system efficiency and reducing environmental footprints. The strategic integration of industrial operations with energy and water production, so-called process integration, can enable simultaneous energy savings, cost reductions, and environmental benefits[3]. Various studies have demonstrated the potential of such integrations. Feng et al.[4] developed a geothermal-driven cascade thermal design using Organic Rankine and Organic Flash Cycles to power an HDH desalination unit, achieving both electricity and freshwater generation with optimized financial performance. Similarly, Sui et al.[5] proposed a multigeneration system combining gas turbine waste heat with Rankine cycles, desalination, and hydrogen production, resulting in enhanced overall system efficiencies and reduced CO_2 footprints. While these studies focus on renewable or combustion-based heat sources, chemical manufacturing processes are another underexplored opportunity for thermal integration. One of the ways to manufacture ATS is using SWAATS technology, which uses sour water stripping gas from a refinery as its feedstock. This technology uses a series of reactive absorption columns where multiple reactions take place to make a water solution of ATS as its final product. The process also contains a furnace, where a mixture of gases composed primarily of hydrogen sulfide is burned to produce sulfur dioxide, which is required further in the process. This unit produces heat, as the flue gas needs to be cooled. To date, no published study has examined the possibility of integrating thermal energy from ATS production with a water desalination process. Therefore, the goal of this study is to investigate the feasibility of integrating the waste heat from ATS production into a thermal or electricity-driven desalination process with a focus on energy efficiency and sustainability.

Methodology

Firstly, a thermodynamic model of the ATS furnace unit was constructed using energy balance and heat transfer equations. As a basis for this model, an existing ATS production unit was used. Ideal complete combustion was assumed, and flue gas composition was calculated using stoichiometric equations. All calculations were performed in MS Excel. The feedstock composition is given in Table I.

Table I
Feedstock composition

	H_2S [%mass]	NH_3 [%mass]	H_2O [%mass]
Feedstock composition (avg.)	80	10	10

The existing unit processes 1 t/h of feed and produces around 5.5 t/h of saturated steam at a pressure of 2 MPa, which is sold to a refinery. The diagram of the existing unit is shown in Figure 1.

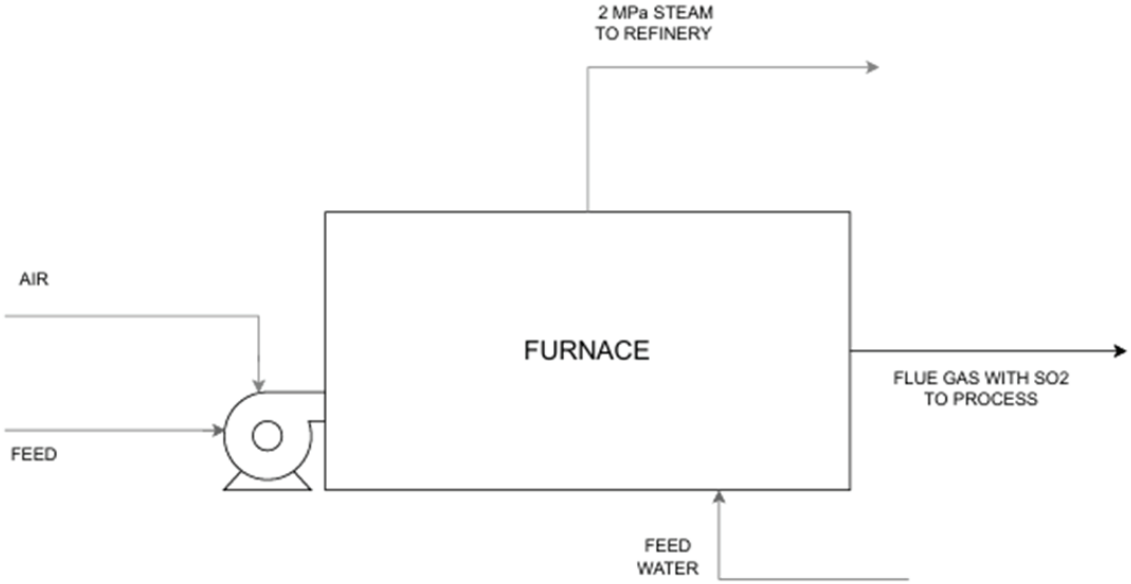

Figure 1. Process flow diagram of the existing unit.

Next, the model was upscaled to produce 8 t/h of steam at a pressure of 3.5 MPa, as per the planned new unit's capacity requirements to process 1.55 t/h of feedstock. For the first alternative, which uses MSF distillation, saturated steam was used. A simple model of MSF distillation was formulated, in which the flashed distillate from each stage preheats the feed and the steam is used in the first stage to heat the sea water to the top brine temperature. The diagram on this process is shown in Figure 2[6].

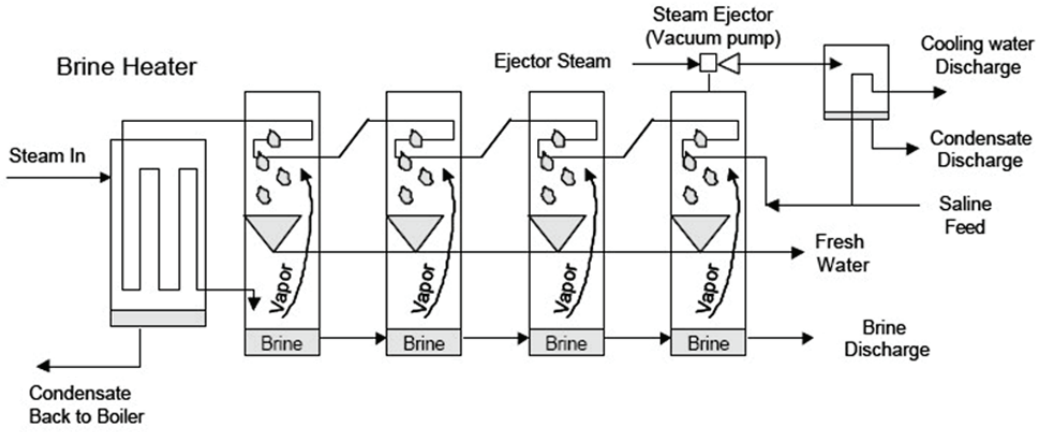

Figure 2. Process flow diagram of MSF distillation[6].

The input data for the calculations are presented in Table II.

Table II
Input data for MSF calculation

Parameter	Unit	Value
Water salinity	[kg/m^3]	35
Number of stages	[-]	15
Top brine temperature	[^{o}C]	105
Sea water temperature	[^{o}C]	20
Heat duty	[kW]	4200
Heat capacity of water	[kJ/kg/K]	4.18
Heat capacity of salt	[kJ/kg/K]	1.53

In the second alternative, a superheater was introduced to increase the enthalpy of the steam entering a condensation steam turbine with a dry condenser operating at a pressure of 50 kPa, to account for the hot climate of gulf countries. Process flow diagram of this alternative is shown on Figure 3.

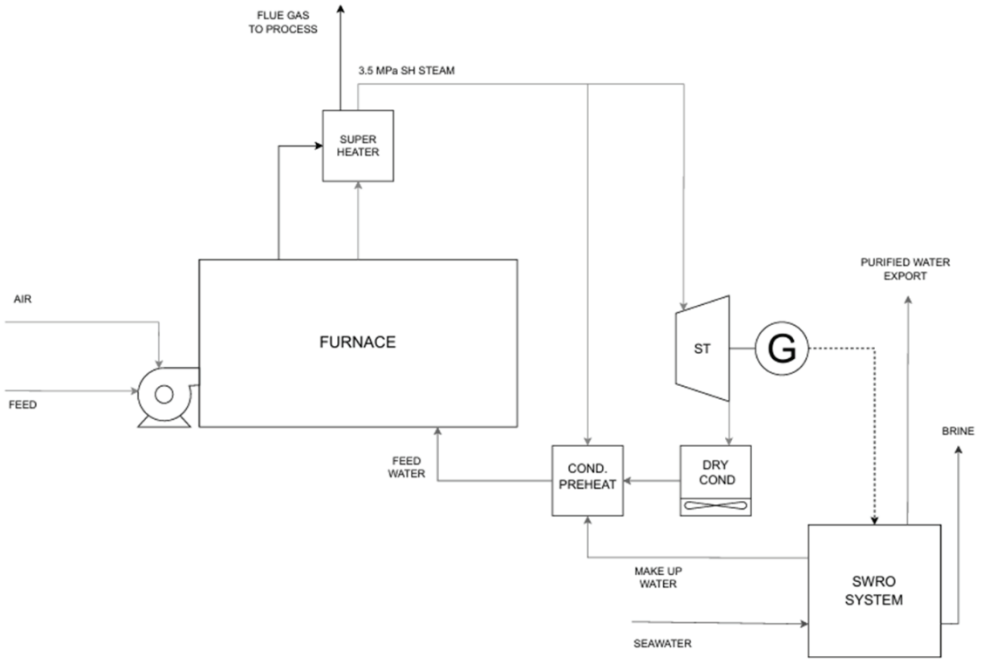

Figure 3. Process flow diagram of ATS furnace with SWRO system (SWRO – sea water reverse osmosis, ST – steam turbine, SH – superheated).

Power generation of the steam turbine was calculated, as well as power consumption of the condenser. Capacity of RO unit was calculated both with an energy recovery device and without it. Finally, the economic feasibility was determined, following the equation below.

$$PBP = \frac{CAPEX}{(C_{water} \cdot V_{water} - OPEX)}$$

PBP – Payback period [year]
CAPEX – Total capital cost of the project [€]
C_{water} – Cost of purified water [€ /m^3]
V_{water} – Volume of purified water [m^3/year]
OPEX – Total yearly operational costs [€ /year]

Results and discussion

Figure 4 shows the fresh water production rate for each of the alternatives. At the considered production scale, Reverse Osmosis is the more efficient and economical choice compared to Multi-Stage Flash desalination. Modern RO plants further reduce energy demand by 60–80% using energy recovery devices (ERDs), which recycle pressure from brine waste to pre-pressurize feedwater. MSF's high thermal energy demand makes it ineffective at small scales, whereas RO's modular design allows for simpler installation, lower maintenance, and scalability. Additionally, RO systems have a smaller footprint, faster deployment, and better adaptability to variable feedwater conditions. For decentralized or small-scale applications, RO offers a sustainable, energy-efficient, and cost-effective solution, while MSF remains viable only for large-scale plants with access to waste heat.

The CAPEX for the steam turbine and condenser was based on real manufacturer offers, while the RO CAPEX and OPEX was based on industry standards and previous projects. Manufacturer offers and previous projects data are both confidential. Price of the purified water product is given by local water authority[7]. From these values, a simple payback period was calculated by the following equation. The payback period was also evaluated for possible increases in OPEX values. This evaluation is shown in Figure 5.

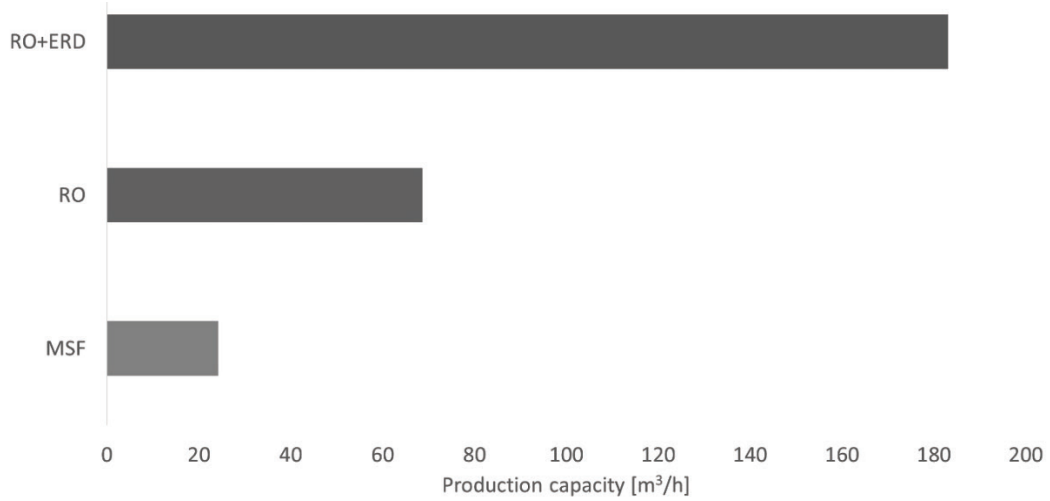

Figure 4. Production capacity for different desalination systems using waste heat from ATS production (MSF-multi-stage flash desalination, RO – reverse osmosis, ERD – energy recovery device).

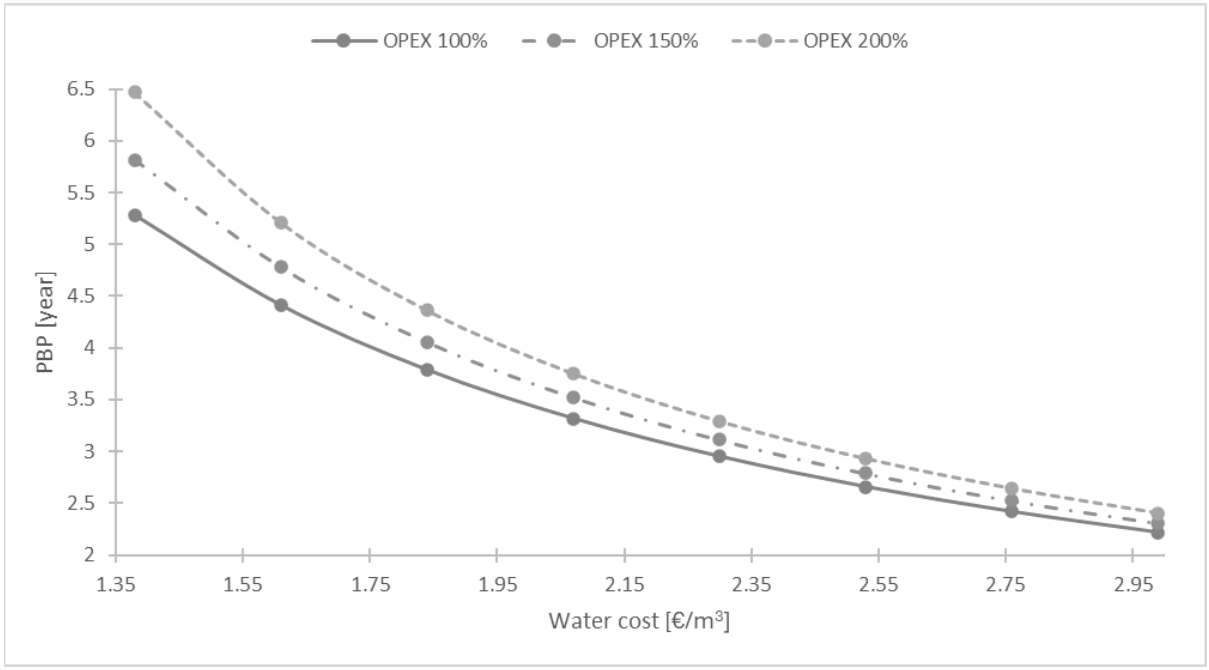

Figure 5. Payback period as a function of water cost with a sensitivity analysis of OPEX value.

The results show that integrating sea water desalination system into ATS production in gulf countries could be a viable solution for utilizing the energy from this process. The energy requirement for MSF distillation in our case came out to be 173 kWh of thermal energy per cubic meter of freshwater produced. This is more than double compared to the values given in literature and shows that this scale is not fit for MSF implementation. While the scale is too small for a MSF unit, RO with its superior energy efficiency due to ERDs and its modular design combined with high commercial costs of purified water in this region seems to be optimal. The project seems economically attractive even with an increase of its OPEX to double.

Conclusions

This novel study focused on integrating fertilizer production plant with desalination unit for the exploitation of underlying synergistic effects regarding the energy efficiency of the integrated plant compared to stand-alone technologies. As found in the study, an MSF unit is too costly and inefficient at the considered plant production scale. On the other hand, the integration of an RO unit powered by Rankine cycle and equipped with ERD showed interesting economic results and represents a viable investment option, especially for regions with water scarcity.

Acknowledgement

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ECONOMY OF THE CHEMICAL INDUSTRY IN NEW CONDITIONS

SOCIAL ASPECTS OF PRODUCTION FROM THE PERSPECTIVE OF CONSUMERS

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Abstract

Currently, significant attention is being paid to the social pillar in building business sustainability. When managing social sustainability, it is important to consider the requirements of customers. However, the perception of the importance of social aspects among customers has not yet been sufficiently explored. Therefore, this article addresses this issue. It presents the results of primary research aimed at revealing the importance of various social aspects associated with production processes from the perspective of consumers of household chemicals and food products. The research involved 200 adult respondents who purchase food, beverages, laundry detergents, and cosmetics. Their responses were processed using exploratory and inferential statistical methods. It was found that, from the customers' perspective, the most important social aspects in production processes are the working environment and conditions, fair wages, education, and training. The perception of importance is also influenced by the type of product being produced and other characteristics of the respondents (gender, education, and age).

Introduction

Sustainability, which many businesses are currently striving for, has three dimensions: care for people (representing care for social justice in relation to products, processes, and systems), care for the planet (including environmental protection), and care for profit (involving efforts for economic stability)[1,2]. Therefore, companies' efforts focus on maximizing profits and market shares, reducing the impact of their products and processes on the environment, and addressing social concerns while maintaining the desired level of product quality[1]. Interest in the dimension of social sustainability is currently growing in sustainability management, as evidenced by the recent increase in publications on this matter[3].

The efforts of businesses towards the social pillar of sustainability influence the perception of the company by various stakeholders. It is important for the company to know and understand this perception so that it can take it into account when improving the management of social aspects. In particular, it can be beneficial to consider the perception of consumers, as they are a crucial group of stakeholders in terms of revenue generation[4]. However, understanding this consumer perception can be challenging, as social sustainability is the least known, most difficult to grasp[5], and therefore the least understood dimension of sustainability[6]. Therefore, a primary quantitative research was conducted to reveal consumer attitudes towards selected social aspects associated with production processes whose outputs are food and consumer chemicals. The article presents the results of this primary research, thereby helping to better understand consumer perception of social sustainability.

Theoretical background

A company's care for social sustainability focuses on issues related to[7,8]:

- workers (including ensuring health and safety at work, fair wages, and education and training),
- consumers (focusing on providing real value through products and consumer protection),
- suppliers, and
- communities (contributing to the development of healthy, productive, and rewarding communities).

These issues, referred to as social aspects, can be understood and categorized in various ways. According to Shaharudin et al. [9], social aspects can be perceived in dimensions:

- safety and health,
- labor rights,
- diversity,
- social responsibility, and
- product responsibility.

According to El Dehaibi et al. [10], these topics include Health and Safety, Family and Culture, Education, Community Support, and Human Rights. According to the authors Padilla-Rivera et al. [11], the thematic areas of social aspects and their content can be illustrated in Table I.

Table I
Social aspect of sustainability[11]

Labor Practices and Decent Work	Human Rights	Society	Product Responsibility
Employment	Investment	Social inclusion (equity)	Customer Health and Safety
Labor/Management Relations	Non-discrimination	Social networks	Product and Service Labelling
Occupational Health and Safety	Freedom of Association and Collection Bargaining	Social cohesion	Marketing Communications
Training and Education	Child Labor	Participation and Local Democracy	Customer Privacy
Diversity and Equal Opportunity	Forced or Compulsory Labor	Anti-corruption	Compliance
Fair distribution of income	Security Practices	Public Policy	Anti-competitive behavior
Quality and Well-being	Human Rights Mechanisms	Compliance	
Employment		Supplier Assessment for Impacts on Society	
		Cultural Traditions	
		Tourism and Recreation	
		Local Communities (Sense of community and belonging)	

If the social pillar of sustainability is understood in the dimensions defined by Padilla-Rivera et al.[11], then labor practices have been the most studied so far. This may be due to the fact that this category includes issues of occupational health and safety, and companies are required to report related impacts[3]. Another reason may be that social aspects associated with labor practices (and production processes overall) are linked to both high risks of negative social impacts and high opportunities for positive social impacts[12]. Therefore, the primary research focused on production processes and the perception of the importance of social aspects associated with them.

Simulation and/or experiment

The primary research focused on the importance of social aspects of production processes from the perspective of customers purchasing food, beverages, detergents, and cosmetics. Quantitative research was conducted in the form of a questionnaire survey, with data collection taking place from December 2023 to February 2024 through electronic and personal interviews.
Respondents assessed the importance of the following social aspects of production processes:

- Place/region of production.
- Contribution of production to the welfare of the given region.
- Fair wages of production workers.
- Working environment and conditions of production workers.
- Scope of social benefits provided to production workers
- Education and skill enhancement of workers in production.

Respondents rated the importance of aspects on a five-point scale (1 = Not important, 2 = Slightly important, 3 = Moderately important, 4 = Very important, and 5 = Extremely important), and their personal characteristics (gender, age, and education) were recorded. The research was conducted among consumers over 18 years old who purchase food, beverages, and consumer chemical products. The quota sampling method used considered

the structure of the Czech Republic's population by gender and age[13]. The questionnaire survey involved 200 Czech respondents, with data collected in groups of 50 questionnaires according to product categories (see Table II).

Table II
Quota Sampling

Quota	Frequency				
	Food	Beverages	Detergents	Cosmetics	*Total*
Men 18–34	6	6	6	6	*24*
Men 35–54	10	10	9	9	*38*
Men 55+	9	9	9	9	*36*
Women 18–34	5	5	6	6	*22*
Women 35–54	9	9	9	9	*36*
Women 55+	11	11	11	11	*44*
Total	*50*	*50*	*50*	*50*	*200*

Data were processed using SPSS and MS Office Excel. Descriptive and inferential statistical methods were applied. Mean, median, and mean rank were used to evaluate the importance of social aspects. The Friedman test (to determine the significant differences among mean ranks) and Kruskal-Wallis test (to determine the significant differences among groups of respondents and/or groups of products) were used at a significance level of 0.05. The structure of respondents in relation to the population of the Czech Republic is presented in Table III.

Table III
Research Sample

Demographic Factor	Group	Frequency (%)		Chi-square Test of Representativity	
		Sample	Population	*Chi-square*	*p*-value
Gender	Men	49.0	49.3	0.007	0.932
	Woman	51.0	50.7		
Age	18–34	23.0	23.0	0.004	0.998
	35–54	37.0	36.8		
	55+	40.0	40.2		
Education	Primary	17.0	46.5	75.697	<0.001
	Secondary	44.5	33.0		
	Tertiary	38.8	20.5		

In Table III, it is evident that the sample of respondents is representative in terms of gender and age, but not according to education. The percentage of respondents with primary education is smaller than that of the entire population.

Discussion and result analysis

The analysis of data obtained from the primary research initially focused on evaluating the importance of the examined social aspects of production processes from the perspective of consumers without considering personal characteristics. The results of the analysis are illustrated in Table IV.
From Table 4, respondents perceive social aspects as moderately important. In terms of ranking, the differences in average values are small, with the median being the same for all aspects except the last one. Based on paired post-hoc testing, a statistically significant difference was only found between the first and fourth aspects. This means that the first four aspects (working environment and conditions, fair wages, education and skill enhancement of workers in production, and the scope of social benefits provided to workers) can be considered more important (and equally important). The “contribution of production to the welfare of the given region” and “place/region of production” are considered by respondents to be less important from the consumer's point of view.

Table IV
The importance of social aspects of production in the entire sample of respondents

Social Aspects of Production	Mean	Median	Mean Rank
Working environment and conditions of production workers.	2.99	3	4.08
Fair wages of production workers.	2.91	3	3.87
Scope of social benefits provided to production workers.	2.83	3	3.71
Education and skill enhancement of workers in production.	2.74	3	3.58
Contribution of production to the welfare of the given region.	2.53	3	3.18
Place/region of production.	2.10	2	2.59

After analyzing the perception of the importance of selected social aspects across the entire sample of respondents, an analysis of responses based on personal characteristics followed. This analysis did not show statistically significant differences based on gender or education. However, it was found that all the social aspects examined are more important for women than for men.

Regarding statistically significant differences based on age, a significant difference was demonstrated only for the aspect “place/region of production.” The perception of the importance of this aspect increases with age.

An interesting conclusion was brought by the analysis of the perception of the importance of social aspects based on the type of product. The result of this analysis is presented in Table V. Although the Kruskal-Wallis test did not show a statistically significant difference in the perception of the importance of individual social aspects, it is clear that the perceived importance of social aspects is higher for food and beverages than for cosmetics and detergents.

Table V
Differences in the perception of the importance of social aspects of production depending on type of goods

Quota	Mean				Kruskal-Wallis Test	
	Food	Beverages	Detergents	Cosmetics	*Chi-square*	*p*-value
Place/region of production.	2.22	2.12	1.98	2.08	1.52	0.68
Contribution of production to the welfare of the given region.	2.58	2.56	2.46	2.50	0.34	0.95
Fair wages of production workers.	2.96	3.10	2.92	2.64	3.40	0.33
Working environment and conditions of production workers.	2.94	3.12	3.08	2.80	2.15	0.54
Scope of social benefits provided to production workers.	2.72	2.82	2.84	2.58	1.53	0.68
Education and skill enhancement of workers in production.	2.98	3.04	2.62	2.66	3.96	0.27

Conclusion

The conducted primary research brought several interesting findings. It was found that the social aspects of production processes are slightly to moderately important from the customers' perspective. For consumers, the social aspects that bring greater benefits to the production workers themselves are more important than those that benefit the local community and/or society. However, this opinion is not entirely uniform, and differences in perception may arise based on personal characteristics. For example, women perceive the importance of social aspects higher than men. However, statistically significant differences according to different groups of respondents are rare.

These summarizing conclusions not only contribute to academic understanding in the field of sustainability and social sustainability of enterprises but can also help managers, especially in chemical and food companies. Specifically, they can show that managing social aspects is also reflected by customers, as a significant group of stakeholders, and that their perception of importance is generally uniform. Improvements in managing social aspects thus appeal to variously defined consumer segments in essentially the same way.

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ACCURACY OF USING INDUSTRIAL AVERAGES IN THE CHEMICAL INDUSTRY

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Abstract

Industrial averages are frequently used for an intercompany comparison or a valuation statement. The value of industry averages can have a significant impact on the value of a business appraisal. Therefore, the research aimed on comparison of industrial averages is conducted. To evaluate the accuracy of using industrial averages, the quantitative research has to be conducted. First, various data sources, whether governmental or non-governmental and national or international, are collected. Second, similarities and differences in the areas of basic financial performance characteristics are detected and analysed. It focuses exclusively on the area of return. The findings show if the usage of industrial averages is accurate. This kind of conclusion has a practical benefit when the intercompany comparison should be conducted or when the averages are a basis for corporate valuations. This could have an impact on decision making of potential buyers, sellers, and valuation statements provided by professional appraisers and valuators. However, the research conducted has its limitations based on data availability.

Introduction

An industrial average expresses the value of a selected indicator for the entire data set representing the given industry sector. This kind of indicator can be used for intercompany comparison. According to Mařík (2018)[1], the comparison proves if the company reaches better or worse results in the area measured by the selected indicator. Specific kinds of averages can be used for relative valuation in the form of multiples how Damodaran (2008)[2] explains. It is one of the methods leading to corporate valuation.

The usage of previously quantified and even publicly available averages is quicker solution than working with corporate market data originally and quantify own multiples. Own work can be limited when the market data is unavailable because of a lack of publicly traded companies and limited market liquidity. This is especially the case of the Czech Republic when it is difficult to follow general recommendations for the quantification of own multiples applied further in the relative valuation. Kislingerová (2001)[3] points out that the average multiple should be based on the data of at least 4-8 companies offering the same product to same costumers having the comparable size and ownership structure. When it is complicated to find comparable companies or there is limited data access the own quantified multiple can be substituted by the industrial multiple (average) as supposed by Mařík (2018)[1] and Kislingerová (2001)[3].

Attention should be drawn that it is recommended to employ the industrial average. Industries do not behave similarly and some industry branches tend to be more vulnerable than the others therefore it is talked about cyclical, neutral, and countercyclical industry sectors as Baele and Londono (2013)[4] or Van Horne and Wachowich (2008)[5] state. First, there is this difference how the companies react to economic fluctuations depending on the belonging to the specific sector. Second, there are significant differences in performance among industries in general how it is highlighted in Bourgeois et al. (2014)[6] or Lee and Alnahedh (2016)[7]. It can be concluded, according to Jackson et al. (2018)[8], company performance is closely linked not only to industry but also to market performance.

It is obvious that it is crucial to work with industrial averages and not global averages because the corporate specifics should be followed. The issue which stays unsolved is that it is impossible to employ Czech market data when the Czech capital market is underdeveloped, has reduced liquidity, and has other weaknesses as explained by Musílek (2015)[9]. There are frequently as an alternative used multiples valid for European or American markets when Czech multiples are not available. International averages are regularly used for domestic valuations which can significantly influenced the corporate value received. It opens a question if it is better to follow European or American data for Czech purposes and if these data pieces can be accurate for the Czech business environment. The research aim focuses on if the development of companies is similar when different averages are compared.

This contribution has a standard structure and consists of four parts. Section 1 sets the research into a broader context and presents the paper aim. The following part focuses on the employed methodology and materials. Finally, Sections 3 and 4 present the results of the research conducted along with their interpretation and conclusions.

Methodology

The aim of the paper is to evaluate the accuracy of using industrial averages therefore the quantitative research has to be conducted. It is essential to have data sources covering different territories which enable to fulfill the aim. First, Czech and international data sources are collected before the comparison could be conducted. Czech datasets published by Ministry of Industry and Trade have had a long tradition since 1990's in the Czech Republic[10]. It could be admitted that European and American datasets employed in this research have not been published by any governmental institution as the Czech data[11]. However, it must be highlighted that the datasets prepared and published by Professor Aswath Damodaran employed in this paper are based on official government sources, sources of rating agencies, and data of stock exchanges. They have had a tradition over one or two decades and they are regularly used by business appraisals and for teaching purposes worldwide. The research is conducted for the individual years 2014-2022. It must be admitted that the year 2023 cannot be included into the analysis because the Czech Ministry of Industry and Trade has only published preliminary and incomplete data referring to this year in the time of paper writing (April 2025). Analysis before 2014 cannot be conducted because Damodaran has published the European data since 2014.

The paper focuses on industry branches belonging to the chemical industry. First, it is essential to define which all industry sectors are involved in the analysis because there may not be general agreement on the definition of the chemical industry. Some approaches may prefer a narrow definition and others a broad definition of this industry. Second, the definition of individual industry branches is also affected by the data sources employed in this research. The data sources used slightly differ in the way how individual industry branches are defined and named. The aim is to ensure maximum consistency between data samples therefore it is necessary to solve some discrepancies. First discrepancy is that the databases of Professor Aswath Damodaran distinguish manufactures of alcoholic and soft beverages although the database of Czech Ministry of Industry and Trade uses only one category presented by manufactures of all kinds of beverages. Second discrepancy is that some Czech main categories according to the classification CZ-NACE[12] involve much more in comparison to the databases of Damodaran therefore the choice is limited only to subcategories as in the case of 20_1 and 22_1.

Table I presents the industry branches analysed according to the data sources used. The left part of the table displays the original classification of CZ-NACE applied to the Czech data. The right part of the table shows the Damodaran classification applied to European and US data. To maintain authenticity, the original names and codes of individual industry branches are followed in Table I. It should be highlighted that more precise matching between industry branches from the different databases cannot be achieved. The Czech sector of manufactures of beverages is once compared to the European and US manufactures of alcoholic beverages and after compared to manufactures of soft beverages. It can be concluded that the research is conducted separately for individual selected chemical industry branches: 10 (54), 11 (28), 11 (29), 20.1 (35), 21 (44), and 22.1 (96). The number without the bracket is the code according to the classification CZ-NACE according to Czech Statistical Office (2025)[12] and the number in the bracket is the code employed by the Damodaran databases.

Table I
Selected industry sectors

Czech Republic		Damodaran Databases	
CZ-NACE	Name	Code	Name
10	Manufacture of food products	54	Food Processing
11	Manufacture of beverages	28	Beverage (Alcoholic)
		29	Beverage (Soft)
20_1	Manufacture of basic chemicals, fertilisers and nitrogen compounds, plastics and synthetic rubber in primary forms	35	Chemical (Basic)
21	Manufacture of basic pharmaceutical products and pharmaceutical preparations	44	Drugs (Pharmaceutical)
22_1	Manufacture of rubber products	96	Rubber & Tires

The data sources employed and analysed industry branches have been introduced in the previous paragraphs therefore it is time to turn attention to the subject of analysis. The subject of the analysis is one specific industrial average. More averages are not selected because of the paper's scope. The selected average belongs to the area of return which is one of the most important areas of corporate financial health. The chosen return ratio is the return on capital ROC whose quantification is presented in the following formula. This indicator is originally used by Professor Aswath Damodaran as the indicator of overall profitability, and it is possible to quantify it precisely

from the Czech input financial data. More frequently used and traditional indicator return on assets defined as EBIT/Assets cannot be employed because the Damodaran source does not provide the input financial data but already quantified indicators.

$$ROC = \frac{EBIT \times (1 - t)}{Assets - (Short - term\ financial\ assets + Cash\ equivalents)}$$

where
ROC – return on capital,
EBIT – kind of profit, earnings before interest and taxes,
t – income tax rate,
Assets – all capital sources including equity and liabilities,
Cash equivalents – cash and all cash equivalents as bank accounts.

The difference between ROC and ROA can be discussed. First, ROC does not take into consideration the effect for the government because the profit in the numerator is already after the taxation. Second, the capital sources in the denominator are limited because short-term financial assets and cash and its equivalents are excluded. This adjustment protects companies with very high or even exceeded liquidity not to decrease the quantified profitability.
The research has to follow several steps. After the acquisition of Damodaran data, the Czech values of the indicator ROC are quantified. The following steps are focused on the data processing. Relative differences of the return on capital (RD ROC) are determined for individual territories (Czech Republic, Europe, and USA). The relative differences are obtained in order to calculate the absolute values of average values of these characteristics for selected time intervals, i.e. absolute values of average values of relative differences AVRD ROC. The relative differences of the return on capital (RD ROC) are constructed as the ratio of the absolute difference between the value of given territorial ROC (Czech Republic (CZ), Europe (EUR), and USA) and the average value of ROC (ROC_{AVG}) for all these territories to the value of ROC_{spread}. The quantification of the relative difference of ROC is displayed in the following formula and the quantification of ROC_{AVG} and ROC_{spread} are explained instantly.

$$RD\ ROC = \frac{(ROC_{TERITORIUM} - ROC_{AVG})}{ROC_{SPREAD}}$$

The average value of ROC (ROC_{AVG}) is just the simple arithmetic average of the indicator for all territories in the given year and its quantification is presented in the formula below.

$$ROC_{AVG} = \frac{ROC_{CZ} + ROC_{EUR} + ROC_{USA}}{3}$$

ROC_{spread} is the difference between the maximum and minimum value of the ROC indicator, i.e. $ROC_{MAX} - ROC_{MIN}$, for all analysed years and all included sectors in this research. ROC_{spread} has the value of 28.71% in this analysis, which is the difference between the minimum value of ROC_{MIN} = 0.01%, detected in the USA territory in 2020 in the industry 22.1/96 (manufacture of rubber products, or Rubber & Tires), and the maximum value ROC_{MAX} = 28.72%, detected in the USA territory in 2022 in the industry 11/29 (manufacture of soft beverages). Since the ROC_{spread} value is intended to fulfill the role of a certain general basal characteristic of the ROC indicator in the analysis performed, a uniform value of ROC_{spread} = 28.71% is used for all territories, years, and industries analysed. For certainty, the following formula presents the quantification of the spread.

$$ROC_{SPREAD} = ROC_{MAX} - ROC_{MIN}$$

Another characteristic received is the absolute value of average value of relative difference AVRD ROC. It is just mathematically determined the absolute value of the previously quantified indicator the relative difference of return on capital RD ROC, so AVRD ROC = |RD ROC|. The purpose of this quantification is to gain average values for the analysed period 2014-2022 which enable the comparison. The part Discussion and result analysis presents only the values of the average value of relative difference RD ROC for each year and each territory included in the analysis and the average value of the absolute value of average values of relative difference AVG AVRD for each territory (time average). The indicator AVG AVRD is just mathematically the simple arithmetic average of the absolute value of average values of relative difference AVRD ROC. The auxiliary indicator ROC_{AVG} which is essential for the quantification of RD ROC and AVRD ROC is not independently presented in the part Discussion and result analysis which subsequently follows.

Discussion and result analysis

The part Discussion and result analysis is dedicated to the presentation of received findings and especially to related interpretations. Tables II – VII display the values of average value of relative difference RD ROC in the given year in the given territory (Czech Republic, Europe, and USA) and the simple arithmetic average of the

absolute value of average values of relative difference AVG AVRD of the indicator ROC in the last column for each territory. Each table is dedicated to one selected industry branch belonging to the chemical industry. Table II focuses on the food industry, Table III and IV display results for alcoholic, respectively soft beverages, Table V presents findings for chemical basic products, Table VI is dedicated to the branch of drugs and pharmaceutical products, and as the last Table VII shows results for the industry of rubber and tires. Attention will be paid not only to different industry branches but especially to differences observed between territories.

European values were consistently closest to the spatial average values in most of the analysed branches, namely in the food industry, alcoholic beverage, soft beverage and drugs and pharmaceutical products. RD ROC ranged from -2.03 to 11.12% and the time average AVRD ROC was 5.63% in the food industry (Table II), RD ROC from -11.41 to 6.34% and the time average AVRD ROC was 5.84% in alcoholic beverage (Table III), RD ROC from -14.42 to 18.39% and the time average AVRD ROC was 12.14% in soft beverage (Table IV), and RD ROC from -4.96 to 13.16% and the time average AVRD ROC was 4.73% in drugs and pharmaceutical products (Table VI).

American values consistently had significant positive differences in these industries, RD ROC ranged from 13.48 to 34.31% and the time average AVRD ROC was 21.77% in the food industry (Table II), RD ROC from 12.26 to 34.70% and the time average AVRD ROC was 19.06% in alcoholic beverage (Table III), RD ROC from 31.28 to 46.38% and the time average AVRD ROC was 37.10% in soft beverage (Table IV), and RD ROC from 7.84 to 23.25% and the time average AVRD ROC was 16.86% in drugs and pharmaceutical products (Table VI).

Czech values had consistently significant negative differences in these sectors, RD ROC ranged from -21.87 to -37.03% and the time average AVRD ROC was 26.95% in the food industry (Table II), RD ROC from -6.61 to -23.65% and the time average AVRD ROC was 14.63% in alcoholic beverage(Table III), RD ROC from -18.92 to -42.03% and the time average AVRD ROC was 29.05% in soft beverage (Table IV), and RD ROC from -12.88 to -29.35% and the time average AVRD ROC was 19.21% in drugs and pharmaceutical products (Table VI). And moreover, Czech values also have consistent (frequently significant) negative differences in the sector of chemical basic products, in which RD ROC ranged from -7.92 to -25.90% and the time average AVRD ROC was 16.46% (Table V).

Table II
Comparison of ROC for food industry

Indicator	Food industry									
	2014	2015	2016	2017	2018	2019	2020	2021	2022	AVG AVRD
RD ROC CZ	-37.03%	-28.78%	-24.75%	-30.50%	-29,49%	-23.16%	-24.18%	-22.77%	-21.87%	26.95%
RD ROC EUR	2.72%	-2.03%	5.86%	11.12%	6,07%	9.68%	8.42%	2.09%	2.68%	5.63%
RD ROC USA	34.31%	30.81%	18.89%	19.38%	23,42%	13.48%	15.77%	20.69%	19.19%	21.77%

Table III
Comparison of ROC for alcoholic beverages

Indicator	Alcoholic beverages									
	2014	2015	2016	2017	2018	2019	2020	2021	2022	AVG AVRD
RD ROC CZ	-23.65%	-12.02%	-18.11%	-23.29%	-17.15%	-6.61%	-8.28%	-8.11%	-14.49%	14.63%
RD ROC EUR	6.34%	-3.27%	-3.77%	-11.41%	-6.54%	-5.64%	-7.58%	-7.18%	-0.79%	5.84%
RD ROC USA	17.31%	15.29%	21.87%	34.70%	23.69%	12.26%	15.86%	15.29%	15.27%	19.06%

Table IV
Comparison of ROC for soft beverages

Indicator	Soft beverages									
	2014	2015	2016	2017	2018	2019	2020	2021	2022	AVG AVRD
RD ROC CZ	-35.43%	-18.92%	-42.03%	-24.90%	-29.87%	-23.77%	-26.30%	-26.91%	-33.27%	29.05%
RD ROC EUR	-10.95%	-12.36%	18.39%	-10.28%	-8.64%	-10.54%	-14.42%	-11.45%	-12.19%	12.14%
RD ROC USA	46.38%	31.28%	23.65%	35.18%	38.52%	34.32%	40.72%	38.36%	45.46%	37.10%

As it will be pointed out further, the situation is different in the sectors of chemical basic products and rubber and tires compared to the previously discussed branches. As for the industry of chemical basic products, as already aforementioned, the Czech values have consistent negative differences, which is the only thing that is consistent with the previously discussed sectors of food industry, alcoholic and soft beverages and drugs and pharmaceutical products. European and American values in the sector of chemical basic products (Table V) reach both positive and negative deviations in individual years. European values of RD ROC were from -22.08 to 24.88%

and the time average of AVRD ROC was 15.29%. American values of RD ROC were from -11.10 to 38.67% and the time average of AVRD ROC was 14.11%. Generally, for this sector, it is valid that there are marginal mutual differences in the time averages of AVRD ROC between individual territories in comparison to aforementioned industry branches in which the differences between territories are more significant.

Table V
Comparison of ROC for chemical basic products

Indicator	Chemical basic products									
	2014	2015	2016	2017	2018	2019	2020	2021	2022	AVG AVRD
RD ROC CZ	-25.26%	-8.89%	-17.69%	-13.77%	-18.56%	-16.06%	-14.06%	-25.90%	-7.92%	16.46%
RD ROC EUR	14.60%	16.55%	16.14%	24.88%	13.42%	12.52%	-4.62%	-12.77%	-22.08%	15.29%
RD ROC USA	10.66%	-7.66%	1.55%	-11.10%	5.13%	3.54%	18.68%	38.67%	30.00%	14.11%

Table VI
Comparison of ROC for drugs and pharmaceutical products

Indicator	Drugs and pharmaceutical products									
	2014	2015	2016	2017	2018	2019	2020	2021	2022	AVG AVRD
RD ROC CZ	-20.24%	-14.78%	-12.88%	-22.44%	-18.13%	-15.44%	-19.11%	-29.35%	-20.51%	19.21%
RD ROC EUR	3.96%	6.94%	-1.01%	3.30%	0.93%	-4.96%	-4.74%	13.16%	3.57%	4.73%
RD ROC USA	16.29%	7.84%	13.89%	19.15%	17.20%	20.40%	23.85%	16.19%	16.94%	16.86%

Table VII
Comparison of ROC for rubber and tires

Indicator	Rubber and tires									
	2014	2015	2016	2017	2018	2019	2020	2021	2022	AVG AVRD
RD ROC CZ	12.12%	14.00%	10.49%	4.75%	7.52%	4.19%	14.29%	3.87%	1.39%	8.07%
RD ROC EUR	-21.81%	-20.95%	-11.08%	2.48%	2.74%	8.13%	3.86%	4.11%	0.59%	8.42%
RD ROC USA	9.68%	6.95%	0.59%	-7.23%	-10.26%	-12.32%	-18.15%	-7.98%	-1.98%	8.35%

As for the branch of rubber and tires (Table VII), Czech values have the highest positive differences in this sector, almost consistently (with the exception of one year when the difference was also positive, but not the highest). Czech values of RD ROC ranged from 1.39 to 14.00% and the time average of AVRD ROC was 8.07%. European values of RD ROC were consistently negative until 2016 and consistently positive from 2017, with the total RD ROC range from -21.81 to 8.13% and the time average of AVRD ROC was 8.42%. American values of RD ROC were (on the contrary, compared to European values) consistently positive until 2016 and consistently negative from 2017, with the total RD ROC range from -18.15 to 9.68% and the time average of AVRD ROC was 8.35%. Generally, this branch has the smallest differences in time averages of AVRD ROC between individual territories compared to all aforementioned analysed sectors.

Conclusion

The aim of the paper was to evaluate the accuracy of using industrial averages when industrial averages from different territories were compared. Findings obtained showed differences between industry sectors according to the employed indicator return on capital ROC. It confirms that it is necessary to distinguish not only between industry sectors but also between territories. The values received in different territories have not differed only in their absolute values but also in the time trends. It points out the potential danger when market data is not available and is substituted by available industrial averages coming even from the different territories for which the market data is accessible.

The research could be expanded to include other territories and other indicators. Indicators do not have to exclusively focus on corporate profitability, and they could also follow other areas of financial health. The alternative areas of financial health could be leverage, liquidity, and efficiency. It also opens the possibility of analyzing other more traditional return indicators than the employed indicator return on capital ROC preferred by Professor Aswath Damodaran.

The research limitations could be detected that different data sources apply different methodology. Differences can be related to the way how industries are defined in the employed data sources. Some data sources can

include in the given industry companies belonging to different industry branches. Another disparity could be detected in average quantification. It is always not evident how averages are quantified. Simple arithmetic average can provide diverse results compared to the weighted average for which the weights are presented by the importance of the company (expressed e.g. by its property, turnover, and number of employees).
Results received in the paper are useful especially for the needs of estimates of parameters needed to calculate the cost of capital, economic costs, and economic added value, as well as for the needs of valuing companies using income methods. Non-appropriate values of industrial averages could influence valuation statements provided by professional appraisers and valuators and this can have a serious impact on decision-making potential buyers, sellers, and courts.

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DEVELOPMENT OF CORPORATE INSOLVENCIES IN THE CHEMICAL INDUSTRY

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Abstract

Companies go through different phases of the business life cycle, such as seed phase, start-up, establishment, growth, maturity, and business exit. Business termination can occur at any time and can take various forms and consequences for stakeholders. Insolvency seems to be the form with the most negative attributes and impacts on different interests' groups. Therefore, the research aimed on insolvency trends is conducted. To detect the insolvency trends, the quantitative research has to be conducted. The time development of corporate insolvencies in the chemical industry is described. Development according to industry branches is analysed from the absolute as well as relative point of view. It should be taken into consideration that the individual industry branches differ in their size and the number of registered business entities. Detected differences between the individual industry branches are pointed out. Possible reasons for the observed differences are highlighted and discussed. The findings show which industry branches are more vulnerable and exposed to the higher insolvency risk. This kind of conclusion has a practical benefit for different groups of stakeholders, namely for potential investors, managers, suppliers, and customers. However, the research conducted has its limitations based on data availability.

Introduction

Insolvency seems to be the phase of the business life cycle with the most negative attributes and impacts on different interests' groups therefore it makes a sense to focus on insolvency trends in different industry sectors. In the centre of interest there are the companies belonging to the chemical industry.

The research aim to analyse insolvency trends in the different industry sectors seems clear but there are difficulties to fulfil such goal when it is a challenging issue to collect required data. Although the Czech Republic has had modern insolvency legal framework since 2008 as stated in Kislingerová at el. (2013)[1] and the Czech insolvency register is one of the most open systems in the world as written in Smrčka (2013)[2] the availability of aggregated data is limited. This issue was pointed out by Kislingerová (2012)[3] who warned that many useful pieces of information enabling the law reform are not published and available. Official statistical sources publish the number of insolvencies (bankruptcies) and their types and the regional distribution among courts, but they do not publish the length of insolvency proceedings, the level of creditor satisfaction, and industry belonging. Czech insolvency proceedings have weaknesses related to these areas such as the long duration of insolvency proceedings (Arltová et al., 2016)[4] or low satisfaction rates of claims (Smrčka et al., 2017)[5].

The information if some industry sectors are more vulnerable and tend to declare more insolvency proceedings than other industry branches could be extremely valuable for interests' groups including potential investors, managers, suppliers, and customers.

This contribution has a standard structure and consists of four parts. Section 1 sets the research into a broader context and presents the paper aim. The following part focuses on the employed methodology and materials. Finally, Sections 3 and 4 present the results of the research conducted along with their interpretation and conclusions.

Methodology

To detect the insolvency trends, the quantitative research has to be conducted. First, it is essential to acquire needed data. The part Introduction has highlighted difficulties with the data accessibility therefore different data samples have to be combined. This research collects various governmental or non-governmental data samples. Own historical research[6] conducted in 2012 was based on the data prepared by the Employment office and published by Ministry of Labour and Social Affairs (2012)[7] followed by extractions from the corporate database Albertina. According to the list of insolvent companies published by the Employment office, the data sample was acquired but the additional pieces of information characterizing individual insolvency cases had to be extracted from different sources such as Albertina. Non-governmental data sources are reports published by the Czech specialized credit agency called Creditreform, later called as CRIF - Czech Credit Bureau which was very active

until 2020. This paper is based on its data following data sources – Creditreform (published in 2014, 2018)[8, 9] and CRIF (published in 2020)[10]. and Since 2020, the international group Credit Bureau has focused exclusively on international comparisons and has not published detailed statistics for the Czech market anymore. The newest publicly available is the data sample published by the group of insolvency and reorganization of University of Economics Prague (project TAČR)[11].

The aim of the research is to analyse the development of corporate insolvencies in different industry branches. The paper focuses on industry sectors belonging to the chemical industry. First, it is essential to define which all industry sectors are involved in the analysis because there may not be general agreement on the definition of the chemical industry. Some approaches may prefer a narrow definition and others a broad definition of this industry. Second, the definition of individual industry branches is also affected by the data sources employed in this research. Own data set and data set published by the TAČR research team enable own industry classification, but the results published by the specialized credit agency do not allow individual industry classification. In this case, the classification employed by the given credit agency must be followed. Unfortunately, even the credit agency does not follow the uniform classification in each analysed year, and it has to be admitted that there are time changes in its applied methodology. It should be concluded that more precise matching between industry sectors cannot be obtained.

The selected industry branches according to the classification CZ-NACE[12] are CZ-NACE 10 Manufacture of food products, CZ-NACE 11 Manufacture of beverages, CZ-NACE 19 Manufacture of coke and refined petroleum products, CZ-NACE 20 Manufacture of chemicals and chemical products, CZ-NACE 21 Manufacture of basic pharmaceutical products and pharmaceutical preparations, and CZ-NACE 22 Manufacture of rubber and plastic products. The part Discussion and result analysis tries to follow the official codes of the classification CZ-NACE. However, when the groups are more widely defined more codes are mentioned for the given case.

Tables presented in the following subchapter display the absolute frequencies of corporate insolvencies in the selected industry branches in given years. The individual industry sectors generally differ in their size and the number of registered business entities therefore there is the need to relativize the data and receive relative frequences. There are more possibilities to express the relative frequency. It would be logical to quantify the relative frequency as the share of insolvent cases on the number of entities belonging to the given industry branch. This approach has several disadvantages. First, the number of insolvent cases compared to the total number of companies is very low. Second, the number of all companies is quite vulnerable but not depending on the insolvency cases but on the other factors such as a voluntary exit from the market and an establishment of new companies. An alternative way to express the relative frequency is to quantify the relative value as the share on total insolvency cases belonging to the sector CZ-NACE C Manufacturing. This approach has the advantage that it is not influenced by the changing number of companies in the given industry, and it even reacts to an increase or decrease of insolvency cases in the given year. When there are no serious industrial structural changes the total number of insolvency cases is just affected by economic cycles and it has an impact on all sectors.

Discussion and result analysis

The part Discussion and result analysis is dedicated to the presentation of received findings. Tables I – IV present the absolute and relative frequencies of insolvency cases in the selected sectors belonging to the chemical industry in particular years. Previous subchapter explained how the relative frequencies could be alternatively quantified. The relative frequency marked with an asterisk * means the relative value expresses the share on the total insolvency cases belonging to the sector Manufacturing. The relative frequency marked with two asterisks ** means the relative value expresses the share on the total companies belonging to the given sector.

Table I displays the oldest data in this paper and it compares two data sources. These two data sources do not cover the exact same time period and had different assumptions. The aim of the Czech specialized credit agency Czech Credit Bureau CRIF was to analyse all insolvency cases therefore the data sample is larger in comparison to the own research whose aim was also to analyse financial characteristics of the insolvent companies therefore only businesses as legal entities (and not self-employed persons) were included. The most insolvent companies belonged to CZ-NACE 10 Manufacture of food products in 2012 and 2013. Other affected branches were CZ-NACE 20 Manufacture of chemical products and CZ-NACE 22 Manufacture of rubber and plastic. The discrepancy between these two data samples in the number of observed cases in CZ-NACE 20 and 22 can be caused by the non-uniform industry classification applied by CRIF aforementioned in the subchapter Methodology. The report of CRIF even specifies the relative frequencies expressed as the number of insolvencies per 1,000 registered companies in a given year in a given sector. According to the procedure of CRIF, the number of registered companies is adjusted for non-entrepreneurial self-employed persons. The relative frequency would have been

6 in CZ-NACE 10 and 6.46 in CZ-NACE 20 in 2012. However, the relative frequency in 2013 showed different numbers (3.85 in CZ-NACE 10 and 5.59 in in CZ-NACE 20). This annual discrepancy (caused by a difference in used bases of 2012 and 2013) proves that the number of registered companies is vulnerable and it has disadvantages when it is used for the development analysis in individual years.

Table I
Corporate insolvencies in the period 2012-2013

CZ-NACE	Name	Own research 2012/3		CRIF 2013	
		Absolute	Relative*	Absolute	Relative*
10	Food products	7	10%	73	12%
11	Beverages	1	1%	0	0%
19	Petroleum	0	0%	0	0%
20	Chemical products	1	1%	47	7%
21	Pharmaceutical products	0	0%	0	0%
22	Rubber and plastic	5	7%	0	0%

Tables II and III present four individual years (2016-2019) according to the results of the Czech specialized credit agency Czech Credit Bureau CRIF which unfortunately did not follow the same methodology therefore the industry classification differs which makes the comparison complicated. The most affected industry branch as in Table I is CZ-NACE 10 merged with CZ-NACE 11 Manufacture of food products and beverages. Industry sectors specialized in the manufacture of chemical products, pharmaceutical products and rubber and plastic reached lower absolute number of insolvency cases in the given time period.

Table II
Corporate insolvencies in the period 2016-2017

CZ-NACE	Name	CRIF 2016			CRIF 2017		
		Absolute	Relative*	Relative**	Absolute	Relative*	Relative**
10, 11	Food products	49	20%	0.19%	33	18%	0.12%
20, 21, 22	Chemical products	18	7%	0.2%	19	10.5%	0.2%

Comparison of Tables I-III has proved the difference between individual industry sectors in the absolute number of insolvency cases. Relative frequencies expressed as the share on the total insolvency cases belonging to the sector Manufacturing display the same level of dependency. It could be stated that some industry branches are more vulnerable and exposed to the higher insolvency risk. Another important factor is the size of the given sector. If the sector is larger and there is the same probability of insolvency a higher number of insolvency cases will be observed in the given sector. Unfortunately, relative frequency expressed as the share on the total companies belonging to the given sector is not available for 2018 and 2019. In 2016 and 2017 this kind of relative frequency reached comparable values for both main sectors (Table II) but in 2013 there were huge discrepancies depending on if relative frequencies were quantified with the use of the base year 2012 and 2013. This precisely does not allow us to conclude that absolute values are primarily influenced by the size of the industry because there could be differences in intensity between years in the given sectors.

Table III
Corporate insolvencies in the period 2018-2019

CZ-NACE	Name	CRIF 2018		CRIF 2019	
		Absolute	Relative*	Absolute	Relative*
10, 11, 12	Food products & Tobacco	20	18.0%	11	8.8%
19	Coke & Petroleum	0	0.0%	1	0.8%
20, 21	Chemical & Pharmaceutical products	3	2.7%	0	0.0%
22	Rubber and plastic	5	4.5%	3	2.4%

Other differences in intensity between years can be observed in Tables I-III. When the absolute numbers are compared there is the significant decreasing time trend in the number of insolvency cases in the individual industry sectors. Although the global economic crisis started already in 2007 in the United States and gradually spread to Europe the macroeconomic indicators witnessed the first deterioration at the end of 2008 in the Czech

Republic and the increasing trend of insolvency cases came delayed. Insolvency declaration generally comes later after first difficulties, and it does not matter if the insolvency is triggered by external or internal factors. It is pointed out that the number of insolvency proceedings is delayed because insolvencies are declared more slowly in the Czech Republic which has the consequence that the Czech companies enter the insolvency proceeding with almost no assets (property emptiness) as confirmed by Čámská (2013)[6], proved by Schönfeld et al. (2019)[13] in the case of companies before the moratorium declaration and Smrčka et al. (2017)[5] in the case of companies with so called virtual headquarters. In the period 2012-2013, still the consequences of the global economic crisis were observed, and it was talked about the crisis in the form of the letter W when after the first deterioration and recovery the second deterioration occurred as described in Kislingerová and Schönfeld (2014)[14]. Although the economy was already recovering after 2013, the number of insolvency proceedings declared still reached high values, and the data shows the decreasing trend and that the lowest numbers were recorded in 2019. These findings are still consistent with the statement that number of insolvency proceedings behaves counter-cyclically according to Yserte et al. (2016)[15] or Lorié and Ciobica (2021)[16].

Table IV
Corporate insolvencies according to TAČR research

CZ-NACE	Name	Insolvencies		Pre-pack	Moratorium	Reorganization
		Absolute	Relative*	Absolute	Absolute	Absolute
10	Food products	17	8.6%	3	1	9
11	Beverages	2	1.0%			
19	Petroleum	0	0.0%			
20	Chemical products	6	3.0%	1		2
21	Pharmaceutical products	1	0.5%	1		
22	Rubber and plastic	12	6.0%		1	3

Table IV presents the most recently published data by the group of insolvency and reorganization of University of Economics Prague. The leading number of insolvencies is repeatedly achieved in the sector CZ-NACE 10 Manufacture of food products but there are also large numbers related to the sectors CZ-NACE 20 merged with CZ-NACE 22 Manufacture of basic chemical products, rubber and plastic. These findings are not fully consistent with the conclusions of Tables I-III. This discrepancy can be caused by several factors such as the different methodology of data collection and different development of insolvency trends influenced by the increasing energy prices having a serious impact on energy-intensive sectors of the chemical industry. It should be noted that the absolute frequencies are low, and none statistically conclusive findings can be obtained when Table IV is compared with the previous results presented in Tables I-III. Table IV still provides additional explanatory power when it does not only focus on the absolute number of insolvencies declared in the given sectors, but it also focuses on the alternative ways of insolvency solution such as prepacks and reorganization. Pre-packs present the term when the insolvency solution is prepared in advance before the insolvency is declared and mostly this solution assumes that the company will continue running its business operations under modified conditions. Reorganization assumes similar way of solution when the main aim is to preserve the company's business activities and keep jobs. The difference is that reorganization is not prepared in advance, but the reorganization plan is developed during the insolvency proceedings. According to findings in Table IV, reorganization principle is more widely applied in the branch CZ-NACE 10 Manufacture of food products.

Conclusion

The aim of the paper was to analyse the development of corporate insolvencies in different industry branches. The most insolvency cases were observed in the sector CZ-NACE 10 Manufacture of food products in all analysed data samples and in this sector the most alternative ways of insolvency solution as pre-packs and reorganizations occurred. Regardless of the sector concerned, the number of insolvencies declared decreased from 2012 to 2019. It could be stated that some industry branches are more vulnerable and exposed to the higher insolvency risk although only absolute frequencies could not confirm this finding because the size of the sector should be taken into consideration. The numbers of companies registered in the given sectors differ and most companies belong to the sector CZ-NACE 10 Manufacture of food products. Reasons why in some industry branches less insolvencies are observed could be that these industries are capital intensive, belong to neutral industry sectors, and its companies are too large to fail. In the case of neutral industry sectors, it is supposed their interconnection to economic cycle. Neutral industry sectors generally face lower frequency rate in the time of the overall economic deterioration in comparison to the cyclical sectors. Capital intensive industry sectors demand more

capital to be invested when the companies are established therefore such business plans tend to be prepared more in detail in comparison to less capital-intensive sectors. More professional managers are also hired in this kind of companies therefore when the company faces any risks then these risks are better controlled and managed. The last reason too large to fail is discussed in institutional economics and it points out when the company is large there are many incentives to keep the company running. These incentives include the need to keep jobs, the effort to preserve supply chains, and the effort of creditors (primarily banks and other institutional creditors) to find a solution to ensure that the company continues, as in the case of insolvency proceedings, the satisfaction rates of claims are very low not only for unsecured creditors but even for secured creditors.

The main paper limitation is the data availability which does not allow any comparison after 2020 and therefore it makes difficult to observe the trends caused by COVID-19, Russian Ukrainian war conflict since 2022, and increasing material and energy prices. The second limitation is that the number of insolvency proceedings declared has not reached values enabling statistical testing.

Although the absolute frequencies of insolvencies declared are low, and none statistically conclusive finding can be obtained these kinds of conclusion are beneficial. Insolvency as the way of the corporate termination has many negative attributes in general. The practical benefit could be detected for different groups of stakeholders, namely for potential investors, managers, suppliers, and customers, whose lives are extremely negatively influenced by corporate insolvencies when they occur.

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PREFERRED INFORMATION AND SOURCES FOR ASSESSING THE REPUTATION OF CHEMICAL COMPANIES AS POTENTIAL EMPLOYERS

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Abstract

Employer reputation represents a key factor in attracting and retaining qualified employees. This study analyses what types of information and which sources of information potential employees prefer when evaluating chemical companies as employers. Primary quantitative research was conducted via an electronic survey of 351 respondents and demonstrated the importance, in particular, of transparency with regard to working conditions, information about safety measures, and opportunities for career growth, these being things which potential employees primarily look for on official company websites, via job portals, or using personal references from current or former employees. The results yielded important practical recommendations for chemical companies in the field of employer branding, which could help companies improve their reputation as employers and in doing so attract and retain high-quality employees. The conclusions reached by the study also suggest how chemical companies can tailor their communication strategies to specific target groups according to their demographic characteristics, thereby significantly strengthening recruitment activities and increasing the attractiveness of chemical companies in a competitive labour market.

Introduction

Employer reputation plays a key role in the labour market, as it influences decision-making among job seekers and the ability of companies to attract and retain qualified employees[1]. This factor is particularly important in the chemical industry, as its socially sensitive focus naturally also affects how companies in this sector are perceived as employers[2]. It is precisely in this sector that assessment of the quality of the working environment, safety risks, environmental responsibility, and career opportunities usually seem to be more important than elsewhere[3]. In today's highly competitive labour market, companies must not only provide high-quality working conditions to secure high-quality employees, but also communicate these conditions effectively.

This study builds on previous research focusing on the information needs of various groups of external stakeholders when assessing the reputation of chemical companies. Whereas the previous analysis focused on general aspects of public perception of the reputation of chemical companies, this study specifically focuses on potential employees and their preferences when obtaining information about companies as potential employers. In the context of the current labour market, where the ability to attract and retain qualified workers represents a strategic challenge for companies, it is essential to understand the factors that influence the decision-making process undertaken by job seekers and to identify the sources of information which they prefer when making these decisions.

The aim of this study is to identify key aspects which potential employees take into consideration when evaluating chemical companies as employers and to determine the most frequently used sources of information. The findings provide chemical companies with practical recommendations for improving their communication strategies and employer branding in order to effectively reach target groups and attract qualified workers.

Theoretical background

Employer reputation as a key factor of competitiveness

Employer reputation has become a key factor which significantly influences the ability of companies to attract and retain qualified and talented employees. The concept of corporate reputation was first defined by Fombrun and Shanley[4], who described it as the overall image of a company which stakeholders form based on the company's long-term activities and its interactions with its environment. In recent years, this concept has developed into specific areas covering various fields and groups of stakeholders, whereas from the perspective of company employees, it is often referred to as employer branding. This is understood to mean the targeted communication of values and working conditions to both potential and existing employees. The aim is to create a positive image of the company on the labour market, making it attractive not only to job seekers but also to current employees[4,5].

A positive employer reputation offers companies a number of advantages. Not only does it help reduce the costs of recruiting new employees, but it also increases the loyalty of existing employees, ensures stability within teams, and contributes to achieving a high overall level of staff quality[6]. Companies with a good reputation can usually choose from a wider pool of applicants, allowing them to select the most talented people[1,3]. At the same time, they report lower recruitment costs, as job seekers tend to actively seek out employers with a good reputation[7]. This effect is particularly pronounced in industries which are perceived as risky or unpopular, such as the chemical industry, where the public is often sensitive to safety risks and environmental impacts associated with this sector[3].

Specifics of the chemical industry from the perspective of employees

The chemical industry is characterised not only by high demands on the technical qualifications of its employees, but also by strict safety standards and environmental challenges. The working environment in this sector is often associated with a higher level of risk, which may influence decision-making among potential[3]. Companies in this sector must therefore actively engage in transparent communication with regard to their safety measures and environmental policies, which can help mitigate negative stereotypes and perceptions of the risks associated with the chemical industry[3]. This is also supported by the results of a study conducted by Walker[8], which confirm that the credibility of information regarding safety and working conditions is a crucial factor in industries perceived as posing a higher risk to job seekers. Open communication, which ensures that the company adheres to high safety standards and takes a responsible approach to environmental challenges, can significantly improve its image and strengthen its position in the labour market[1].

Sources of information which influence decision-making among job seekers

In today's digital age, the way job seekers obtain information about potential employers has changed significantly. Apart from traditional information channels, such as official company websites and job advertisements, informal digital channels are playing an increasingly important role[1]. These include reviews of employers on platforms such as LinkedIn and Indeed, or discussions on social networks which provide job seekers access to authentic opinions from former and current employees. According to a study by Walker[8], this type of information source is becoming increasingly popular among younger job seekers and is often perceived as more trustworthy than official corporate communications. This trend is important for companies because it means that their digital reputation and the way they communicate with their stakeholders on public platforms have a direct impact on their ability to attract talented new employees[7,9].

A company which neglects to manage its online reputation properly risks job applicants forming a negative impression of its working conditions or culture. On the contrary, organisations which actively use modern communication channels to disseminate authentic and transparent information can improve their attractiveness on the labour market. This strategy not only increases confidence among potential employees, but also strengthens the overall reputation of the company as an attractive and responsible employer[5].

Research methodology

The primary objective of this research was to determine what types of information and which sources of information potential employees prefer when assessing the reputation of chemical companies as employers. The research was conducted in two phases. First, a qualitative preliminary study was prepared on the basis of review of the professional literature, which was then conducted in the form of eight individual in-depth interviews. The interviews were conducted using a pre-prepared set of questions aimed at identifying the factors which potential employees consider important when assessing the employer reputation of chemical companies and their preferred sources of information. The results of this qualitative survey formed the basis for creation of a questionnaire for follow-up quantitative research.

Primary quantitative research was conducted using an electronic survey. Due to limited time and personnel resources, respondents were selected by means of purposive sampling on the basis of their availability, where a large proportion of those chosen were university students. The aim was to ensure the widest possible range of responses from respondents of different age groups, educational backgrounds, and genders. A total of 351 fully completed questionnaires were obtained. Due to the uneven structure of the sample, the data obtained were weighted during statistical processing in such a way as to ensure that the responses reflected the demographic structure of the Czech population by gender and age as at 31 December 2022[10]. This approach helped align the results more closely with quota sampling, which better represents the situation within the overall population.

IBM SPSS Statistics 24 software was used for statistical processing of the obtained data. Descriptive statistics were used for the basic description of the sample — primarily absolute and relative frequencies, averages, medians, and standard deviations.

The Friedman test was used to verify statistical assumptions and analyse data, along with post-hoc tests, which allowed us to identify differences between the individual evaluated aspects. The Kruskal-Wallis test was also used to identify differences between independent groups of respondents (e.g., by age, gender, or education) and the chi-square test to assess the association between categorical variables. The statistical significance of all results was assessed at a 95% significance level ($p < 0.05$).

Result analysis

Analysis of the results focused on identifying key factors influencing perception of the reputation of chemical companies from the perspective of potential employees and the preferred sources of information sources which these job seekers most often use when searching for information about employers. Respondents rated individual aspects of employer reputation using a four-point scale (1 = not important at all, 4 = very important) and subsequently indicated the sources of information used, whereas they were able to select multiple options. The results were analysed separately for individual aspects of reputation assessment and for preferred sources of information.

The Friedman test verified that respondents do not perceive all aspects of reputation examined in this study as equally important ($p < 0.001$). Post-hoc analyses allowed these aspects to be ranked according to their weighted average ranking from most important to least important. The results are summarised in Table I

Table I

Results of the evaluation of the importance of aspects for the assessment of the reputation of a chemical company from the perspective of potential employees

Aspect	weighted relative frequencies of importance levels [%]				Median	Weighted average ranking
	4	3	2	1		
Health risks	**82.2**	**16.6**	**0.4**	**0.8**	**4**	**7.58**
Amount of wage/salary	**79.4**	**18.0**	**1.7**	**0.8**	**4**	**7.37**
Benefits for employees	66.2	25.1	7.5	1.2	4	6.47
Opportunity for career growth	58.8	27.5	10.8	2.9	4	6.04
Company results (profit or loss)	50.9	39.4	8.4	1.3	4	5.77
Tradition and overall reputation of the company	52.8	35.5	9.3	2.4	4	5.74
Availability of the company	46.7	63.2	8.3	1.8	3	5.73
Vision of the company – vision of the future	43.3	43.9	11.6	1.2	3	5.41
Company's position on the market	45.7	39.2	10.0	5.1	3	5.38
The company's attitude towards ecology	44.5	37.9	13.9	3.7	3	5.29
Production processes, technology used	46.8	32.0	16.6	4.6	3	5.22

Source: Own.

It is clear from Table I that potential employees in chemical companies consider information about health risks, salaries, benefits, and career opportunities to be the most important. Of the areas surveyed, they are least interested in the employer's attitude toward ecology and production technology.

Another area examined was respondent preferences for sources of information (see Figure 1). This analysis reveals the communication channels which are important to potential employees when searching for information about a company.

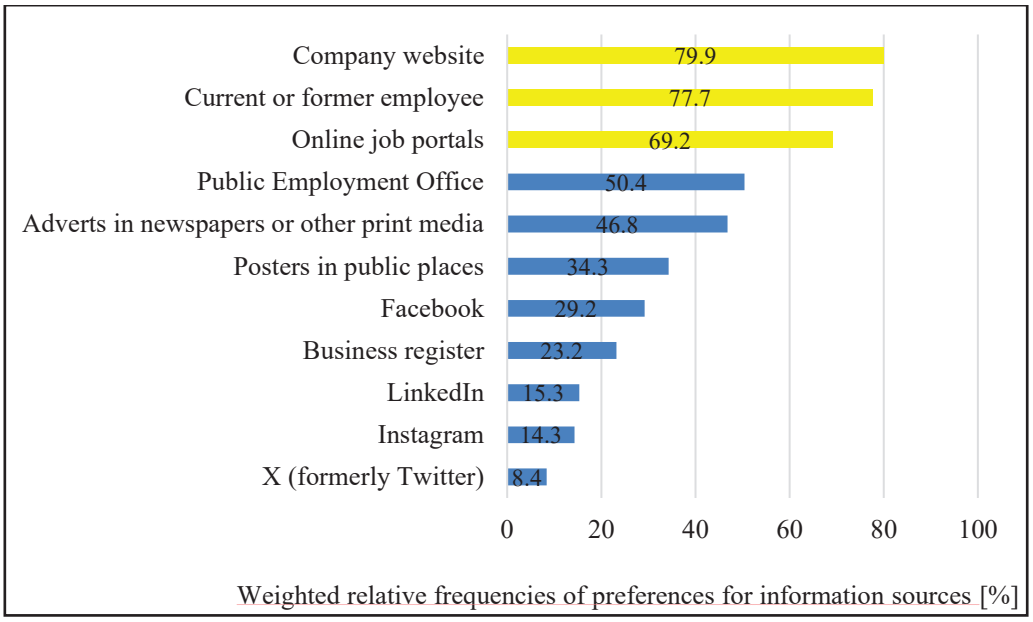

Figure 1. Preference of information sources among potential employees of chemical companies

Figure 1 shows that the most preferred means of communication when looking for information about a potential employer are the company's website, current or former employees, as well as advertising websites. Somewhat surprisingly, social networks, primarily Social Network X, Instagram or LinkedIn, can be considered the least preferred communication channels when searching for information about employers.

The possibility of formulating recommendations on the right communication strategy for the target companies required an analysis of differences in the perceived importance of aspects of employer reputation depending on the demographic characteristics of the respondents. The results are shown in Table II.

Table II

Results of the analysis of differences in the perceived importance of aspects for assessing the reputation of a chemical company depending on demographic factors

Reputation assessment aspect of a chemical company	**Demographic distribution**		**Test**	
	Gender		Kruskal-Wallis test	
	Man	Woman	χ^2	sig.
Availability of the company	135.6	**161.8**	8.50	0.004
Production processes, technology used	138.5	**158.6**	4.77	0.029
Benefits for employees	139.9	**157.0**	4.21	0.040
Reputation assessment aspect of a chemical company	Age		Kruskal-Wallis test	
	<42	>42	χ^2	sig.
Opportunity for career growth	**187.5**	134.6	27.59	<0.001
Benefits for employees	**173.1**	139.5	12.32	<0.001
Production processes, technology used	**163.9**	142.6	4.09	0.043
Reputation assessment aspect of a chemical company	Education		Kruskal-Wallis test	
	Without matriculation	With high school diploma and higher	χ^2	sig.
Production processes, technology used	126.4	**157.2**	9.41	0.002
Opportunity for career growth	127.9	**156.6**	8.97	0.003
Benefits for employees	133.1	**154.3**	5.41	0.020
Reputation assessment aspect of a chemical company	Professional education in chemistry		Kruskal-Wallis test	
	Yes	No	χ^2	sig.
Tradition and overall reputation of the company	156.9	**181.1**	4.00	0.045

Source: Own.

Table II shows that the perceived importance of some aspects of a chemical company's reputation as an employer varies statistically significantly by the demographic characteristics of the respondents. The most statistically significant differences were found in terms of employees' ratings of the importance of information about production processes and benefits, which are more important to women under 42 with a college degree than to men over 42 without a high school diploma. Career growth opportunities are also rated as more important by younger respondents with higher education than by those with primary education. The accessibility of the company is also more important for women than for men, and interestingly, respondents without a chemistry background place more importance on tradition and the overall reputation of the company.

The final area of analysis was to examine differences in preferences for information sources depending on demographic factors (see Table III).

Table III

Results of the analysis of differences in preferences for information sources depending on demographic factors

Preference of information sources	**Demographic distribution**		**Test**	
	Gender		χ2-test	
	Man	Woman	χ^2	sig.
Posters in public places	23.5	**37.6**	7.28	0.007
Instagram	14.1	**26.2**	6.89	0.009
Public Employment Office	38.3	**52.5**	6.41	0.011
Preference of information sources	Age		χ2-test	
	<42	>42	χ^2	sig.
Adverts in newspapers or other print media	24.4	**58.2**	40.28	<0.001
Instagram	**33.7**	5.7	39.22	<0.001
Company website	**95.9**	71.5	38.26	<0.001
Online job portals	**87.6**	61.4	31.02	<0.001
LinkedIn	**28.0**	7.0	24.06	<0.001
Public Employment Office	37.8	**57.0**	12.04	0.001
Posters in public places	23.8	**41.1**	11.25	0.001
Preference of information sources	Education		χ2-test	
	Without matriculation	With high school diploma and higher	χ^2	sig.
Online job portals	59.2	**80.0**	12.30	<0.001
LinkedIn	4.2	**22.1**	10.89	0.001
A person who has worked or is still working in the company	64.8	**83.9**	11.82	0.001
Company website	73.2	**87.9**	8.34	0.004
Adverts in newspapers or other print media	**54.9**	35.7	7.96	0.005
Business register	12.7	**27.1**	5.70	0.017
Preference of information sources	Professional education in chemistry		χ2-test	
	Yes	No	χ^2	sig.
Company website	**97.3**	81.6	10.05	0.002
Online job portals	**89.2**	72.2	8.28	0.004
Instagram	**32.4**	18.1	6.42	0.011
LinkedIn	**28.4**	15.9	5.24	0.022

Source: Own.

Table III shows that preferences for information sources differ statistically significantly by gender, age, educational attainment and chemistry background. Posters in public places and information from the employment office are more preferred by women aged 42 and over; company websites, job portals and LinkedIn are more used by people aged 42 and under with higher education and chemistry background; and Instagram is a more important information source for women aged 42 and under with chemistry background; advertisements in newspapers or other printed sources are preferred by respondents over 42 with less education, and people

with more education like to hear the opinion of current or former employees compared to people with less education who prefer information from the company register

Discussion

This study confirmed that, when assessing chemical companies as potential employers, individuals place the greatest importance on salary, employee benefits, perceived health risks, and prospects for career advancement. Digital sources of information – especially company websites, job portals, and personal references – play a crucial role in decision-making among candidates. Traditional methods, such as advertisements in print media or information from job centres, are less relevant, especially among younger respondents.

Analysis of differences between groups of respondents according to their demographic characteristics revealed important correlations. Younger applicants under the age of 42 show a significantly stronger preference for career advancement and digital information channels, such as job portals, social media (particularly Instagram and LinkedIn), and personal recommendations. In contrast, older respondents more often use traditional sources such as job centres, newspaper advertisements, or posters in public places — i.e. channels associated with a higher degree of stability and availability of information in the offline environment. This necessitates a differentiated approach to communication strategies – while a presence on digital platforms is crucial for younger audiences, older generations are more likely to be reached by more conservative forms of communication.

Significant differences were also observed according to gender, education, and professional qualifications. Women placed greater emphasis on employee benefits and the accessibility of the company, while men rated production technology more positively. Respondents with a higher level of education more often rely on professional information channels such as LinkedIn, the commercial register or official company websites. In contrast, people without an academic secondary education trust personal recommendations or advertisements in traditional media more. In terms of expertise, candidates with a background in chemistry are more demanding in terms of the quality and transparency of communication, especially in the fields of safety and technology.

Chemical companies should therefore tailor their employer branding strategy to individual target groups. Active work on digital reputation, transparent communication of benefits and working conditions, as well as differentiation of communication channels according to demographics, can significantly contribute to the effectiveness of recruitment activities.

Although the study has provided valuable insights, its limitations should also be mentioned. The first limitation is the sample of respondents itself. Although 351 responses were analysed, the sample cannot be considered to be fully representative. However, the impact of a higher proportion of students among respondents was partially eliminated by weighting the data according to the age and gender structure of the population (Czech Statistical Office, 2023). Nevertheless, it is possible that certain preferences (e.g., emphasis on career growth or digital resources) were reflected in the results due to the specific characteristics of the sample investigated.

Another limitation is the use of an online questionnaire survey. This method of data collection may have attracted mainly technologically literate respondents, which may have slightly increased the preference for digital information sources. Respondents who prefer traditional approaches may have been underrepresented in the sample.

Another partial limitation may be the use of exclusively non-parametric statistical tests (the Friedman test, and the chi-squared test), which, although appropriate for the nature of the data, need not necessarily capture deeper interactions between variables. More advanced models (e.g., regression analysis or segmentation using clustering) could be applied in future research.

We recommend expanding the research with the aid of qualitative methods such as in-depth interviews or focus groups, which would allow for a deeper understanding of the motivations and information strategies of job seekers. It would also be interesting to conduct longitudinal monitoring of the development of information behaviour over time, especially in connection with the rapid development of digital trends.

Another direction could be international comparison, which would offer a broader context for understanding employer reputation in different cultural and economic environments. It would also be interesting to compare individual segments of the chemical industry (e.g., pharmaceuticals, petrochemicals, or plastics), which may differ in terms of both the nature of the work performed there and their requirements for employees.

Conclusion

This study contributes to a deeper understanding of how potential employees perceive the reputation of chemical companies and which factors influence their decision-making with regard to their potential future employment. The findings show that, apart from the quality of working conditions and benefits offered, the way

in which this information is communicated also plays a key role. The credibility and accessibility of information — especially via digital channels — represent an important element in the attractiveness of the given employer. The results also underscore the need to personalise approaches to communication in order to ensure that they reflect the demographic characteristics of job seekers. Companies that want to reach a wide range of candidates should actively manage their online reputation, provide transparent and relevant information, and use an appropriate mix of communication tools. This will not only increase their chances of successful recruitment, but also promote long-term trust and loyalty among employees.

From the point of view of strategic human resource management, it is clear that employer branding is no longer merely a matter of marketing presentation, but an important element of competitiveness in the labour market. The results of this study should therefore be seen as a starting point for designing effective recruitment and communication strategies which reflect current workforce preferences and adapt to the dynamic evolution of the working environment and technology.

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THE CURRENT STATE OF SLOVAK WINEMAKING AS A SECTOR OF TRADITIONAL BIOTECHNOLOGY

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Abstract

Slovak winemaking, as a representative of the traditional sector of classical biotechnology, currently faces numerous economic challenges and opportunities, having already undergone a long and demanding journey. This article analyzes the current state of Slovak winemaking as an economic sector with a significant impact on the local economy. The article primarily focuses on the development of wine production in Slovakia over the past three decades, examining trends in domestic consumption, consumer preferences for quality, grape prices, production costs, and the effects of climate change on harvests, all of which influence the industry's competitiveness. The aim of this article is to provide an objective perspective on the current state and economic outlook of Slovak winemaking, identify the main challenges, and propose potential measures to enhance its competitiveness and ensure sustainable development.

Introduction

Slovak viticulture and winemaking have undergone significant changes over the last three decades. Following the fall of socialism, the industry shifted from the mass production of wines of questionable quality to the production of limited volumes of wines with excellent quality that are capable of competing with those from leading wine-producing countries in international competitions. This is particularly true in the category of dry white wines, where Slovak wines are currently regarded among the best in the world. However, the overall situation is not as optimistic as it may seem at first glance. Although the quality of Slovak wines has improved significantly, viticulture, which serves as the production base of the industry, is currently in a highly complicated situation. The price of grapes, which are the sector's main raw material, has for a long time failed to reflect the actual costs of vineyard operation and the investments needed for sustainable development. As a result, many grape growers have gradually abandoned cultivation, leading to the decline or disappearance of numerous vineyards. At present, the Slovak Republic has just over 9,000 hectares of vineyards in active production (Trubačová, 2025), while at the time of its accession to the European Union in 2004, it was granted planting rights for 22,227 hectares. For context, before the breakup of Czechoslovakia, Slovakia had more than 32,140 hectares of cultivated vineyards in 1985 (ZVVS, 2025). This illustrates a rapid decrease in vineyard area and, consequently, in production capacity within a single generation. It should be noted, however, that not all of the original vineyard areas, which exceeded thirty thousand hectares, were located in places suitable for producing wines of outstanding quality. The current state of viticulture has resulted from a combination of several factors, which together led to a decline in the total area of productive vineyards. Given that the current area represents less than one third of the vineyard land that existed at the end of the Czechoslovak federation, and that today the existing vineyards are largely concentrated in the most favorable locations, any further significant decrease in area is unlikely. In addition, newly planted vineyards are gradually entering their productive stage, contributing to the renewal and rejuvenation of the vineyard base. These new areas are planted with well-regarded grape varieties that enjoy stable market demand and are located in sites with favorable natural conditions. The situation is further complicated by the fact that one of Slovakia's most valuable wine regions, the Malokarpatská area, is situated next to the capital city of Bratislava. Due to increasing migration and demand for housing, the area has come under pressure from real estate development. Many vineyards that were abandoned after the dissolution of agricultural cooperatives were gradually left uncultivated, reclassified from agricultural to construction land, and consequently lost permanently. In addition to the generally rising production costs due to inflation, grape growers face substantial expenses for chemical treatments used to protect vines from fungal diseases and pests. Public financial support also still has space for improvement to make a tangible difference for those working in viticulture. From the perspective of viticulture as the main source of raw materials for winemaking, the current state may not be ideal, but it can be considered relatively stable. The winemaking sector, which processes the output of viticulture, faces a somewhat different yet equally challenging situation. After the economic transition of the 1990s and the decline of vineyard areas, domestic wine production decreased. Moreover, much of the wine produced during that period was of average or below-average quality when compared to current expectations. The transition to modern wine production became more prominent

after the beginning of the new millennium, with the emergence of a new generation of professionally trained winemakers, many of whom gained experience abroad. Over the course of approximately ten years, Slovakia evolved from a country producing mostly average quality wines to a dynamic wine-producing nation capable of competing with some of the world's best, particularly in the category of dry white wines. Although Slovak wines have reached the level of international quality standards, overall production volumes have declined considerably, and this trend has not yet been reversed. Even though per capita wine consumption has decreased significantly over the past decade, and domestic consumers now tend to prefer smaller quantities of wine with better quality, domestic wine production continues to fall short of meeting national demand.

Results and Discussion

Viticulture and winemaking have a long-standing tradition in Slovakia (Ladvenicová et al., 2022a). Vineyards account for approximately 1% of the country's agricultural land, and the entire territory of the Slovak Republic is divided into six viticultural regions (Ladvenicová et al., 2022b). Based on the most recent statistical data, it is evident that vineyard area continues to decline. As of July 31, 2024, the total registered vineyard area in Slovakia was 13,003.08 hectares. In the previous year, 2023, this figure was higher by 196.35 hectares, indicating a year-on-year decrease of 1.5%. Of the 13,003.08 hectares registered in 2024, 11,215.23 hectares were in productive use. This category also recorded a year-on-year decline of 736.72 hectares, which represents a 6.2% decrease compared to 2023. In addition to the reduction in existing productive vineyards, there was also a notable decrease in vineyards under planting (i.e. non-productive vineyards). This category fell by 47.8% year-on-year, from 664.17 hectares to 347.15 hectares. This may be interpreted as a result of previous plantings reaching the fruit-bearing stage, while new vineyards are no longer being established in the same quantities. This situation may, among other reasons, be caused by declining interest among growers to establish new vineyards due to high financial demands and relatively low profitability. The only monitored indicator that recorded an increase was the number of registered winemakers, which rose to 874 in 2024, representing a year-on-year increase of 9%. Of this number, 517 winemakers also cultivated vineyards (Trubačová, 2025). It can thus be inferred that 357 winemakers active on the market do not grow grapes and therefore must purchase the raw material. An interesting general trend in the alcoholic beverage market is the continuous decline in overall alcohol consumption, which also affects grape wine. A noteworthy pattern is the consistent 10% annual decrease in domestic wine consumption observed since at least 2021, with the most recent data showing a sharp 34% drop in 2023 compared to the previous year. This significant decline is likely driven in large part by general price inflation, which forces consumers to reduce spending on luxury goods, including higher-priced wines. As a result, consumers increasingly opt for lower-cost, medium-quality wines, most of which are imported. This trend is likely one of the main factors behind the current negative balance in Slovakia's foreign trade in wine, as well as the substantial growth in wine imports observed in recent years (Trubačová, 2025).

Table I
Wine Consumption in Slovak Republic

Indicator	M. j.	2019	2020	2021	2022	2023*
Total consumption	tis. l	77977.0	70642.0	71565.0	64633.0	42927.0
Consumption per capita	1	14.3	12.9	13.2	12.3	7.9
Consumption per capita from 18 years**	1	17.6	15.9	16.3	14.7	9.8

(Modified table by author according to Trubačová, 2025).
Note.: *in 2023 change in consumption calculation (Statistical Office of the Slovak Republic)
** Trubačová calculation

The largest group of wine consumers within the Visegrad Group countries, including Slovakia, consists of individuals who consume wine on 2 to 5 days per year, representing 18.42% of the population. The second-largest group, accounting for 16.58%, includes consumers who drink wine 1 to 2 days per week. The third group, comprising 16.38% of the population, consists of individuals who consume wine 2 to 3 days per month (Bírová et al., 2024). In 2023, the per capita consumption of grape wine in the Slovak Republic was 7.9 liters. When adjusted to include only adults aged 18 and over, the figure increases to 9.8 liters per person. Total wine consumption in 2023 amounted to 429,270 hectoliters of grape wine. At the same time, domestic wine

production continued to decline, reaching only 254,364 hectoliters in the 2023/2024 fiscal year. This represents a year-on-year decrease of 23.3%, or 77,142 hectoliters compared to the previous year. Despite this, the average annual production is generally estimated at around 300,000 hectoliters (Trubačová, 2025). In terms of pricing, the average price of red wine without geographical indication rose by 11.3% year-on-year in 2024, reaching €1.70 per liter. The average price of quality wines in 2024 was €2.68 per liter, representing a 1.8% increase compared to 2023 (Čičmanec, 2025). Slovak wineries predominantly relied on debt financing, which exceeded equity capital. However, the overall value of assets and their main components has shown consistent long-term growth. A similar trend has been observed in the development of equity, liabilities, and their subcategories. Fixed assets have continued to dominate over current assets in the asset structures of Slovak wine enterprises (Ladvenicová et al., 2022a).

Table II
Imports of Wine and Wine Products to the Slovak Republic

Item Code CS	Name	Unit	2020/21	2021/22	2022/2023	2023/2024	2023/24 / 2022/23 (%)
2204 10	Sparkling wine	hl	23837	25619	32391	25143	-22.4
		thous. €	10062	10580	15489	12609	-18.6
2204 21	Wine up to 2 l	hl	296196	254105	245835	283676	15.4
		thous. €	39747	35614	41358	47811	15.6
2204 22+29	Wine over 2 l	hl	369295	298284	289349	450555	55.7
		thous. €	10314	16755	21075	34534	64.0
2204 30	Grape must	hl	70353	53116	45602	27419	-9.9
		thous. €	3222	6328	5899	4301	-27.0
2204	Total	Hl	759682	631125	598011	786793	31.5
		thous. €	73659	65587	79421	94920	19.5
2205	Vermouths	hl	5866	6580	8756	10972	25.3
		thous. €	1100	1163	1404	1947	38.7
2009 61	Grape juice	hl	18276	23773	14544	15012	3.2
		thous. €	943	1309	1705	1877	10.3

(Modified table by author according to Trubačová, 2025).

In contrast to the decline in domestic wine production, wine imports to Slovakia increased significantly. In the 2023/2024 season, imports rose by 31.6 percent compared to the previous year, representing an additional 188,782 hectoliters and bringing the total volume of imported wine to 786,793 hectoliters. More than half of this volume consisted of wine transported in containers larger than two liters, often in the form of bulk shipments delivered in tankers. At the same time, Slovakia exported 492,866 hectoliters of wine, which represented a year-on-year decrease of 9.5 percent. Overall, considerably less grape wine was exported than imported. The result was a negative foreign trade balance amounting to 63,982 euros, and this deficit worsened by an additional 18,053 euros compared to the previous year (Trubačová, 2025). An analysis of export and import developments in wine trade within the European Union showed that, with the exception of Hungary, the EU's trade balance with the Visegrad Group countries, including Slovakia, has remained persistently negative. Hungary is the only member of the V4 group with a consistently positive trade balance in wine (Rogovská, 2018). In terms of comparative advantages, Slovakia shows the strongest position in wine trade with the Czech Republic and Poland. In contrast, Slovakia holds a comparative disadvantage in wine trade with Hungary, as Hungary has a competitive advantage not only within the Visegrad region but also on a global level (Bírová and Rovný, 2024). According to Valach (2023), however, the food industry in Slovakia, including the wine sector as a branch that processes grapes, is generally considered relatively prosperous.

Table III
Exports of Wine and Wine Products from the Slovak Republic

Item Code CS	Name	Unit	2020/21	2021/22	2022/2023	2023/2024	2023/24 / 2022/23 (%)	2023/24 Wine of Slovak origin
2204 10	Sparkling wine	hl	1760	222	677	821	21.3	-
		tis. €	231	338	520	610	17.3	-
2204 21	Wine up to 2 l	hl	61222	59311	66728	45099	-32.4	-
		tis. €	7354	7358	9449	6934	-26.6	-
2204 22+29	Wine over 2 l	hl	441172	480289	475408	445467	-5.9	-
		tis. €	21875	27832	23386	23759	1.6	-
2204 30	Grape must	hl	2961	5247	1572	1479	-5.9	-
		tis. €	561	1348	1378	1151	-16.5	-
2204	Total	hl	506715	545089	544407	492866	-9.5	69282
		tis. €	29554	31836	33433	30830	-7.6	6399
2205	Vermouths	hl	211	175	181	215	18.8	-
		tis. €	26	33	41	54	31.7	-
200961	Grape juice	hl	185	530	304	105	-65.3	-
		tis. €	26	69	60	34	-43.8	-

(Modified table by author according to Trubačová, 2025).

The Slovak wine sector was subject to detailed analysis in 2018 by Rogovská, resulting in a comprehensive SWOT evaluation presented in Table IV. Since then, the situation has changed slightly, as domestic production has continued to decline while wine imports have increased. In addition, the area of fruit-bearing vineyards has decreased, indicating that the negative trend is ongoing. Several findings from the SWOT analysis remain particularly relevant from a long-term perspective. Among the main strengths are the favorable natural conditions for grape cultivation and the historical international success of Slovak wines at prestigious events. These factors continue to represent important comparative advantages. In contrast, the most persistent weaknesses include slow utilization of financial support from both national and European Union sources, insufficient vineyard renewal, and inadequate marketing. These issues are considered to be the most serious and long-standing challenges. Slovakia has consistently struggled to draw on EU funds efficiently. The area of newly planted vineyards continues to decrease, and the promotion of Slovak wine, although it is objectively of high quality, remains underdeveloped. Nevertheless, these weaknesses can also be interpreted as opportunities. There is potential for improved marketing and presentation of wines produced in Slovakia, as well as its wine-producing regions. The export activities of small and medium-sized wineries could benefit from the creation of a national wine cluster and simplified access to European subsidies, particularly for smaller and newly established producers. Among the most significant threats are strong foreign competition, especially in the form of inexpensive imported wines, increasing production costs, and a range of related issues commonly referred to as challenges associated with the business environment.

Table IV
SWOT analysis of the Slovak wine sector according to Rogovská

Strengths	Weaknesses
• appropriate natural conditions for the cultivation of grape vines • orientation towards the production of wines of better quality • orientation towards the production of wines of better quality • awards from international exhibitions and competitions • varied variety • healthy banking sector, use of credit • healthy banking sector, use of credit • the possibility of drawing funds from the EU and from the state	• slow spending of financial support from the state and the EU • slow and insufficient recovery of vineyards • insufficient R&D expenditure and their inadequate connection to the wine industry • underutilized use of capacities in the wine industry • insufficient marketing • missing human resources • high cost of revenues • low competitiveness on domestic and foreign markets • weak cooperation of companies in membership in sales organizations • unregulated ownership relationships in the land market • unclear legislation • the split of the industry into primary production and the processing industry • unwillingness of individual winemakers for cooperation
Opportunities	**Threats**
• free production capacities • building the brand „Slovak wine“ • developing old traditions • the increasing willingness of consumers to pay more for quality and Slovak products • the utilization of the potential for agrotourism development • creation of a wine cluster • awards from international exhibitions and competitions • economic growth and increase the population’s purchasing power • improving the use of EU funds • rising R&D expenditure • product innovations (bio, organic production) • support for „court sales“ • educating the consumers for loyalty to domestic products • increasing consumption of wine • new form of sales (internet) • rigorous monitoring of wine quality	• cheap foreign competition • business policy of supermarkets • weather risk • changes in legislation • unequal EU support • inadequately functioning legal environment (law enforcement, corruption) • growth of input prices (energy) • lack of loyalty of Slovak consumers • missing human resources • clientelism and administrative difficulty in obtaining EU and state support

(Rogovská, 2018).

Based on the findings discussed above, it can be concluded that the situation in the winemaking and viticulture sector in the Slovak Republic remains quite challenging, particularly for domestic producers of grape wine who are also engaged in vineyard cultivation. Nevertheless, there are signs of gradual stabilization, as evidenced by

the emergence and steady establishment of professional wineries that produce high-quality wines and are involved in the renewal of original vineyard plantings.

Conclusion

Based on the data presented, the current situation in the Slovak wine sector can be considered complex, mainly due to the long-term decline in vineyard plantings and the subsequent continuous decrease in domestic wine production. Recent data on new vineyard plantings indicate that many of the newly established vineyards have already reached the fruit-bearing stage and have replaced older vineyards with grape varieties that no longer meet market demand. However, the area of newly planted, yet non-productive vineyards is currently only half the size compared to previous periods, which reflects a gradual slowdown in new vineyard establishment. In wine production, the trend also points toward decreasing output, with producers increasingly focusing on high-quality wines. This appears to be the only viable path for domestic producers to succeed in a highly competitive market environment, where the import of large volumes of low-cost, average-quality wines makes the production of lower-quality domestic wines economically unsustainable. The import of inexpensive foreign wines has continued to rise year-on-year and now represents a substantial share of total wine sales in the country. This existential necessity, combined with strong competitive pressure, has led to a situation in which mostly well-established and competitive enterprises remain active in the Slovak viticulture and winemaking sector. If these enterprises are able to maintain their market position, and if appropriate government support helps to improve the business environment, it is highly likely that internationally recognized and influential wineries may emerge from the territory of the Slovak Republic in the future.

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ESG AND PROJECT FINANCING IN THE CHEMICAL INDUSTRY

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Abstract

ESG is a comprehensive approach to evaluating companies based on their environmental and social performance and how they are governed. This approach is supported by international commitments such as the Paris Agreement, but also by EU legislation. Financial indicators are key in making decisions about the development of companies and the financing of investment projects. Nowadays, indicators related to the impact of investment activities on the environment, society and corporate governance are also increasingly being reflected, ESG is becoming another key indicator in the assessment of investments. This paper aims to map the impact of ESG on project financing from the perspective of banks and from the perspective of companies in chemical industry. Based on structured interviews, it will be assessed to what extent the ESG approach influences the evaluation of project proposals when considering financing from the perspective of banks, and to what extent ESG influences the evaluation of investment proposals from the perspective of chemical industry companies.

Introduction

ESG (Environmental, Social, Governance) is a comprehensive approach to evaluating companies based on their environmental and social performance and how they are governed and managed. This approach is supported by international commitments such as the Paris Agreement, but also by European Union (EU) legislation, e.g. in the form of the Corporate Sustainability Reporting Directive. Financial indicators have been and are key in making decisions about the development of companies and the financing of investment projects. Nowadays, indicators related to the impact of investment activities on the environment, society and corporate governance are also increasingly being reflected, ESG is becoming another key indicator in the assessment of investments. This paper aims to map the impact of ESG on project financing from the perspective of banks and from the perspective of companies in chemical industry. This research is motivated by the observation that ESG considerations are shifting from optional to essential components in strategic planning and financial management within these sectors.

The aim is to find out to what extent this approach influences the behaviour of banks, particularly when financing investment projects through bank loans, and to what extent companies, particularly in the chemical industry, have had to adjust their perspective and practices related to financing towards improving their approach to sustainability.

Literature Review

The growing significance of Environmental, Social, and Governance (ESG) factors in project financing has garnered extensive scholarly and professional attention. The conceptual basis of ESG aligns with broader sustainable development theories, emphasizing that economic activity should balance profitability with social welfare and environmental stewardship. Armstrong (2020) underscores that ethical considerations are integral to understanding the role of ESG, asserting that responsible behaviour enhances corporate reputation and long-term financial performance. The evolution of ESG from a risk management perspective to a strategic value driver reflects an increased recognition of its relevance in modern corporate governance.

Camara (2023) explores the systemic interaction between corporate governance and ESG, highlighting how effective governance structures underpin sustainable practices. He points out that transparent decision-making, stakeholder engagement, and accountability are vital for embedding ESG into corporate culture. This aligns with the findings that companies with mature ESG frameworks tend to perform better in terms of stakeholder trust and financial outcomes.

Regulatory drivers play a pivotal role in shaping ESG practices. The European Union's directives, including the Corporate Sustainability Reporting Directive (CSRD) and the EU taxonomy for sustainable activities, aim to unify reporting standards and improve the comparability of ESG data across firms and sectors. The recent Omnibus regulation seeks to simplify compliance, particularly for small and medium-sized enterprises, and to mobilize capital for sustainable investments.

The literature emphasizes that robust regulatory frameworks encourage companies and financial institutions to adopt consistent metrics, fostering transparency and investor confidence. These standards serve as a foundation for integrating ESG into risk assessments and project evaluation processes.

Assessing ESG performance involves qualitative and quantitative methods. Clément et al. (2022) conducted a systematic review of **ESG scores** used in academic literature, noting the diversity of rating agencies and methodologies, which can lead to discrepancies and challenges in comparability. Their analysis advocates for harmonized measurement standards to facilitate reliable assessment and decision-making.

The integration of ESG factors into project development and financing is increasingly recognized as essential for risk mitigation and value creation. Studies suggest that companies with strong ESG profiles are better positioned to attract investment, secure favourable financing conditions, and mitigate environmental and social risks associated with projects.

The recent focus on green bonds and sustainability-linked loans reflects a financial-market evolution toward sustainable investment products. Atlas Metrics (2024) discusses the linkages between the Corporate Sustainability Reporting Directive (CSRD) and the Sustainable Finance Disclosure Regulation (SFDR), emphasizing their role in promoting transparency and responsible investing.

Despite progress, literature acknowledges persistent barriers, including fragmented standards, high implementation costs, and limited internal expertise. Firms, especially smaller ones, face challenges in collecting accurate ESG data and integrating sustainability into strategic processes.

Nevertheless, opportunities abound. Technological tools, such as business intelligence and data analytics, promise improved ESG data availability, and reliability. Furthermore, growing investor demand for responsible investments incentivizes companies and banks to deepen ESG integration.

Within the chemical industry, ESG considerations are particularly critical due to environmental impacts and regulatory scrutiny. Research indicates that chemical companies adopting sustainable practices can gain competitive advantage and improved access to green financing. Similarly, banks actively incorporate ESG assessments to align their lending portfolios with sustainability goals, which enhances their market positioning and risk management strategies.

The financial sector is increasingly reflecting the requirements of ESG principles when providing financial products and services. Banks and insurance companies not only declare their support for green investments, but in some cases, they are committing to moving away from financing activities with high greenhouse gas emissions, such as coal mining and processing.

Banks modified their products based on ESG principles, currently there are available the **green products** like:

- Green, social and sustainable bonds
- Green Credits
- Credits for financing of:
    - Renewable energy sources
    - Support for increasing energy efficiency
    - Green buildings
    - Projects focused on water or waste management and reducing the climate impact in agriculture
    - Social entrepreneurship
    - Obtaining certification of sustainability
    - Sustainable mobility
    - Circular economy
    - Pollution prevention
    - Projects to promote the use of recycled materials and advanced recycling technologies
    - Projects to reduce the risks associated with extreme weather events and protect biodiversity
    - Biotechnical measures to respond to climate change
    - Projects to improve the welfare of farm animals and produce healthier food
    - Sustainability Linked Interest Rate Swap
    - Financial and operational leasing for the acquisition of assets contributing to sustainability
    - Combination of credits with green subsidies
- Support of education
- Consulting.

This shift is part of a broader global trend towards sustainable financing, which aims to support environmentally friendly projects and at the same time contribute to achieving long-term sustainability in the economy. Recent empirical studies (McKinsey & Company, 2023) confirm that ESG integration leads to better risk-adjusted returns for investors and more resilient corporate performance.

The research focuses on assessing the rules, the form of methodologies and the reflection of ESG rules in the approach to project financing in the banking sector of the Czech Republic. It provides an overview of supported activities of individual banks and products to support sustainability. It also provides the opinion of chemical industry companies on how much this change has affected or limited the financing of development projects in their case and to what extent they take the ESG approach into account when approving new investments.

Methodology

This research is based on qualitative analysis through structured interviews with key stakeholders in the banking and chemicals sector in the Czech Republic. Banks with a significant market share and manufacturing companies in the chemical industry, among the most important producers, were selected for the research. The interviews were conducted online in March and April 2025. Respondents were professionals involved in investment project evaluation, ESG management and strategic planning in selected banks (3 respondents) and chemical companies (3 respondents). The aim of the interviews was to gain insights on:

- general approach to ESG
- integration of ESG into strategy and follow-up processes, product definition of banks/chemical companies
- the impact of ESG on financing conditions
- organisational arrangements for integrating ESG principles
- perceived barriers and facilitators to ESG integration
- an estimate of the future evolution of the impact of ESG on financing.

The data collected was analysed to assess the extent to which ESG principles were integrated into strategy and routine processes in both groups, identifying common patterns, differences and emerging trends in ESG-related practices. A limitation of this research is the small number of respondents and further cross-sectional quantitative research would be desirable. However, the structured interview format provides a more detailed insight into the issues, a more detailed view of the attitudes of both banks and chemical industry companies and is a good basis for further detailed research in this area.

Results

Influence of ESG on Banking Sector Practices

Qualitative interviews with banking experts showed that ESG factors have gone from peripheral considerations to becoming core elements of loan and project evaluation. ESG principles are incorporated into banks' strategy documents and subsequently become a standard part of defining both deposit and loan products, but also in setting internal processes within banks and towards the external environment. Banks also include ESG in their overall strategy, and ESG is included in lending policies and the design of new green investment instruments. Bank respondents indicated that ESG criteria are now embedded in their formal funding assessment frameworks, particularly for risk assessment. This is particularly relevant for large infrastructure projects with high environmental impact. In particular, several respondents highlighted the inclusion of ESG ratings from recognised agencies, which serve as complementary tools alongside traditional financial analysis.

Banks also indicated that they are developing internal policies and dedicated teams to standardise ESG assessments. Some banks have established sustainability committees to oversee ESG integration and monitor ongoing compliance. It has also been noted that the introduction of digital tools and data analytics is facilitating more comprehensive, and timely ESG assessments. For example, banks are increasingly requiring clients to submit sustainability reports or disclose ESG information as part of the funding application process, highlighting the importance of transparency. This increases the pressure on credit clients, who are required to take a similar approach and incorporate ESG principles into their policies and procedures. Banks are already playing an important role in promoting sustainability and have set a strong foundation in the ESG area by modifying their strategies and setting up internal methodologies and are ready to continue this approach.

Implementation of ESG by Chemical Companies

Chemical companies, ranging from large multinationals to national manufacturers, have acknowledged that ESG considerations are now key in shaping corporate strategies and operational practices. Most companies have implemented ESG strategies in line with international standards such as the Global Reporting Initiative (GRI) or the European Union taxonomy. Many respondents highlighted ongoing investments in cleaner production technologies, improved waste management and reduction of greenhouse gas emissions. However, the

introduction of ESG principles is reflected in practice by a focus on individual investments, particularly in the environmental field, leading to a reduction in energy intensity, and an increase in the share of renewable sources. Social responsibility initiatives such as community involvement and employee welfare programmes are also coming to the fore. There is an increasing emphasis on good management practices to meet the expectations of stakeholders, business partners and, not least, banks in the case of financing.

Access to project funding often depends on demonstrating concrete ESG results. Several companies reported using external consultants to audit and verify ESG disclosures, recognising that the credibility of reporting affects investor and creditor confidence. They also stated that presenting ESG achievements helps to attract new investment and can lead to better terms when negotiating financing.

However, the data also shows that some firms are dissatisfied with some of the legislative enforcement practices of ESG principles. They are particularly concerned about the administrative complexity, ambiguity in requirements, changes in requirements and the lack of space to put these principles into practice. They also have a negative perception of the minimal consideration of the specifics of individual industries, where companies in the chemical industry face a much greater challenge in decarbonisation, reducing energy intensity and in other procedures changing production processes.

Challenges in ESG Adoption

Both sectors have highlighted barriers to the comprehensive implementation of ESG measures. The lack of universally accepted standards and measurement frameworks was an overriding issue, making comparisons and comparability between companies and sectors difficult. Respondents highlighted that the current changing environment for the implementation of ESG principles is fragmented, making it difficult to develop a long-term strategy in this area and to develop proposals for implementation.

Cost implications were another concern. Implementing advanced environmental management systems, upgrading production facilities and improving reporting infrastructure entails significant costs.

Changing conditions and the need to refresh expertise in ESG principles further slowdown implementation and increase costs. ESG reporting is administratively demanding. Many organisations do not have sufficient internal capacity or knowledge to effectively and comprehensively integrate ESG considerations into all their core activities and decision-making processes. This shortcoming underscores the need for training and for capacity building.

In comparison to chemical companies the banks integrated ESG principles into their strategies systematically based on the recommendation of their mother banks few years ago and currently ESG indicators are key in area of evaluation of investment proposals and in area of new bank products. Chemical companies also recognized the ESG as key indicators, but implementation of such indicators in their strategies is not such advanced and systematic. They implement investment projects focused on environmental improvement, reducing of energy but there is necessary the systematic approach. On the other side in chemical industry is really complicated transition to green production and implementation of ESG principles and the changed condition on European and nation level also complicate the planning and financing of this changes.

Discussion

The results show a clear trend: in the Czech chemical industry and banking sector, ESG integration is now essential for project financing. This shift is in line with the global movement towards sustainable finance and reflects the growing influence of regulatory frameworks and stakeholder expectations.

Banks are gradually integrating ESG considerations into their risk management and credit assessment. This development not only reduces financial risk by taking into account long-term environmental and social factors, but also strengthens their reputation as responsible lenders. The use of ESG ratings and financial products linked to sustainability demonstrates a proactive approach to aligning banking practices with sustainability objectives.

Chemical companies recognise that demonstrating ESG compliance serves several strategic purposes: securing access to favourable financing, enhancing reputation and ensuring long-term business continuity. Incorporating ESG into their strategic planning demonstrates a fundamental transformation from traditional profit-focused models to sustainability-oriented approaches.

Despite positive developments, significant obstacles remain. The absence of standardised ESG metrics complicates efforts to compare and benchmark sustainability performance, leading to potential inconsistencies in assessment and reporting. This fragmentation and the changing regulatory environment impair the ability of financial institutions to reliably incorporate ESG factors into decision-making.

Cost remains a tangible barrier, especially for smaller companies that may lack the financial and human resources needed for complex ESG initiatives. In addition, internal capacity to understand, implement and report on ESG remains uneven, underscoring the importance of capacity building programmes.
Given these challenges, industry stakeholders and regulators should work to harmonise standards and available tools for ESG measurement Greater awareness and education on ESG benefits and implementation strategies could accelerate adoption, leading to more sustainable investment flows and innovation in green technologies.
The evolving regulatory environment, including directives such as the CSRD, is putting pressure on companies to improve transparency and accountability for ESG practices. Such regulations promote comparability and credibility, thereby enhancing investor confidence. They also incentivise companies to implement comprehensive ESG management systems, potentially reducing the perceived risks associated with sustainable projects.
Going forward, the integration of ESG principles into project finance in the Czech chemical industry is likely to deepen, although the uptake will probably be slower than originally anticipated due to the Omnibus. Technological advances in data collection and analysis will facilitate more accurate ESG assessments. Moreover, as international investors increasingly demand ESG-compliant investments, local companies will need to adapt their practices to remain competitive.
In addition, the rise of innovative financial products such as climate bonds and sustainability-linked loans presents an opportunity for both sectors to access new sources of capital that are aligned with the sustainability goals. Policy makers and industry associations can support this transition by setting clear guidelines, promoting transparency and offering technical assistance.

Conclusion

With the gradual introduction of ESG principles into banks' strategies and subsequently into the new financing rules, both on the resource side (green bonds, sustainable deposit products) and on the lending side, which take into account not only economic returns but also the focus of investment projects and their non-financial evaluation according to ESG scores, there is a significant shift in the external financing options for companies. This change also affects the decision-making on sources of financing in chemical companies. As production in chemical industry enterprises is often energy intensive and material inputs are very often fossil-based, the chemical industry is considered to have problems meeting the new requirements based on the non-financial criteria. It is a major challenge for companies and banks to find a compromise, as the outputs of the chemical industry are crucial to the economy not only in their own right, but also as inputs to the automotive industry and other manufacturing sectors. It is desirable to focus and strengthen technological development towards sustainable technologies applicable specifically to the chemical industry.
Integrating ESG factors into project finance processes is changing the chemical industry and the banking sector in the Czech Republic. Both stakeholders recognise the importance of sustainability for long-term competitiveness and risk mitigation. While progress has been made, significant challenges remain in the areas of standardisation, measurement and organisational alignment.
Promoting common ESG standards, raising awareness and developing robust reporting mechanisms to enable deeper integration of ESG into project evaluation and financing, and a clearer view of the long-term progress of putting ESG principles into practice are essential for further development. Such developments will not only benefit environmental and social objectives, but also strengthen financial stability and investor confidence.

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MANAGEMENT OF SELECTED SOCIAL ASPECTS IN A CHEMICAL COMPANY THROUGH COOPERATION WITH A HEALTHCARE FACILITY

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Abstract

Social factors include the relationships between a company and its employees, customers, communities and society and ensure ethical behaviour in areas such as human rights, working conditions, community impact and partnerships. In this context, workforce regeneration, particularly through collaboration with health care facilities, represents an important social aspect, although it remains under-researched in the literature. This paper addresses this gap by outlining the steps to establish a health facility that collaborates with a chemical company to manage workforce regeneration of workers, particularly in production processes. The article is based on a literature review and primary qualitative research, including a study in a physiotherapy facility. The research provides a proposed framework for the establishment of a healthcare facility that respects the social responsibility of both partners, including strategic marketing analysis, legislative requirements and business planning. The implementation of these steps can improve the management of social aspects, which will benefit both chemical companies and healthcare facilities. The proposed guidelines are transferable across industries.

Introduction

In recent decades, there has been an increasing focus on sustainable development in all aspects of human life, the very concept being characterized as progress that can improve the quality of life, enabling people to live in a safe and healthy environment while enhancing the social, economic and environmental aspects of present and future generations.[1]Within the framework of sustainable development, social aspects are also very often analyzed in companies with industrial processes, where most studies focus on measuring social areas such as employment, health and safety, which includes areas such as education or regeneration that directly affect the working conditions and quality of life of employees.[2,3,4]Therefore, social aspects are linked to different stakeholders, including workers, companies, customers and local communities.[3,4] Causal relationship diagrams between social factors show that worker health and safety are closely linked to overall business performance and should therefore be systematically integrated into sustainability strategies.[3]

This area is often addressed and attempted to be codified, but despite efforts to integrate social considerations into the sustainability framework, many key elements are overlooked.[2,5]As the current literature shows, workforce regeneration is often overlooked,[6,7]even though it plays an important role in the long-term sustainability of the enterprise.[4,8]

Studies show that human resource management is closely related to the management of social aspects, and both together can affect the long-term sustainability of the enterprise.[2]

The importance of social aspects is often overlooked in the context of quality management, which primarily focuses on optimising processes, minimising errors and ensuring high standards of products and services.[9]Although this approach is necessary to maintain competitiveness, it does not always adequately reflect wider social factors such as working conditions, work-life balance or the promotion of workforce regeneration.[4,9]In contrast to quality management, social management brings a more specific perspective that encompasses the mental well-being of employees, improving working conditions and reducing the negative impacts of the work process on their health and productivity.[1,4]While quality management is primarily concerned with outputs and efficiency, social management emphasises employees, thereby contributing to greater satisfaction, stability and resilience of the enterprise.[4,9]

This article deals with social aspects in the dimension of employees, specifically the aspect of workforce regeneration, which is also related to the quality of life and health of employees. Workforce regeneration is a key aspect of the sustainability of industrial enterprises that needs to be further investigated.[6,7]Since the literature has not yet addressed how to effectively link enterprises with external health facilities to manage workforce regeneration, the aim of this article was to propose a methodological procedure that summarizes the different actions that need to be taken in establishing and setting up the processes of a health facility in the field

of physiotherapy that is being established to help manage social aspects in a chemical enterprise. Primary qualitative research through a case study methodology was conducted to accomplish the objective.

Research Methodology

The objective of the primary research was to present a complete description of the process of setting up a health care facility, business planning, meeting and complying with legislative regulations and requirements in health care and business, and setting quality and risk management policies in a specific physiotherapy facility.
The selected non-state private outpatient rehabilitation facility that was the object of investigation in the case study is now in its third year of business and currently has a total of 5 physiotherapists working in the facility. The facility currently has 234 linked birth numbers for which it reports the care provided to the insurance company. Although the outpatient facility is not accredited, its operator has made the adjustment for quality and safety of care just through accreditation standards according to to the Joint Accreditation Commission, o.p.s. The legal form of the health facility is a limited liability company.
The research activity was conducted by studying literature, books and scientific articles, observation, analysis of internal documents of the facility, study of legislation and interviews at a specific non-state private outpatient physiotherapy facility. The research part of the case study was described anonymously with the consent of the managing directors of this facility.
The research investigation took place from December 2023 to March 2024, during which a total of 8 sessions were conducted with the facility operator to gather relevant information through guided interviews, observation and analysis of specific internal documents of the facility.

Analysis of Results

As a result of the analysis of the primary research results and their comparison with the literature, a methodological approach for business planning, establishment and start-up of a physiotherapy clinic to help manage the social aspects in the chemical company was developed.

A methodological procedure for setting up and running a physiotherapy clinic
The methodological procedure includes the following steps to be taken before the actual start-up of the business, i.e. planning the business, setting up the company and then standardising the procedures and processes of the facility, including their implementation.
The individual steps are divided into three logical units according to the logical sequence of individual activities and their grouping. The first phase is the **prephase of creating the organisation - planning the business** (marked with the letter **A**), the second phase is already the **phase of creating the organisation - setting up the facility** (marked with the letter **B**) and the last phase is **creating the internal organisation - the system of operation** (marked with the letter **C**).

A) PRE-PHASE OF ORGANISATION FORMATION - BUSINESS PLANNING
The essentials that a prospective entrepreneur should clarify or analyse before starting a health care business are listed below.
This part of the whole process of setting up a health organization to collaborate in managing the social aspects in a chemical enterprise involves initial thought preparation and management planning. It is necessary to clarify what all needs to be arranged before the actual establishment of the facility and what will be required during the implementation of the actual plan.

Here are the steps that need to be defined at the very beginning of the establishment of the facility, i.e. during the business planning:

- Defining the vision, mission, strategic objective and sub-objectives to achieve it
- Choosing a business plan, creating a SWOT analysis
- Creation of a business plan, including budgeting, calculations and determination of return on investment
- Setting marketing strategy
- Choosing the status of a legal or natural entity according to the business plan

The general steps described above must be carried out before the actual establishment of the organisation, however, if the healthcare organisation intends to primarily or largely focus its activities on cooperation with a chemical company, it is necessary to modify these steps according to this intention.

The first step is to **define the vision, mission, strategic objective and sub-objectives** to achieve it. Above all, for the vision, it is essential for a functioning collaboration that the visions of both the enterprise and the medical device are aligned, especially that the vision of the medical device matches the vision of the enterprise. It is necessary to declare that this is first and foremost a primary collaboration between the health facility and the chemical company.
The second step in the start-up process is the **creation of a business plan**, which includes the facts regarding the establishment, the strategy of the business, the goals and the means to achieve them. The business plan description includes, for example, a description of the organizational chart, the location and size of the business, and the range of services the facility will provide. It is essential here to identify the hole in the market that is not filled by physiotherapy services.
The next step is to **create a business plan, determine the necessary budgets, calculate costings and determine the return on investment**. Here it is advisable to outsource and use the services of economic experts, which can avoid the risk of losing the whole project.
Setting up a marketing strategy is specific here, since in cooperation with the company the facility will preferably have patients who work in the company and the company doctor will refer these patients to this medical facility on the basis of an agreement.
The choice of a legal entity or corporate status is a more advantageous option here, as if the owner of the health care institution dies, the institution does not cease to exist and is taken over by a new owner, so helping to manage the social aspects in the company would still be possible.

B) THE ORGANISATION FORMATION PHASE – SETTING UP THE ESTABLISHMENT
If the entrepreneur decides to run the business and represent their company as a legal entity in the future, the following few steps need to be taken for its successful establishment. This part is already of an administrative nature and includes administrative and executive activities related to the actual establishment and building of the facility.

Here are the steps involved in the administrative and executive part of creating an organisation, i.e. creating a business:

- ❖ Establishment of a legal entity
- ❖ Filing an application and registering the health facility with the regional authority
- ❖ Registration of the health facility
- ❖ Arranging compulsory insurance for the health facility
- ❖ Selection of premises for the future HH
- ❖ Finding future collaborators of the ZZ

The first step in setting up a facility is to establish a legal entity.
This process consists of several sub-steps, which include the following sequence of activities:

- Establishment of a memorandum of association (2 or more persons in the establishment), in the case of one person, a deed of incorporation
- Registration with the bank
- Registration with the Trade Licensing Office, obtaining a legal entity ID number
- Registration in the Commercial Register
- Registration with the tax office
- Registration with the Czech Social Security Administration
- Registration with the health insurance office[10,11,12]

The next step in the process of establishing a health care facility is to **submit an application for a licence to provide health care services and the process of registering the health care facility with the relevant regional authority**.
The application step is very specific and is characterized by the following activities:

- Submission of a form to the regional authority, Department of Health, entitled Application for Authorisation to Provide Health Services.
- Payment of the administrative fee of CZK 1,000

The following documents must be attached to the application:

- Information on the appointment of **a professional representative**, approved **technical, material and personnel equipment of** the facility, confirmation **of the integrity and professional training of** all staff, **approval of the premises**, valid **operating rules of** the facility, etc.

- Proof of the professional, specialised and medical competence of the applicant's physiotherapist or the professional representative of the PH
- Authorisation of the physiotherapist or professional representative to work without professional supervision and evidence of at least 1 year of experience in the field[11,12]

Next comes the **registration of the ZZ with the regional authority, Department of Health**, which consists of three successive parts.

- **The first phase** is the inspection of the physical, technical and personnel equipment of the facility, and the type and scope of health care provided.
- **The second stage** consists of the submission of the consent and the receipt for payment of the administrative fee, the certificate of medical fitness of the applicant or the professional representative, the submission of the lease or sublease agreement or the extract from the land register.[11,12]
- **The third stage** is securing **contractual relations with insurance companies** (in the case of provision of care through public health insurance) through an application and tender procedure under the Reimbursement Decree. Alternatively, setting the prices of the services provided for self-payers.[13]

Before the actual start of the physiotherapy business, it is also necessary for the provider to arrange compulsory **insurance** for the NHS, according to Act No. 372/2011 Coll., on Health Services, which constitutes the next step in the process of establishing the facility.[14,15]

Regarding **the choice of premises for the operation of the health facility**, in relation to the cooperation between the health facility and the company, it would be appropriate if the facility were located within or near the premises of the company and the chemical company rented to the health facility, at a favourable price, the premises owned by the company.

The selection of associates can be handled through outsourcing, whereby the owner of the facility must then decide how many associates will be needed at the facility to ensure that the facility is able to provide care preferably to the facility's associates, but also to the public.

Once all the legislative and administrative requirements have been met and the business has been authorised to operate in the healthcare sector, specifically here in the field of physiotherapy, the next step is to set up processes in terms of the quality and safety of the care provided and to fulfil the purpose for which the healthcare institution is established, namely to help manage the regeneration of the workforce.

C) THE PHASE OF SETTING UP THE INTERNAL ORGANISATION – THE SYSTEM OF FUNCTIONING

In this phase, it is already about setting up the functioning system of the facility, i.e. setting up the process system of the facility. Here, processes are set up starting with ordering patients, selecting appropriate types of therapies, how to inform and educate patients and last but not least setting up quality and risk management.

A possible process of **setting quality** in a health care facility is setting according to the **Accreditation Standards for Outpatient Health Care Facilities according to the Joint Accreditation Commission, o.p.s.**, which includes all legislative requirements for setting minimum quality and safety of services in health care facilities and prevention of risks associated with health care, including the National Safety Goals developed by the Ministry of Health.

The path to setting up the operation of safe processes related to care, through which the health care institution will help to manage the regeneration of the workforce, is possible through the health care facility's application and compliance with the quality and safety management standards (**Accreditation Standards for Outpatient Health Care Facilities according to the Joint Accreditation Commission, o.p.s**.) and **the National Safety Goals by the Ministry of Health of the Czech Republic**, which include the five most important areas in terms of the issues of adverse events and risks that must be taken into account when providing health care services. The sectoral safety objectives also include all the legislative requirements for setting the minimum quality and safety of services in health care facilities and preventing risks associated with health care.

The following table (Table I) describes which National Safety Goals and Accreditation Standards apply to the operation of an outpatient healthcare facility, with each group of standards mentioned below divided into further sub-standards that have conditions of achievement expressed according to indicators.

For outpatient facilities, a total of 56 standards divided into 9 groups are set. The accreditation standards are only a way to set up a quality and safe ambulatory facility, but it is not necessary to participate in the

accreditation process, on the other hand, the National Safety Goals are mandatory to meet and four are given for ambulatory facilities.

Table I: Establishing Quality and Risk Policies in an Outpatient Facility

Quality and Risk Policy in a Healthcare Facility	
National Safety Goals	**Quality and Safety Management Standards**
NSG 1: Safe Patient Identification	Quality and Safety Management Standards
NSG 3: Implementing Optimal Hand Hygiene in Healthcare Providing	Diagnostic Care Standards Healthcare Continuity Standards
NSG 4: Safe Communication	Standards for Respecting Patients' Rights Standards of Management Human Resource Management Standards Standards for Information Collection and Processing Standards of Anti-Epidemic Measures

Source: Joint Accreditation Commission, 2019; Ministry of Health of the Czech Republic, 2015.

In addition to the above-mentioned requirements that must be met, it is necessary to set up processes based on this legislation, which each facility already creates itself.

In the case of cooperation between a healthcare facility and a chemical company, it is necessary to set the way in which the healthcare provided to patients will be reimbursed.
In view of the cooperation with the chemical company and the help with managing the regeneration of the workforce, it is most advantageous for the company and the healthcare institution to provide the following types of care on a reimbursement basis:[14]

- The company doctor, after examination, sends the worker to the medical institution for rehabilitation, and then the performed procedures are reimbursed by the public health insurance, based on the claim form prescribed by the doctor.
- If the worker wants extra services, such as physical therapy, for example, ultrasound therapy, and the doctor does not provide a claim form for this care, the worker pays for the care himself or herself, and is therefore a self-payer or participates only partially in the payment of the care, as the health insurance company pays part of the reimbursement.

In the case of cooperation with a chemical company, it is necessary to identify areas for rehabilitation according to the company's employees' problems and their state of health and the impact of the work environment on their physical difficulties or even occupational diseases. It is necessary to determine which regeneration techniques or physical rehabilitation will be necessary according to the survey of the regeneration needs of the employees.

After setting up all the processes that will take place in the facility, it is also necessary to **set up the control of their progress**. Each health facility is obliged to report once a year on its functioning and provision of care directly to the Ministry of Health of the Czech Republic. The facility can set the metrics for its processes itself, but the easier way is through the application, implementation and subsequent reporting of the fulfilment of accreditation standards according to the Joint Accreditation Commission, o.p.s.

For a more in-depth introduction to the issue, here are four standards with established indicators to meet.
Standard 21: Access to care is organized in the facility to meet the needs of patients.
Standard indicators:
The facility regularly evaluates the functionality and effectiveness of the care delivery system and adjusts the system as appropriate. The facility has a telephone or e-mail appointment system in place.
Waiting times for patients are acceptable, monitored, and minimized because patients are always scheduled for an agreed upon time.
In this case, the facility's collaboration with the business allows the facility to set operating hours for two shifts, with 2-3 physiotherapists providing care in each shift. The chemical company's staff will therefore be able to come in after their working hours or on their days off.[16]

Standard 30: The facility has an effective patient education system in place.
Standard Indicators:
The patient's need for education, ability to receive education, and willingness to receive education are assessed and documented.
Patient education is documented and patients are informed of their health status and confirmed diagnoses
Patients are informed about rehabilitation procedures and how they can regain, maintain or improve their functional abilities.
The treatment and patient education provided should have an impact on the chemical company, such as reassigning the worker to another job where he or she would exert less effort and not exacerbate his or her physical decompensation.[16]
The management of the chemical company must ensure that the medical facility is functional and helps in managing the social aspects, especially for the aspect of workforce recovery, the following two standards cover this issue.
Standard 2: The facility has an internal audit of the quality and safety of services provided, this activity is planned and carried out by designated persons.
Standard Indicators:
The facility has a process for auditing activities, these are conducted by designated persons, and the findings of the audits are used to improve quality and safety in the facility.
Audit findings are communicated to chemical plant management.
Standard 42: The management of the ZZ is actively involved in the management of the quality and safety of the services provided.
Standard Indicators:
Facility management is actively involved in the planning of the quality and safety management program, particularly in prioritizing such a program and allocating resources for its implementation.
Facility management actively oversees the implementation of the quality and safety management programme.
The management of the establishment shall regularly review the outputs and results of the quality and safety management programme.
Facility management shall use the outputs and results of the quality management programme for decision-making. [16]

Discussion

This research demonstrates that establishing and operating a physical therapy facility in the context of working with a chemical company presents several key considerations.
One of the most important factors influencing the establishment of a health care facility is the legislative requirements. Strict regulations ensure high quality care and patient safety, which is an undeniable advantage. On the other hand, the process of registering and approving a healthcare facility proves to be administratively demanding, time-consuming, and, moreover, with an uncertain outcome as to whether the whole process will be successful. It therefore poses a significant risk to the entire fulfilment of the vision of helping to manage the social aspect of workforce regeneration in a chemical company.
The cooperation between a health facility and a chemical company is very specific and it is necessary for both parties to adapt to the other, otherwise effective cooperation is not feasible. This is primarily a problem of contractual relations with insurance companies, since, due to the failure to conclude contracts with all the contracting insurance companies, the facility will not be able to treat the patients of all the insurance companies. The company must also respect that the healthcare facility is governed by standards and mandatory legislation, so there must always be an agreement and understanding of the needs and limitations of both parties, whatever the cooperation.
From a business perspective, healthcare is a very specific sector. While the general rules for doing business are well described and there are many sources of information, the specific business of healthcare requires specific knowledge and understanding of the regulations. However, in the case of setting up a healthcare facility to collaborate in managing the social aspects of a chemical business, there is no methodological guidance. The publication is therefore useful in this regard.
Another aspect may be the establishment of cooperation with the health insurance company, which is essential for the financial sustainability of the health facility. However, insurance companies do not currently enter into new contracts with providers, which means that the only option is to buy out the contractual relationship from an existing facility. This limits the access of new entrants to the market and creates a situation where the availability of healthcare can become dependent on existing capacity. The option, however, is for the chemical

company to be the payer for healthcare in a rehabilitation facility that will partner with the company. However, such an option would be financially draining for the company.
Another interesting aspect is the absence of external audits in smaller facilities. Operators often set their own internal processes, which, while allowing flexibility, increases the risk that some aspects of quality and safety are not sufficiently controlled. In this case of cooperation between the company and the health facility, it would be advisable to introduce audits carried out by the company itself in addition to internal audits, so that there is ongoing evidence of the fulfilment of the health institution's vision and the effectiveness and functionality of the cooperation in managing the social aspects of the company.

Conclusion

The results of the primary research show that the current system of providing physiotherapy services is complex and regulated, which ensures a high level of quality, but at the same time poses significant barriers for new health care providers. For a new health facility being established for collaborative management of social aspects in a chemical company, the establishment process is complex, lengthy and with uncertain outcomes, and there is no methodological guidance available for collaborative establishment. However, it also emerged, specifically from the case of the physiotherapy clinic under study, that even if it is a smaller type of facility, it is possible to set up a process to operate efficiently and sustainably.
The article provides a practical guide that includes all the requirements, legislative regulations or other recommendations to establish and set up a quality and safe physiotherapy clinic that will cooperate in managing the social aspects in a chemical company.
If all legislative issues are met by the medical facility and the collaboration is designed with maximum consideration for the needs of the chemical enterprise, this collaboration can contribute significantly to the management of social aspects in the enterprise.

Limits

The limitation of this paper is that the proposal is theoretical and the methodology is not implemented. After implementation in practice, i.e. real cooperation between a health care facility and a chemical enterprise, the methodology could be modified, extended and supplemented.

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MARKET ANALYSIS METHODOLOGY FOR ASSESSING THE MARKET POTENTIAL OF INNOVATIONS IN THE CHEMICAL INDUSTRY

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Abstract

This article presents a comprehensive and empirically validated methodology for the strategic market analysis required to assess the commercial potential of innovations, with a specific application to the chemical industry. A structured analytical framework is proposed, built upon an extensive literature review and a series of in-depth expert interviews. The framework enables early-stage research and development (R&D) projects to better align with market expectations by systematically evaluating external environments, customer segments, and competitive dynamics. The methodology was validated using a case study focused on the innovation of ACF series indoor air filters. This case study confirmed the approach's effectiveness in guiding strategic innovation decisions, enabling a clear path from research concept to market evaluation and strategic recommendation.

Introduction

Innovation management increasingly necessitates a close alignment between research and development (R&D) investments and validated market needs. Nevertheless, many firms encounter challenges in implementing structured methodologies to assess the innovation potential during the early stages of technological development. This issue is particularly critical in the chemical sector, where prolonged development cycles and significant compliance costs amplify the risk of market misalignment[1]. Recent literature emphasizes that market-driven approaches, alongside strategic foresight mechanisms, are essential to mitigate the risks of innovation failure[2].

Modern global markets are characterized by volatility, rapidly evolving technologies, shifting regulatory landscapes, and complex customer expectations. Addressing these dynamics requires robust predictive tools that integrate macroeconomic trends, competitive pressures, and customer behavior[3]. For instance, studies in biotechnology and green chemistry underscore the importance of the early integration of market signals to enhance innovation adoption rates[4,5]. This article is based on a master thesis defended at the University of Pardubice, which analysed the market application of an intended innovative indoor air filtration technology using ACF-based filters using a structured analytical framework. The aim of this paper is to present a practical tool for researchers and innovation managers to systematically evaluate market conditions prior to full commercialization.

Preparation of the proposed methodology

The market analysis methodology presented here was designed through a three-step process that included both theoretical insights and empirical validation. The primary objective was to enable researchers to assess the market potential of emerging technologies, particularly in the context of the chemical industry.

The process of developing the proposed methodological framework can be summarised in the following steps:

1. **Formulation of the problem to be solved and information requirements –** The need to identify the market situation was formulated to assess the market potential of the intended innovation of ACF series air filters.
2. **Conducting a literature search** – First, a literature search was conducted to identify existing theoretical approaches to market analysis to determine the market potential of various innovations[6,7]. The methodological basis of our proposal is based on the principles of strategic marketing analysis[8], augmented by recent contributions focusing on the commercialization of innovations[9,10]. The literature search allowed for a strengthened selection of analytical dimensions. For example, Sarigiannidis et al.[11] highlight the importance of structured segmentation and foresight in market diagnostics, and Teirlinck and Poelmans[7] document the success of open innovation strategies based on early market assessment.
3. **Consultation of the process and content of the partial analyses with experts –** In order to anchor the methodology in practice, several interviews were conducted with experts in applied – research and experts

from companies engaged in commercial market analyses (e.g. UNICO). Based on the feedback, the analytical framework was refined into a multi-level structure (see Figure 1).

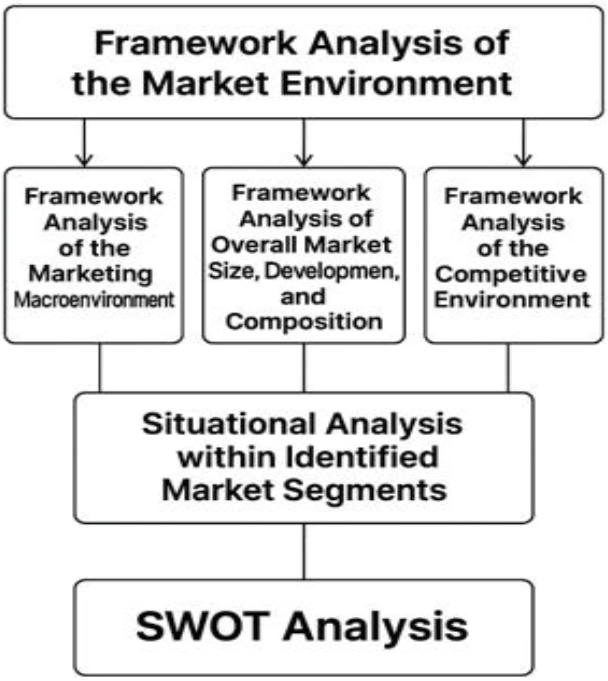

Figure 1. Diagram of a market analysis to assess innovation potential

Based on the experience gained from the practical application of this methodology in assessing the market potential of the intended innovation of the ACF series of indoor air filters, the content of the analyses of the proposed framework was specified and discussed. The results are summarised in the following chapter.

The final concept and discussion of the results

In the practical application and refinement of the basic concept of the proposed analysis, the funnel principle, i.e. proceeding from more general to progressively narrower and more specific information, has proved useful.

In line with our proposed approach (see Figure 1), we recommend first conducting a **Framework Analysis of the market environment**, which is elaborated in detail within the framework of the Framework Analyses of (1)the marketing macro-environment, (2)the overall size, development and sweetening of the market, and (3)the competitive environment.

In the practical application of these analyses, it has proved necessary to first clarify precisely the expected technological application of the intended innovation and the appropriate geographic area. Furthermore, it has proven to be:

1. ***In the framework analysis of the marketing macro-environment***

- Understand the current scientific and technological environment and to identify trends (e.g. the use of smart technologies, the emergence of hybrid (combinable) filters, etc.).
- Evaluate the legal (regulatory) environment and expected future changes (e.g. EPA Indoor airPLUS certification in the USA; LEED (Leadership in Energy and Environmental Design), etc.).
- Assess the socio-cultural environment (e.g., level of awareness in the area, desire for a healthy lifestyle, desire for a sustainable lifestyle, level of association of 'breathing clean air contributes to overall health', etc.).
- Identify related demographic trends (e.g. increase or decrease in the proportion of people with health problems, etc.)

- Map the ecological and natural environment (e.g. possible impact of natural disasters, impact of depletion of non-renewable resources, etc.).

2. ***In the framework analysis of the overall size, development and composition of the market***

- Determine the current (past market size in terms of sales) overall and in different geographic areas
- Find the expected market size in future years overall and by different geographic areas and assess the expected development – determine the rate of market growth or decline
- Identify the key drivers of market growth (decline)
- Identify the key end-users of the intended technological innovation

3. ***In the framework analysis of the competitive environment***

- Identify competing technologies and their share of the total market
- Identify key competitors and their market share

The next step should be a **Situation Analysis within the identified market segments.** For each of the sub-segments identified above, the key users of the intended innovation should be identified:

- Key factors of the marketing macro environment for the segment
- The size, development and specific market characteristics (needs) of the segment
- The competitive environment within the segment

The results of the analyses are reflected in the resulting **SWOT analysis**, which is recommended to be compiled both for the whole analysed market and for each identified market segment.

Although the current literature recognises the growing importance of alternative strategic analysis frameworks such as SOAR (Strengths, Opportunities, Aspirations, Results) and NOISE (Needs, Opportunities, Improvements, Strengths, Exceptions), this research has deliberately retained the **SWOT** framework as a key tool for synthesising the results of market analysis. In the specific context of assessing the market viability of **ACF-based air filtration innovations** - targeting distinct sectors such as industrial manufacturing, public transport and commercial buildings - SWOT has proven to be more effective in explicitly identifying potential risks to adoption, barriers to market entry and competitive threats that are key to the early stages of innovation decision-making[12,13].

In contrast, the **SOAR** framework, although increasingly used in organizational development and appreciative inquiry, tends to emphasize vision and aspiration over risk diagnosis. Studies such as Stavros and Cole[14] and Stavros and Sutherland[15] note that SOAR excels at linking internal capabilities to future goals but lacks the structural robustness to deal with external constraints or competitive benchmarking-both of which are necessary for strategic market planning to commercialize innovation.

Similarly, the **NOISE** framework, while useful in dialogues involving stakeholders, does not offer the same level of operational granularity for multi-segment comparative diagnostics. Its strength lies in innovative workshops and qualitative exploration of needs, not analytically driven segmentation strategies[16].

In this study, SWOT was particularly advantageous due to its ability to integrate data from the **PESTEL and Five Forces** analyses and offer a structured synthesis that matched well with expert expectations and strategic assessment needs (Antonini et al., 2025). The method's widespread popularity, ease of adaptation, and proven applicability in industrial innovation further solidified its selection[13,17].

Although the SOAR and NOISE frameworks were briefly piloted and checked for comparative purposes, SWOT analysis was retained in this research as the superior strategic synthesis tool due to its analytical neutrality, comparability across segments, and resonance with evaluation standards in commercial innovation assessment.

Conclusions

This study presents a validated and practically applicable framework for early strategic market analysis that is targeted to the chemical industry conditions and specifically focused on the evaluation of innovations in the field of activated carbon-based indoor air filtration (ACF). The proposed methodology combines macro-environmental assessment, situational analysis of identified market segments, and synthesis through SWOT analysis. By

combining the principles of strategic marketing with empirical findings from expert interviews and case studies, the framework enables more informed decision making in the early stages of the innovation cycle. The case application has shown that the structured use of this methodology promotes a better alignment of technological development with current market conditions, thereby increasing the chances of successful commercialisation. The benefits of the conducted= study can be summarised in the following points:

- It will allow targeting technological innovation efforts to the most promising market segments.
- Avoid segments with minimal chance of success and therefore allocate resources appropriately.
- Adapt the implementation of technological innovation directly to the situation and requirements of a given prospective market.
- Focus further research in the right direction.
- Create the basis for further detailed analyses that can lead to market evaluation of the innovation.
- It is the basis for assessing the commercial application of the innovation and can therefore be the basis for grant funding. projects or collaborative projects between researchers.

Despite the positive results, several limitations of this study should be mentioned:

- **Sector specificity -** The framework has been developed and validated in the context of one industry sector (chemistry and air filtration), which may limit its transferability to sectors with different dynamics, e.g. biotechnology or healthcare.

- **Data sources -** Some of the underlying data in the case study was based on secondary data and expert estimates, which may reduce the accuracy of the predictions in a rapidly changing market environment.

- **SWOT as the only synthesis framework** - Although SWOT provides strategic clarity, it may lack the ability to capture more subtle market signals or non-linear trends if not complemented by dynamic analytical tools.

To expand the application potential of the methodology and overcome the above limitations, we recommend the following research directions:

- **Cross-disciplinary validation** - Validation of the framework in other areas such as green chemistry, medical technology or environmental engineering where innovation cycles and regulatory requirements are different.

- **Integration of quantitative predictive methods** - Incorporating techniques such as Monte Carlo simulations, real options analysis or market scenarios to enhance the predictive accuracy of analyses.

- **Combining SWOT with other frameworks (SOAR, NOISE)** - Hybrid models can provide a more balanced view combining risk diagnostics (SWOT) with a focus on vision and stakeholder engagement (SOAR/NOISE), especially for innovative projects in the public domain.

- **Longitudinal studies** - Application of the methodology on time series (ex-post) to validate the predictive parts and calibrate the different tools of strategic analysis.

- **Use of Artificial Intelligence** - Incorporation of machine text processing tools (e.g. NLP for trend tracking, sentiment analysis) can increase the efficiency and timeliness of environmental scanning and improve the real-time adaptability of the framework.

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EXPLORING SUSTAINABLE PACKAGING INNOVATIONS: ARE BUSINESSES ADDRESSING ALL KEY ASPECTS?

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Abstract

Businesses are increasingly adopting sustainable packaging innovations to minimize their environmental and societal impact. A key question remains whether businesses consider all key aspects of sustainable packaging. Understanding corporate preferences can highlight underutilized areas of sustainable redesign that require greater support to achieve truly effective packaging solutions. This study explores the adoption of sustainable packaging innovations in the Czech FMCG sector, with a particular focus on the chemical industry (household chemicals and cosmetics). A literature review identified 26 types of packaging innovations, followed by an empirical study involving 253 Czech FMCG manufacturers from the food and chemical industries. The findings reveal that manufacturers primarily concentrate on improving packaging protection, enhancing handling, reducing material usage, and using recyclable materials. Conversely, innovations involving renewable packaging materials and reusable packaging options remain less widespread. A comparison of the chemical and food industries indicates several differences that are discussed.

Introduction

In today's business environment, companies increasingly recognize the importance of adopting sustainable innovation strategies to minimize the negative social and environmental impacts of their operations and, consequently, to enhance overall business performance[1]. Sustainability-oriented strategies are transforming corporate philosophies and business models in ways that enable the achievement of specific social and environmental values alongside economic profit[2]. While such strategies should ideally encompass all business processes, sustainable packaging innovations often represent the first tangible step in demonstrating corporate social responsibility.

Focusing on sustainable packaging redesign appears to be a logical choice for companies operating in the fast-moving consumer goods (FMCG) sector, as consumers are increasingly concerned about the sustainability of current packaging solutions[3]. This strategy can also facilitate market expansion, as sustainable packaging enhances the perceived value of products among socially responsible consumers[4]. Similarly, eco-labels on packaging can serve as effective marketing communication tools to raise consumer awareness of a company's sustainable innovations[5]. Significant incentives for implementing sustainable packaging in consumer goods markets may also originate from other stakeholders within the supply chain. Gustavo et al.[6] emphasize the role of retailers in driving changes in packaging design. Likewise, Zhang et al.[7] identify sustainable packaging design and the use of eco-labels as key criteria in the selection of private-label suppliers by retailers. Finally, companies are increasingly compelled to adapt their activities to comply with tightening legislative requirements[8].

When implementing sustainable packaging, manufacturing firms most frequently focus on reducing packaging material usage, promoting packaging reuse, and enhancing the recyclability of packaging waste[9,10]. However, their preferences are primarily influenced by the economic evaluation of innovations. According to Molina-Besch and Pålsson[11], companies tend to prioritize redesign tools with clearly defined economic benefits (e.g., optimizing the amount of material used or improving packaging fill rates). The potential for cost reduction associated with packaging is often a sufficiently attractive reason for companies to undertake redesign efforts[12]. Moreover, companies are generally more inclined to invest in innovations that have previously yielded high returns[6].

Reducing packaging weight is also a preferred redesign strategy, as noted by Collado-Ruiz and Avendaño[13], since it not only offers environmental benefits but also reduces logistics costs. In contrast, switching to recycled materials (typically more expensive than virgin materials) is often not supported for economic reasons. The fact that the amount of material used affects both environmental impact and company costs leads to a preference for material-saving strategies in sustainable packaging redesign. However, such changes are only pursued if they do not compromise product protection and shelf-life standards[14].

Previous research[15] in Czech chemical industry enterprises revealed that material changes were the most applied redesign tool five years ago. Nevertheless, innovations aimed at reducing the total amount of material used in packaging (such as introducing bulk packaging or altering packaging shapes) were considered the most successful. The primary focus on the economic benefits of packaging redesign likely explains why certain packaging attributes with significant societal impact remain overlooked. According to Molina-Besch and

Pålsson[11], innovations that reduce environmental impacts during the product's consumption phase (such as improved dosing or enhanced communication functions) are particularly underutilized.
Understanding corporate preferences can highlight underutilized areas of sustainable redesign that require greater support to achieve truly effective packaging solutions. Therefore, the aim of this paper is to identify the areas in which sustainable packaging innovations for FMCG products have been implemented in the Czech market over the past five years (2020–2024), and to uncover the specific characteristics of manufacturers in the chemical industry (household chemicals and cosmetics) through a comparison with other key FMCG producers (food and beverages).

Research methodology

To achieve the research objectives, a quantitative study was designed in the form of a questionnaire survey conducted among Czech companies operating in the FMCG markets (producers of food, beverages, household chemicals, and cosmetics). Data collection was based on information available in the public database of Czech business entities (ARES)[16]. The sampling frame included 10,722 companies with the most common forms of business in the Czech Republic (s.r.o., a.s., k.s., v.o.s.) operating in the following sectors: manufacturing of food products (CZ-NACE 10+), manufacturing of beverages (CZ-NACE 11+), and manufacturing of chemicals and chemical products (CZ-NACE 20+). Considering the required sample size (267 companies, based on Cochran's formula[17]) and an expected response rate of 30% (based on prior experience with similar studies), a random sample of 1,000 companies was contacted with a request to participate in the research.
Random selection was ensured by arranging all entities in the sampling frame in a randomized order. Companies were contacted sequentially via telephone or email. Entities that were unsuitable for the research (e.g., not producing FMCG), undergoing liquidation, or lacking contact information in publicly available databases or on company websites were replaced by the next entity in the sequence until the target of 1,000 contacted companies was reached. Contacted companies were asked to designate a suitable respondent based on the information sought, and the selected respondent was then sent a link to an electronic questionnaire. This approach ensured the anonymity of data collection. To improve the response rate, non-respondents were contacted again if they failed to complete the questionnaire within the specified timeframe. Data collection took place between January 20, 2025, and March 21, 2025. A total of 253 fully completed questionnaires were obtained, corresponding to a response rate of 25.3%.
At the beginning of the survey, companies were introduced to 26 types of packaging innovations across six key areas of sustainable packaging redesign. The specification of innovations in each area was based on a literature review and previous research by the authors[18]:

- protecting the product and minimizing its waste (Protect),
- safe and user-friendly product handling (Handle),
- clear and trustworthy communication (Inform),
- reducing the consumption of resources and waste (Reduce),
- reusability of packaging after its primary product has been emptied (Reuse),
- recyclability of packaging waste (Recycle).

A complete list of the examined innovations is provided in Table II in the Results and Discussion chapter. Respondents indicated for each innovation, using a binary scale (0/1), whether they had implemented it in the past five years (2020–2024). They were also given the opportunity to report additional sustainable packaging innovations not listed in the questionnaire. However, only two respondents used this option, and in both cases, the reported innovations could be categorized under one of the 26 predefined items during data preparation.
At the end of the survey, company size was determined according to the EU methodological guidelines[19] through questions regarding the number of employees and annual turnover. Companies also identified their primary business sector, which was categorized for research purposes into two groups: chemical companies (household chemicals and cosmetics) and food companies (food and beverages). Table I presents the structure of the research sample according to the monitored characteristics.

Table I
Research Sample

Size of company	Frequencies in the group (%)		
	Food and Beverages	Household Chemicals and Cosmetics	*Total*
Micro	45	54	*47*
Small	31	32	*31*
Medium-sized	19	14	*18*
Large	5	0	*4*
Total	*86*	*14*	*100*

The data were analyzed using exploratory and inferential statistical methods in IBM SPSS Statistics 24. In the first step, a multiple response analysis was conducted to identify the types of innovations most frequently implemented by companies. In the second step, the analysis focused on identifying the areas of sustainable packaging redesign in which companies had innovated. For this purpose, a new binary variable (0/1) was calculated for each area, taking the value of 1 if the company had implemented at least one innovation in that area. The subsequent analysis of these new variables enabled the identification of the most frequently targeted areas of packaging innovation and allowed for the determination of the average number of areas in which companies implemented innovations. The results of this analysis directly reflect the diversity of approaches among companies toward sustainable packaging redesign and address the main research question of this study: *Are businesses addressing all key aspects of sustainable packaging innovations?* The statistical significance of observed differences between chemical and food companies was tested using the chi-square test (for differences in frequencies) or the ANOVA test (for differences in means).

Results and Discussion

An exploratory data analysis revealed that 215 out of 253 companies (i.e., 85%) participating in the study had implemented at least one sustainable packaging innovation in the past five years. This figure suggests a high level of engagement among companies in sustainable packaging innovations for FMCG products. However, this value is likely to be biased, as the lack of packaging innovation was one of the main reasons for the low response rate. Considering the total number of companies contacted, the actual proportion of companies implementing innovations likely falls somewhere between 22% and 85%.

To identify corporate preferences regarding the types of packaging innovations adopted, only those companies (N = 215) that reported at least one innovation implemented between 2020 and 2024 were analyzed. Table II compares companies from different sectors based on the types of packaging innovations introduced. The observed differences in company frequencies were tested using the chi-square test.

As shown in Table II, the most frequently implemented innovations in both sectors were those aimed at enhancing product protection (against external influences) or extending shelf life. These innovations target the core protective function of packaging, which not only reduces environmental (product waste) and social (product safety) impacts but also significantly contributes to the economic sustainability of the product (e.g., fewer losses due to damaged or re-packaged goods, extended distribution and storage periods)[18]. Conversely, the least frequently adopted innovations involved the use of alternative materials such as biodegradable or compostable packaging. This is attributed to technological barriers[20] and the underdeveloped municipal waste management infrastructure in the Czech Republic, which is not yet adequately equipped to handle such materials[18]. Reusable packaging innovations were also less commonly implemented, particularly in the food and beverages sector.

A distinctive feature of chemical companies is their more frequent implementation of additional innovations in the area of protecting the product and minimizing its waste (e.g., better portioning, ensuring full product usage, packaging sizes that prevent waste), as well as in safe and user-friendly product handling (e.g., child-resistant closures, packaging made from health-safe materials). These innovations are typically more accessible and expected in the household chemicals and cosmetics sector, as they are closely linked to product usability in households (e.g., dosing) and to reducing the risk of accidental ingestion by vulnerable populations[18]. The low adoption rate of health-safe packaging materials in the food and beverage sector is likely due to stricter regulations, which may leave little room for further innovation in this area[21]. Manufacturers of household chemicals and cosmetics also more frequently explore reusable packaging options (e.g., refillable packaging for households) or reformulate products to reduce packaging material requirements (e.g., by lowering water or solvent content, introducing waterless products). These specific innovations also enable significant material and energy savings in logistics by reducing product volume and weight[22].

Table II
Packaging Innovations Implemented in Companies from the Food and Beverages (F&B) and Household Chemicals and Cosmetics (HC&C) Sectors

Area	Type of Innovation	Frequencies of Companies (%)			Chi-square test	
		F&B	HC&C	*Difference*	χ^2	*p*
Protect	Increasing product protection or shelf life	61	60	*-1*	0.00	1.000
	Better dividing product into doses	22	57	*35***	16.78	<0.001
	Ensuring complete product consumption	17	51	*34***	17.59	<0.001
	Packaging size preventing product waste	18	40	*22***	7.33	0.007
Handle	Shape optimization for easy and safe handling	20	34	*14*	2.67	0.102
	Easy and safe closures	27	37	*10*	0.96	0.326
	Child-resistant closures	3	31	*29***	30.89	<0.001
	Packaging from health-safe materials	21	49	*28***	10.78	0.001
Inform	Information on product and packaging handling	15	26	*11*	1.71	0.192
	Information on product/packaging sustainability	18	31	*14*	2.61	0.106
	Packaging from lighter materials	22	23	*1*	0.00	1.000
Reduce	Material savings through structural packaging changes	22	31	*10*	1.07	0.302
	Material savings in packaging through product innovation	2	17	*15***	11.54	0.001
	Increased packaging fill for material savings	12	23	*11*	1.95	0.163
	Shape optimization for better fill of tertiary packaging	17	9	*-8*	0.92	0.337
Reuse	Refillable packaging for households	6	20	*14**	5.67	0.017
	Refillable packaging in stores	8	3	*-5*	0.47	0.495
	Returnable packaging	12	23	*11*	2.26	0.133
Recycle	Packaging from ecologically certified materials	18	31	*14*	2.61	0.106
	Packaging from more easily recyclable materials	22	23	*1*	0.00	1.000
	Other packaging innovations for easier recyclability	24	23	*-1*	0.00	1.000
	Packaging from recycled materials	19	17	*-2*	0.01	0.935
	Reduction of non-renewable materials in packaging	11	17	*7*	0.68	0.410
	Compostable packaging	11	6	*-5*	0.33	0.568
	Biodegradable packaging	5	3	*-2*	0.01	0.911
	Other innovations for easier waste sorting	8	20	*12*	3.68	0.055

Note: ***p<0.001, **p<0.01, *p<0.05

The above findings indicate that in the food and beverages sector, most companies innovate packaging primarily to increase product protection or shelf life (61%), while other types of innovations were reported by fewer than quarter of respondents. In contrast, companies in the household chemicals and cosmetics sector demonstrate a higher degree of creativity across nearly all areas of sustainable packaging redesign. A follow-up analysis of the number of innovation areas targeted by companies revealed that chemical companies more frequently combine innovations from multiple areas. While the average number of innovation areas for food companies was 2.76, it reached 3.83 for chemical companies. This difference is statistically significant at the 0.1% level (F = 19.31; df_1 = 1; df_2 = 213; p < 0.001). Table III summarizes the types of innovation areas targeted by companies in each sector. Differences in company frequencies were again tested using the chi-square test.

Table III shows that the most widely adopted innovations in both sectors are those focused on protecting the product and minimizing its waste (72% in F&B, 97% in HC&C). Conversely, innovations aimed at clear and trustworthy communication (25% in F&B, 43% in HC&C) and reusability of packaging after its primary product has been emptied (20% in F&B, 40% in HC&C) are the least implemented. The adoption rate of these innovations depends on the business sector; in particular, companies in the chemical industry show significantly higher implementation rates in the Protect, Handle, and Reuse categories. However, it cannot be conclusively stated that company preferences differ solely based on industry. Rather, the results suggest that sustainable packaging innovations have received considerably more attention in the chemical industry in recent years.

Table III
Areas of Sustainable Packaging Redesign Implemented in Companies from the Food and Beverages (F&B) and Household Chemicals and Cosmetics (HC&C) Sectors

Area	Frequencies of Companies (%)			Chi-square test	
	F&B	HC&C	*Difference*	χ^2	*p*
Protect	72	97	*25***	8.73	0.003
Handle	48	80	*32***	10.96	0.001
Inform	25	43	*18*	3.80	0.051
Reduce	48	63	*15*	1.93	0.165
Reuse	20	40	*20**	5.49	0.019
Recycle	62	60	*-2*	0.01	0.954

Note: ***p<0.001, **p<0.01, *p<0.05

The findings of this study confirm previous research[6,11,12,13,15], which indicates that companies tend to favor innovations that not only reduce environmental impacts but also yield economic benefits. However, the chemical industry has seen a notable shift in the diversity of implemented innovations over the past five years. For example, compared to a previous study[15], there is now a much stronger emphasis on improving packaging recyclability for household chemicals and cosmetics (60% of companies introduced innovations in this area in the past five years). This is a relatively high proportion, considering that such innovations are typically associated with increased costs[13]. Nevertheless, this result is likely influenced by increasingly stringent packaging legislation[8].

Despite these developments, the current state of sustainable packaging innovation among FMCG manufacturers cannot yet be considered satisfactory. Greater emphasis should be placed in both sectors on innovations that enhance packaging communication regarding sustainable product use. These are low-cost innovations that can significantly improve both the social and environmental sustainability of packaging. Additionally, new approaches to reusable packaging should be explored, as the existing methods have not yet achieved widespread practical application and thus have limited impact on reducing the environmental burden of packaging waste.

Conclusion

The aim of this study was to identify the areas in which sustainable packaging innovations for FMCG products were implemented in the Czech market between 2020 and 2024, with a specific focus on the household chemicals and cosmetics sector. Our findings revealed that the most frequently adopted packaging innovations targeted product protection and waste minimization. In contrast, innovations aimed at improving the communicative function of packaging or introducing reusable packaging systems were significantly less prevalent. Innovations in the areas of protection, handling, and reusability were notably more widespread among chemical industry manufacturers. However, company preferences across sectors did not differ substantially.

This study has several limitations. First, its geographical scope - being limited to Czech companies - may restrict the generalizability of the findings to other regions. Second, although the response rate was relatively high given the nature of the respondents, it still poses a limitation in terms of sample representativeness. Furthermore, the specific characteristics identified in chemical companies may not be solely attributable to the industry type but could also be influenced by other unobserved factors (excluding company size, which was comparable across sectors in this study). For future research, we recommend expanding the geographical scope to include additional regions to enhance the generalizability of the results. It would also be beneficial to incorporate other variables into the analysis that may influence inter-company differences, such as the degree of integration of sustainability principles into corporate strategies or prevailing economic conditions.

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CIRCULAR ECONOMY IN THE CHEMICAL INDUSTRY: OPPORTUNITIES AND SOLUTIONS

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Abstract

The circular economy is becoming a key concept in the transformation of the chemical industry towards a more sustainable and resource-efficient use. This paper focuses on concrete and operational examples of circular solutions implemented in chemical company, bringing both economic and environmental benefits. The potential of closed-loop material flows in chemical operations will be examined in more detail, in particular closed loops of materials, catalysts and solvents. Attention will also be paid to wastewater management possibilities, closed material loops of packaging materials. Specific corporate measures reflecting R-strategies usable in the conditions of chemical production and products will be presented. Regulatory, technology, market and economic challenges that may impact the wider implementation of these approaches will also be discussed.

Introduction

The circular economy (CE) is based on processes in which products at the end of their useful life or during the production and post-production phases of the life cycle are transformed into resources for different or the same purposes and thus re-entered into circulation. At the same time, this reduces the waste that would otherwise be generated from the original products[1]. According to Korhonen et al.[2], CE uses closed material cycles, which link sustainable production and consumption processes while reducing the consumption of primary resources and minimizing waste. Reike et al.[3] add that for the most efficient use of resources and minimization of environmental impacts during the product life cycle, a key stage is the design of products that allow for their reuse, recycling and regeneration. The importance of circular product design was also confirmed by Bakker et al.[4] The economic perspective was described in their work on circular business models by Bocken et al.[5]. Murray et al.[6]promote ecological and social perspectives, where CE must also be seen as a tool for maximizing the functioning of the ecosystem and improving people's living conditions.

For the implementation of a CE, knowledge and life cycle analysis are essential to identify input and output flows and activities that consume resources and raw materials and have different outputs and environmental impacts[7]. The pre-production phase of the life cycle includes the acquisition of raw materials and resources, research, development and design of the product, which affects its future possibilities for reuse, recycling and waste minimization. In the production phase, the main processes are primarily the production of the product itself, or its distribution. In the product use phase, the product is used by the end customer, who must decide how to end its life cycle[8]. Cao and Folan present a simplified division of the product life cycle into phases: BOL (The beginning-of-life phase); MOL (The middle-of-life phase) and EOL (The end-of-life phase), and in Fig. 1 they illustrate these three-product life phases[9]. The diagram shows material and information flows, as well as possible ways of ending the life cycle, which often create material loops, returning material back to the life cycle.

For the successful implementation of CE, every effort should be made to ensure that the product does not end its life cycle by disposal but can be used again in whole or in part in an appropriate manner. Various methods of reuse or recycling, or other forms of so-called R-strategies, are used for this. Potting et al.[10] ranked 9 R-strategies according to priority into 3 categories: smarter use of products and production; extending the life of the product and its parts; and efficient use of materials.

In the first category, the R-strategies are considered priority: *R0 – Refuse* = Make the product redundant by abandoning its original function or by offering the same function with a completely different product. *R1 – Rethink* = Increase the intensity of product use (e.g. through product sharing or multifunctional products). *R2 – Reduce* = Achieve higher efficiency in production or use.

The second category of strategies is based on the options: *R3 – Reuse* = Reuse of products by another user, if the product is still in good condition and able to perform its original function. *R4 – Repair* = Repair and maintenance of damaged products so that they can continue to perform their original function. *R5 – Refurbish* = Renovate an old product so that it can be used again. *R6 – Remanufacture* = Use a part of a no longer functional product and reuse it for a new product that performs the same function as the original. *R7 – Repurpose* = Use a non-functional product or its parts for a function other than its original use.

The third category contains the last two R-strategies: *R8 – Recycle* = Processing materials to obtain a material of the same or lower quality. *R9 – Recover* = Burning materials with energy recovery.
(Potting et al., 2017)

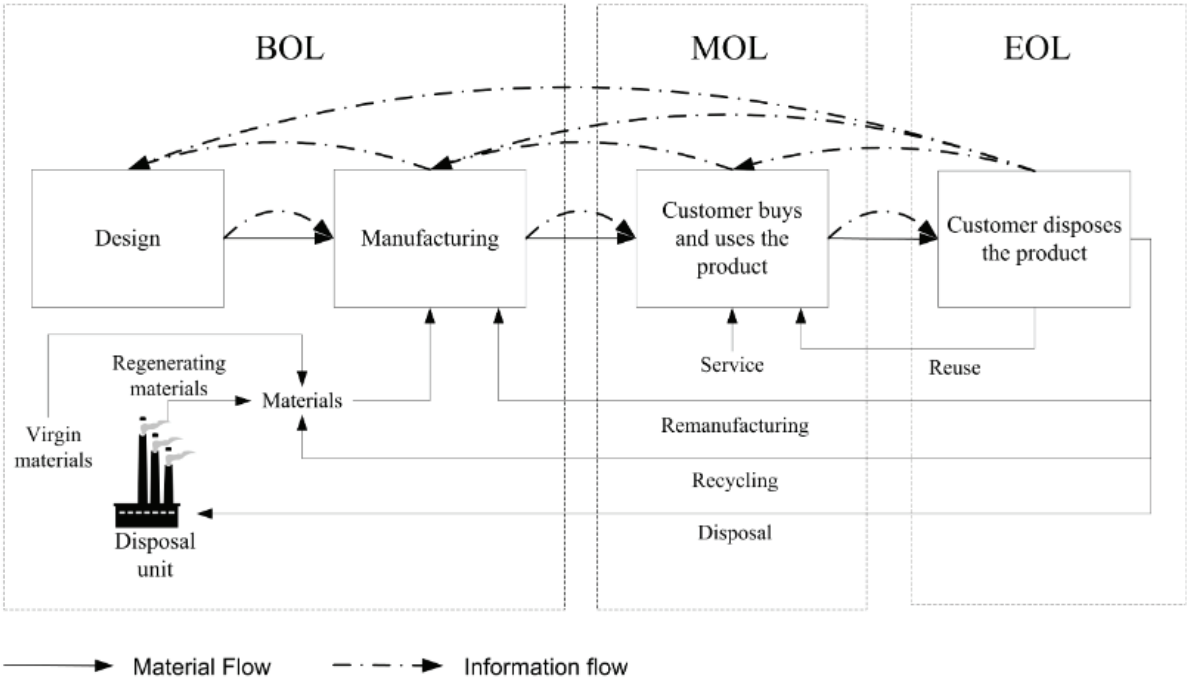

Figure 1. Life cycle phases and closed loops[9]

Ang et al. described material loop models in these categories, where the priority for CE is the use of short loops in the first category of R-strategies. Medium loops for the second category of R-strategies are considered less efficient, and long loops for the Recycle and Recover strategies are considered the approaches with the lowest circularity[11].
R-strategies are a key tool of CE. The greatest emphasis should be placed on preventing waste and optimizing the use of materials already in the design and production phase. Although R-strategies offer many possibilities, their use in practice depends, among other things, on the economic, technological or even legislative conditions of the given company, which limits their different possibilities of practical use in different sectors.

Circular opportunities, solutions and barriers

With the increasing demand (and therefore production) and use of chemicals, the chemical industry has a high impact on the environment, but it does not receive as much attention as it should, both in academic research and in systematic policy initiatives in the field of CE. The chemical industry is characterized by high consumption of chemicals, emissions of varying degrees of toxicity, waste generation and not fully traceable ways of dealing with the end of the life cycle of chemicals. For these reasons, ways are being sought and introduced to implement circular solutions and thereby reduce the problems, but also to reduce dependence on non-renewable resources[12].
In the field of chemicals, Ang et al. identified realized opportunities within the short loop of R-strategies. For the *Refuse* strategy, it is primarily about eliminating the consumption of solvents, catalysts and energy through an alternative synthetic process. They found dozens of examples of the use of new biocatalysts, ionic and metal catalysts, which reduce the volumes of conventional catalysts used so far. They also describe examples of alternative syntheses using nanoparticles. For the *Reduce* strategy, it is possible to achieve a reduction in solvent, catalyst and energy consumption through an alternative synthetic process and to achieve savings by using microwaves in syntheses, photosynthetic catalysis, microreactors, ultrasound radiation and many others.
Within the medium loop, the literature focuses mainly on the *Repair* strategy, specifically for catalyst recovery or regeneration of used solvents using distillation, organic solvent nanofiltration or membrane pervaporation.
Strategies within the long loop are already used in practice and are mainly *Recycle*, consisting in obtaining various forms of waste (e.g. metals, organic solvents) from wastewater, or for the *Recover* strategy, incineration of waste streams and unused substances for the purpose of obtaining energy. (Ang et al., 2021)[11].

Water and wastewater itself play a significant role in chemical production. Water is used in large quantities, both as a raw material, often as a solvent or for separation or cleaning processes and finally as an energy and temperature medium. Large amounts of wastewater can also be used in cooling processes or in steam generation. This circular process can ensure a significant reduction in wastewater production in companies[13, 14].
Wastewater is treated using physical, chemical and biological processes not only to remove organic and inorganic compounds, but also to recover various metals, such as copper, zinc, arsenic, nickel or iron[15].
Packaging and transportation offer greater potential for circular solutions than the product or materials themselves. Reusable returnable transport items (RTIs), complemented by some Industry 4.0 technologies such as tracking chips, represent an effective solution to reduce the environmental burden while maintaining the safety and health of customers[16].
Based on the areas listed above, there are many opportunities for the chemical industry to apply CE principles. Whether it is in the pre-production phase, production or distribution, there are good practice examples that some R-strategies can be practically implemented.
Despite increasing interest in CE strategies, the chemical industry faces numerous obstacles to their practical implementation. Chemical formulations often consist of complex mixtures, which complicates the separation and recovery of individual components. Impurities or trace contaminants may render recovered chemicals unsuitable for reuse, particularly in high-purity applications such as pharmaceuticals or electronics[17,18]. The presence of hazardous substances presents significant challenges. Reprocessing or transporting such materials poses health, safety, and environmental risks[19]. Moreover, stringent regulations such as the EU's REACH legislation strictly govern the handling, reuse, and disposal of hazardous chemicals, often limiting feasible CE pathways[20]. One major legal barrier is the reclassification of recovered chemicals as “waste,” which subjects them to more restrictive regulation than their virgin counterparts[21]. Ambiguity in regulatory language around the status of recycled chemicals further hinders their market reintroduction[22].
Most chemical manufacturing systems are linear and lack the infrastructure to support closed-loop recovery, particularly for solvents, catalysts, and intermediates. Transitioning to such systems is capital-intensive and technologically demanding[23]. Furthermore, recycled feedstocks may vary in composition, affecting product quality and process stability[24]. Circular alternatives often face unfavourable economics. Virgin petrochemical materials remain inexpensive, undermining the competitiveness of recycled inputs[25]. Simultaneously, many advanced recycling technologies (e.g., pyrolysis, chemical depolymerization) remain cost-intensive and have yet to scale industrially[17,18]. There is also a lack of industry-wide standards and certifications for recycled chemicals, leading to uncertainty in quality and performance among industrial customers[26]. This lack of trust hampers demand and adoption of CE-derived inputs.

Research methodology

To confirm the theoretical basis of the possibilities of circular solutions in industrial chemical companies, two complementary forms of research were used. First, examples of good (and bad) practice from chemical companies operating around the world were researched to identify functional R-strategies. Based on the content analysis of websites, social media, annual, press and other published reports and information from companies, functional circular solutions were identified. Attention was paid not only to the essence of the implemented circular solutions, but also to the achieved state of implementation, identified benefits and affiliation to individual R-strategies.
The resulting set of good practice examples was the basis for compiling the questions for the second part of the research in the form of qualitative research with representatives of a large chemical manufacturing company. The intention was to address representatives of a multinational corporation with demonstrable experience with circular activities and the life cycle of products. The pre-selection of the company was also carried out based on the assumption that a large multinational company would have sufficient resources to identify and decide on the adoption of circular measures at the company level.
Based on the theoretical basis, the qualitative research was conducted as a structured individual interview with managers of a chemical company producing basic chemical products (basic chemical products). The respondents were company managers co-responsible for taking relevant measures to reduce material consumption, energy, environmental management and production management. The research was conducted in the period February 2025 - March 2025. The information obtained was processed using content analysis. The first set of questions examined the company's overall approach to implementing circular and related sustainable measures that the company took in connection with ESG and SDG processes. The second set of questions examined the measures taken in connection with the implementation of environmental solutions in comparison with existing examples

of good practice identified in the research part of the research. The third set of questions focused on the opportunities and constraints that affect the possible implementation of CE measures.

Research findings

The first set of questions confirmed that company representatives do not view the implementation of circular solutions solely as environmental initiatives. Compliance with legislation, stakeholder pressure, and efforts to strengthen market competitiveness also play significant roles. CE principles are embedded in the company's corporate strategy as part of its ESG policy. The company currently meets all regulatory requirements without difficulty and has voluntarily adopted additional CE measures that, while not yet legally mandated, are positively received by business partners and support entry into new international markets.

Respondents indicated that CE measures—particularly resource and material reuse—generate significant operational cost savings. Rising prices of input commodities such as water, energy, and packaging materials make the long-term application of CE principles economically advantageous. A core driver of the company's circular transformation is its in-house research, which develops innovative products and technologies aimed at reducing or reusing resources (Rethink).

The second part of the survey revealed that the company implements several CE measures. In production, it primarily focuses on minimizing waste generation by optimizing manufacturing processes. These efforts emphasize reducing input consumption and environmental impact (Reduce). The company is also gradually introducing recycling, regeneration, and reuse of chemicals and solvents. When replacing equipment, it selects systems that enable the separation and recapture of chemicals for reintegration into closed loops—provided the solutions are cost-effective compared to purchasing virgin materials. However, extended material loops are hindered by the REACH regulation, which requires the registration and evaluation of all substances, including recycled ones. This makes the use of recycled chemicals subject to the same time-consuming and costly procedures as new substances.

Due to the large volumes of water required for production and operations, implementing water circulation would necessitate significant investment in high-capacity water management systems.

Packaging represents another area with potential for circularity. The company applies CE principles across transport, storage, and consumer packaging. Reuse of primary packaging is only feasible when safety can be ensured, which often involves complex cleaning, leak testing, and compliance with ADR, CLP, and REACH labeling. Secondary and tertiary packaging offer greater flexibility, with fewer legislative barriers. For these categories, the company uses returnable transport items (RTIs) internally. However, RTIs are not used for external deliveries and are not planned for near-term implementation due to high logistical costs—particularly for imported raw materials from Asia, where reverse logistics would be prohibitively expensive. The company employs reusable materials (primarily plastic and cardboard) until they are no longer viable (Reuse), at which point they are recycled (Recycle). Recycled materials, such as from damaged pallets, are used by external partners to manufacture products like chipboard (Remanufacture).

In waste management, the company applies circular practices where technologically and legally feasible, focusing on material recycling, energy recovery, and wastewater management. However, chemical waste is often classified as hazardous under EU Directive 2008/98/EC and relevant national regulations. This entails stringent requirements for labeling, storage, and transportation, and such waste may only be handled by specialized entities. The company recycles non-hazardous material waste wherever possible (Recycle) and cooperates with an external recycling partner to maintain a company-wide system. It has eliminated landfill disposal to reduce environmental impacts and improve efficiency.

Wastewater treatment is also a key component of CE implementation. The company operates two separate sewage systems: one for chemical (process) wastewater and one for stormwater and sanitary water. Chemical wastewater must undergo pre-treatment by the company and further purification by a municipal facility before discharge, as required by law. For the second system, a closed water circuit enables partial recirculation and contributes to water savings. However, chemical extraction from wastewater is not practiced.

Remanufacturing and repurposing strategies are not routinely applied. In limited cases, manufacturers accept returns of unused materials, semi-finished, or unsold products. The company also explores the secondary resources market to find uses for surplus inventory.

The third part of the research identified several barriers to further CE implementation. The most critical is regulatory compliance for hazardous and chemical substances, which are often excluded from reuse and require incineration or specialized disposal. In addition, many chemical substances are transformed or degraded during use, making long material loops infeasible.

Economic barriers also persist. Virgin petrochemical-based materials are typically cheaper than recycled alternatives, and chemical recycling technologies (e.g., pyrolysis, depolymerization) remain expensive and

scalable only to a limited extent. Technical and infrastructural challenges further impede circularity. Closed-loop systems for solvent or catalyst recovery are rare and require costly modifications. Moreover, substituting virgin materials with recycled inputs may compromise process efficiency and product quality. As a result, the company uses recycled feedstocks in chemical production only to a very limited degree.

Discussion and result analysis

This paper examines the practical application of CE principles in a chemical manufacturing company, revealing the complex relationship between environmental, economic and regulatory factors. The implementation of CE measures is not seen solely as an environmental initiative; it is also aligned with regulatory compliance obligations, stakeholder expectations and strategic objectives within the company's environmental, social and governance (ESG) policy. The foundation of circular solutions is the company's own research, which develops innovations to reduce or reuse resources.

Key findings show that CE practices contribute significantly to operational cost savings, particularly in the context of rising input prices such as energy, water and packaging materials. The company has integrated CE strategies into its manufacturing processes by focusing on waste minimization (Reduce), gradually introducing chemical reuse and recycling where economically feasible, and optimizing facilities to enable closed systems.

However, significant obstacles remain. REACH and other legal requirements treat recycled substances on an equal footing with virgin materials, requiring costly and time-consuming registration and approval. This limits the feasibility of long circular loops, especially when handling chemicals that degrade or transform during use. In water management, although partial recirculation systems are in place, full reuse is hindered by high infrastructure and operational costs.

Packaging is a more flexible area. While the reuse of primary packaging is limited by safety and labelling requirements, secondary and tertiary packaging allows for greater circularity. Reusable transport items (RTIs) are effectively used internally, although reverse logistics challenges prevent wider use in external supply chains.

Waste management reflects a selective but proactive approach. Material waste that is not classified as hazardous is consistently recycled, supported by collaboration with specialist partners. The company has eliminated landfilling and prioritizes energy recovery and material recycling where regulations allow. Hazardous waste remains a major challenge due to strict EU classification and treatment requirements.

Although strategies such as remanufacturing and reuse are used on a case-by-case basis, they are not yet systematically implemented. Attempts to return unused materials or products to suppliers or secondary markets remain limited in scope.

Overall, the company demonstrates a structured and multifaceted CE approach, but further progress is limited by systemic regulatory, economic and technical barriers. Addressing these challenges will require policy adaptation, investment in scalable recycling technologies and enhanced cross-sectoral cooperation to support the circular economy in complex industrial environments such as chemical manufacturing.

Conclusion

Based on a content analysis of the collected data, the company's proactive approach to exploring CE opportunities can be positively evaluated. Circular measures are implemented rationally and in accordance with economic efficiency, although the company faces several general barriers common to the processing industry, as well as specific challenges related to the nature of chemical production, chemical substances, and associated regulatory requirements.

The results of this pilot study cannot be generalized, as the company's approach to CE is strongly influenced by its specific financial, market, technological, and resource conditions, as well as other operational constraints.

However, the company's economically driven and context-sensitive approach to CE transformation—considering factors such as operational conditions, energy intensity, resource availability, access to alternative energy and water sources, and emission levels—can be viewed as potentially generalizable. Finally, the proactive role of management in advancing the company's strategic CE goals, aligned with the objectives of the Paris Climate Agreement and a broader commitment to industrial sustainability, is also noteworthy.

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ECONOMY AND MANAGEMENT OF RAINWATER AND WASTEWATER UTILIZATION IN TOURISM: STRATEGIES, TECHNOLOGIES, AND CURRENT STATE IN SELECTED TOURIST DESTINATIONS

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Abstract

Effective water resource management is a key aspect of sustainable tourism development. This article analyzes the economic and managerial approaches to the use of rainwater and wastewater in tourist facilities, focusing on modern technologies and strategies implemented in selected tourist destinations. It compares the current state of water recycling and reuse across different regions, identifies key challenges, and evaluates the effectiveness of applied solutions from both economic and environmental perspectives. Special attention is given to the potential of rainwater utilization to reduce potable water consumption and to innovative wastewater treatment systems. The findings highlight the importance of intelligent water resource management in the context of sustainable tourism and provide recommendations for improving water management practices in tourist facilities.

Introduction

The use of wastewater and rainwater in tourist destinations is an important topic, as tourism often causes increased pressure on water resources, especially in areas with limited water supplies (eg islands, mountain areas, Mediterranean destinations). Modern technologies and approaches try to improve the sustainability of tourism and minimize negative impacts on the environment.
The mountain area has its own specifics - especially limited water resources, higher seasonal load (eg in the winter season), sensitive natural environment and often complex terrain. All of this puts greater emphasis on the careful management of water.
Here is an overview of technologies and approaches to the use of wastewater and rainwater specifically for mountain tourist areas.

Wastewater recycling in mountain accommodation facilities
Decentralized wastewater treatment plants (small WWTPs)

- Suitable for mountain hotels, cottages, ski resorts,
- They can be modular, easy to operate and operate even in winter conditions,
- For example membrane bioreactors (MBR)-high quality of purified water, the possibility of its reuse:
  - Snowmaking of the slopes,
  - Irrigation of greenery around the accommodation,
  - Flushing toilets.

Heat recovery from waste water

- For example the water from the hotel showers is first cooled and the heat is used to preheat the other water,
- It reduces the energy demand in places with more expensive energy sources.

Catching rainwater in a mountain environment
Collection of rainwater from the roofs of mountain huts, hotels, cable car stations

- The water is cleaned and stored in underground tanks (protected against frost),
- Usage:
  - WC, cleaning, washing of equipment (eg skis, bikes),
  - Storage water for firefighting purposes (important in remote areas),
  - In the summer months for irrigation, or replenishment of mountain lakes.

Natural and ecological solutions
Root treatment plants (wetlands)

- They work well in smaller settlements, at ecological huts,

- Low operating costs, high resistance, natural integration into the landscape,
- In winter, they may have limited effectiveness, but they can be combined with other systems.

Green roofs and permeable surfaces

- They retain precipitation, improve the microclimate and insulation,
- Prevents excessive runoff of water from steep slopes and erosion,
- Independence from long-distance water supplies (which is logistically and economically demanding in the mountains),
- Reduction of the risk of floods and erosion during torrential rains,
- Increased resistance to drought in the summer months,
- The possibility to promote the destination as "eco-friendly" – a powerful marketing tool.

The importance of decentralized water management in tourist locations

Decentralized systems use rainwater and greywater collection as well as small-scale treatment plants (e.g. MBR, roots treatment plants, SBR) directly at the point of consumption – an ideal solution for mountainous and remote tourist destinations. For example, a pilot study of greywater with MBR showed that a 30 m^3/day system for a hotel achieves a return on investment in three years and effectively reduces energy consumption by up to 35% (Hedregodt et al., 2017).

Technological solutions: MBR, SBR, wetlands, bioelectrochemical systems

- Membrane bioreactors (MBR) offer high quality purified water suitable for reuse in irrigation, flushing or snowmaking. MBR technology has been shown to be effective in treating municipal and industrial wastewater, particularly due to its compact design and ability to remove high organic loads (Judd, 2016),
- Sequential batch reactors (SBR) and wetlands have shown lower environmental impact in mountainous areas with climate challenges (SciTech et al., 2023),
- Bioelectrochemical systems (e.g. microbial fuel cells – MFCs) are a promising solution with the possibility of generating electricity while treating water (Sustainability et al., 2023).

Rainwater harvesting and utilization

Rainwater harvesting systems have great potential in reducing drinking water consumption. However, their implementation faces technical and economic challenges, especially in mountainous areas. Rooftop water retention with filtration, sedimentation and UV treatment is suitable (Ghaitidak & Yadav, 2021). Green roofs and infiltration areas are also important, improving the microclimate and retaining rainfall (Mentens, J., Raes, D., & Hermy, M. (2006).

Social and economic aspects

Research shows that public perception of recycled water affects the level of technology adoption. Concerns about health risks are often an obstacle even where recycled water is intended for technical use only (KD et al., 2023). Therefore, an information campaign and transparent communication of benefits are important in tourist areas.

Integrated management and smart systems

The GST4Water model integrates rainwater and greywater systems with digital monitoring and applications for real-time consumption management (Cipolla et al., 2018). The Swiss KREIS-Haus project shows the practical use of decentralized water collection and recycling with a high level of energy efficiency and educational potential (McBean et al., 2025).

Research methodology

Based on theoretical knowledge gained through a literature search, we proposed two different ways of using wastewater for two different tourist destinations. In the first destination, we collect water from sinks, showers and wellness areas, without any toilets. In the second destination, in the High Tatras, we collect rainwater.
Academic research and studies from relevant research areas, climate change, climatic phenomena, climate manifestations, and adaptation and mitigation measures are used to address the validity of theoretical assumptions regarding the formulation and implementation of relevant decisions in the field of wastewater use in practice.

Simulation and experiment

Design of a system for the use of wastewater and rainwater for a mountain hotel in Špindlerův Mlýn

Basic data (assumption):

- Hotel capacity: approx. 60–100 beds,
- Restaurant, wellness, showers, WC,
- Year-round operation, peak in winter.

Wastewater recycling (grey water)

What we collect:

- Water from sinks, showers, wellness (without toilets).

Technology:

- Modular gray water recycling system (e.g. AQWISE, Hydraloop or local solution from ENVI-PUR),
- Filtration, biological cleaning, UV disinfection,
- Water reuse tank - min. 5 m^3.

Usage:

- Flushing toilets, cleaning work,
- Irrigation of greenery in the summer season,
- Possibility of future expansion to snowmaking (in cooperation with the ski resort).

Capture and use of rainwater

Technology:

- Collection from roofs (if possible from several objects of the hotel complex),
- Pre-cleaning (filters, sedimentation),
- Underground tank 10–15 m^3 – insulated against frost,
- Controlled use using a pump and sensors.

Usage:

- WC flushing (in addition to gray water),
- Washing outdoor surfaces and equipment,
- Water reservoir for fire fighting,
- Irrigation in summer.

Natural solution for cleaning the rest of wastewater

- If the hotel is not connected to the central sewage system:
  - Compact waste water treatment plant (MBR or SBR system) with a tank for reuse,
  - Possibility of combination with a root treatment plant (small wetland) for biological treatment,
- If it is connected → at least pre-treatment of gray water before discharge.

Smart management and monitoring

- Water consumption sensors,
- Application for operational monitoring (levels, water quality, leaks),
- Involvement in sustainable certification - e.g. Green Key, EU Ecolabel.

Approximate costs (without subsidies):

Table I

Item	Price (approximate)
Gray water recycling unit including installation)	1,500,000 CZK
Rain tank + filtration	900,000 CZK
Smart monitoring system	300,000 CZK
Root treatment plant / MBR system	1,000,000 CZK

Subsidies: Programs such as the Environmental Operational Program (OPŽP) or the Modernization Fund often cover 40–70% of the investment. Possible despite the National Recovery Plan.

Marketing bonus

- The hotel can use the ecological system as part of the brand:
  - "Accommodate with a clear conscience",
  - Green Hotel certificate,
  - QR codes with information about water savings in showers or toilets,
  - Use in communication with eco-tourists or school groups.

Design of a system for the use of wastewater and rainwater for a hotel in Štrbské Pleso

Prerequisites:

- 70–100 beds, restaurant, wellness, sauna, winter operation key,
- Location near the lake → emphasis on absolute environmental friendliness,
- Connection to public infrastructure is possible, but limited.

Gray water recycling (showers, sinks, wellness, swimming pool - without toilets)
Technology:

- Advanced MBR system (Membrane bioreactor) – (ASIO, Wabag, Veolia),
- UV disinfection + activated carbon,
- Storage tank (6–10 m^3), insulated against frost.

Use of recycled water:

- Flushing toilets,
- Cleaning of wellness and outdoor spaces,
- Irrigation of green areas (in summer),
- Possible snowmaking of a smaller slope (if the composition is appropriate).

Collection and use of rainwater
Construction:

- Collection from sloping tin roofs → gutters → filter,
- The first precipitation goes to the bypass (the so-called first flush), then to the underground tank (10–15 m^3),
- Filtration, UV treatment.

Usage:

- WC flushing (extra charge),
- Stock for fire tank,
- Washing water for bikes, boots, skis,
- Possibility of use in the technical background (maintenance, washing of equipment).

Wastewater treatment plant and eco-infrastructure

- Due to the location, a highly efficient biological treatment plant, e.g. with tertiary cleaning (chemical stabilization P, UV),
- Alternatively, a compact MBR system with outlet to the sewage system,
- For eco-hotels: decorative root cleaning zone (for summer, at the entrance).

Smart monitoring and environmental education

- Monitoring of water consumption, leaks, quality of recycled water,
- Display on the touch panel in the entrance hall,
- Educational info-zone: How much water is saved daily, compared to normal operation,
- Suitable for eco-certification: Green Key, EU Ecolabel, Naturland.

Approximate costs (without VAT, without subsidies):

Table II

Item	Price (approximate)
MBR treatment plant with a capacity of 15–20 m³/day	2,000,000 CZK
Gray water system (filtration, tank, distribution)	1,500,000 CZK
Rainwater system (filtration, tanks)	900,000 CZK
Monitoring, sensors, applications	350,000 CZK
Green roof or wetland zone (optional)	3,000,000 CZK

Funding options: Slovak Environmental Funds, Recovery and Resilience Plan of the Slovak Republic, EU funds (INTERREG, OP KŽP, LIFE), Possibility of connection with an eco-tourism or education project

Marketing and added value

- The hotel becomes a "model ecological operation" in TANAP,
- Possibility to get support from the national park and the municipality,
- Promotion via "eco-travel" portals,
- Interest of schools, universities, companies in the excursion → educational potential.

Acknowledgement

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EFFICIENCY OF REVERSE LOGISTICS PROCESSES IN AN INDUSTRIAL ENTERPRISE

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Abstract

The article analyzes current practices in the processing of recycling and reuse of materials and identifies key areas for improvement. The aim of the article is to propose a proposal for streamlining reverse logistics processes and optimizing product flows in the context of sustainable development of an industrial enterprise. The methods used are based on identifying ways in which reverse logistics can support sustainability, increase process efficiency and contribute to the overall improvement of supply chain management in a modern industrial environment. The conclusions and recommendations that will emerge from this article will be based on real findings from the studied enterprise. The implementation of these recommendations should not only increase the efficiency of reverse logistics processes, but also support the principles of the circular economy and contribute to reducing the environmental burden.

Introduction

Logistics is seen as a broad and complex process that involves planning, implementing and controlling the efficient movement and storage of goods, services and information between points of origin and consumption. Its main objective is to meet customer needs. This concept encompasses various aspects, from the management of internal and external material flows to the environmentally responsible processing of return flows[1].

Logistics in a manufacturing company is an integrated system that ensures the optimal flow of materials, information and value from suppliers through the production process to the customer. The active and passive elements of this system must be coordinated with each other to jointly achieve the set logistics goals while minimizing overall costs[2].

According to Rogers and Tibben Lembke in 1999, Reverse logistics isa new type of logistics that differs from conventional logistics in that it returns goods from theretailer or customer to the manufacturer. The planning and execution of the flow of raw materials, work-in-process, finished goods, and related information from the point of consumption to the point of origin to create value or cost-effective disposal of products or goods is known as reverse logistics[3]. According to (Sharma, 2019)[4], Reverse logistics is an essential component of the supply chain that includes a series of actions that occur after the sale of a product to restore the value of the product and end its life cycle. Reverse logistics is a process that includes all the actions of effective planning, implementation, and control, cost-efficient flow of raw materials, inventory processes, final results, and related information from the point of consumption to the point of origin. Reverse logistics also includes managing damage-related returns, recycling, recalls, seasonal inventory, and restocking[5].

Creating and implementing a quality methodology according to ISO9001 standards into quality processes creates the basic prerequisites for successful growth of companies and increases their competitiveness. Changing the methodology creates the prerequisites for converting the quality system to the needs of the current market situation[6]. Reverse Logistics include collection, sorting, recycling, redistribution, and disposal[7].

Reverse Logistics reflects a strategic concept in modern supply chain management that integrates collecting, processing, and returning unsold or unused products into the production or distribution cycle[8].

Large and medium-sized companies are not the only ones contributing to environmental improvement. Many small-scale industries depend on government subsidies to operate, which is one of the causes of industrial pollution. They often ignore environmental regulations and release highly toxic gases into the atmosphere. Environmental management principles are applied in all aspects of the supply chain, such as design, manufacturing procurement, assembly, packaging, logistics, and distribution, in Green Supply Chain Management (GSCM) practices. However, GSCM practices have yet to be widely applied in developing countries and small and medium-sized enterprises. The rate of GSCM implementation is lower in small-scale enterprises than in large and medium-sizedenterprises[9].

The logistics industry, integral to economic and everyday activities, significantly contributes to environmental degradation and resource consumption. The sector faces increasingly stringent environmental regulations due to its impacts on traffic congestion, safety, and pollution, alongside a growing demand for sustainable logistics solutions. Con-sequently, companies are adopting Green Logistics strategies to meet these demands.

Logistics in a manufacturing enterprise is an integrated system that ensures the optimal flow of materials, information and value from suppliers through the production process to customers. The active and passive elements of this system must be coordinated with each other to jointly achieve the set logistical goals while minimizing the overall2. Reverse logistics is an integral part of the supply chain. It encompasses a series of activities that take place after a product is sold to restore its value or end its life cycle. It is the process of effectively planning, implementing and controlling the cost-effective flow of raw materials, inventory, finished products and related information from the point of consumption back to the original source[10].

Discussion and result analysis

Figure 1 shows five main areas: returns, reselling, repairs, replacement and recycling. Each of these areas represents a specific stage of processing a good or material that supports a circular economy and reduces environmental impact.

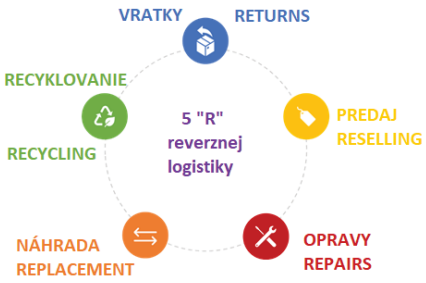

Figure 1. Five main areas of reverse logistics

While returns and exchanges are a strength for larger retailers, they are a problem for smaller retailers – mainly due to limited resources and a lack of volume discounts. The rise of e-commerce has further exacerbated the difficulty of returning goods, with 10% of in-store purchases and a whopping 30% of online purchases being returned. A study of the returned goods market revealed that 95% of these products are not returned due to any fault or error on the part of the manufacturer or retailer, but purely due to the personal decision of the end customer. Such products can be easily resold, as they are flawless and fully functional.

A company can increase its revenue by repairing defective or damaged goods, which can then be returned to the original owner or sold to a new customer as a refurbished product. Customers often prefer to have goods repaired rather than pay more for a new product. In addition, some customers do not mind receiving a discount on products that look and function like new.

Customers may sometimes request an exchange/replacement due to size issues or color preferences. Providing quick and easy exchanges leads to increased customer loyalty. On the contrary, cumbersome exchange policies and procedures can lead to a decrease in customer satisfaction and, consequently, their loyalty.

Recycling and disposal are important not only for compliance with legal regulations, but also due to the growing popularity of sustainable businesses. Recycling also leads to a significant increase in profit.

As part of the research, we selected a company that belongs to the SK NACE classification in section C – Industrial production, specifically to subcategory 27.33.0 – Manufacture of electrical installation equipment. The process of handling complaints and returns (products that the customer wants to return within 1 year of the product invoice) in the company begins with receiving a request from the customer, which usually comes by e-mail. This must contain all the necessary details, such as the material reference, invoice number or delivery note, number of pieces and, in the case of a complaint, a description of the defect. Based on this information, an internal record is created in the table, while other necessary data is added from the Systems Application Products in data processing system, in particular the customer number and the amount for which the goods were sold. This data is important for assessing whether the goods in question will be sent for expert examination (if the goods exceed the unit price of €100). If the complaint is caused by incorrect material in the packaging, the packaging is marked with the correct name of the goods, but its contents do not correspond to what was supposed to be there, a credit note is issued for this goods directly from the factory. The customer keeps the goods and does not have to send them back. After collecting all the necessary information, the complaint or return is entered into the Green Plant system.

This system generates a document containing important data for complaints, for example, information on whether the product is still under warranty and whether it needs to be sent for expert assessment and therefore

"GP" in other words expertise, for returns the number of units that can be returned is indicated, or information on whether the goods were purchased within the last 12 months and whether they can be accepted back as stock goods. After checking this document, the data is then entered into the Bridge Front Office system, where a case is opened associated with the person who reported the complaint or return. If it is already possible to clearly determine at this stage that the error occurred in production, a complaint is also opened and directed directly to the production department. After processing the data and evaluating it, the customer is contacted with information on the method of resolution. If the goods are not sent for expertise, the customer is informed that a credit note will be issued to him. At the same time, he is obliged to store the claimed goods for a period of three months in case the manufacturer subsequently requests them for a detailed examination. If the goods are sent for expert examination, the customer will be sent a generated GP document, which they must print and insert into the package together with the product. The customer is also asked to send the data necessary for picking up the package, i.e. the exact address, contact person, dimensions and number of packages, as well as their weight. In the case of a rejected return, we will try to find out whether the product could still be accepted and we will contact the warehouse via an additional e-mail with a request for its approval or information about the possibilities of its return. In the event that the warehouse repeatedly refuses to accept the product back, we have another option to verify the situation with local production or the warehouse. Sometimes it may happen that the product in question can be used in production or for a specific project that is planned. If it is found that the production department can use the goods, we can hand them over to them, which will prevent the complete rejection of the goods for the customer, who is then forced to keep the product in stock. If all methods are rejected, an explanation is sent to the customer stating the reason for the rejection. In the case of an accepted return, a GP document is also sent to the customer, which must be included in the package, and the same data necessary for ensuring transportation is requested. After the shipment is delivered to the central warehouse in Hungary, a physical inspection of the goods takes place. In the case of returns, in addition to the product itself, the condition of the packaging is also checked, for example, damage to the box or description of the packaging, which could prevent further sale. If everything is in order, a credit note is issued to the customer. In the case of complaints, professional tests are carried out to determine the defect that was reported. If the device is working properly, the customer is informed that no defect has been confirmed, and the goods will be returned to him. If the fault is proven, a credit note is issued for the goods and the customer is informed of the result of the completed complaint procedure.

Companies place great emphasis on proper packaging of goods to ensure their protection during transport to customers. When choosing packaging materials, they take into account several factors, such as the size, weight, shape and fragility of the product, as well as the conditions in which it will be transported. The aim of packaging is not only to prevent mechanical damage to the goods, but also to ensure their stability during handling, storage and transport. For this purpose, the company mainly uses cardboard boxes and wooden crates. Cardboard boxes are an ideal solution for smaller and medium-sized products that are not extremely susceptible to damage. This type of packaging is light, strong and allows easy handling. For larger or heavier products, wooden crates are used, which provide greater strength, durability and stability during transport. Wooden packaging is particularly suitable for special equipment that does not have its original packaging or is custom-made. To prevent damage to the goods during transport, the company uses various types of protective filling materials. For products that are not particularly sensitive to shock or mechanical damage, air cushions - plastic bags filled with air - are most often used. This material effectively absorbs minor shocks and is particularly suitable for transporting products such as switches or other electrical components. For more sensitive equipment that can be damaged even by minor shocks, the company uses bubble wrap. This material provides excellent protection because its air bubbles absorb shocks and prevent mechanical damage. Bubble wrap is most often used for transporting fragile items such as card readers, electronic devices or other components that require increased protection against shocks. Given the current emphasis on environmental sustainability, we suggest that the company consider replacing classic plastic bubble wrap with more environmentally friendly alternatives, such as bubble-structured packaging paper, recycled cardboard or biodegradable cellulose filling materials. Such a step would contribute to reducing plastic waste and improving the environmental profile of the company. When transporting large and heavy products that are packed in wooden boxes, polystyrene chips or so-called flo-paks are used as a filling material. This material perfectly adapts to the shape of the transported object and fills the free space in the package, thereby preventing its movement during transport. Polystyrene filling is used mainly when transporting custom-made engines, generators or other industrial equipment that do not have the original packaging from the manufacturer. When shipping larger quantities of goods, a palletization system is used, which ensures efficient arrangement of products on the pallet in order to ensure stability and safety during handling and transport. When placing goods on a pallet, the company follows the principle of weight distribution - heavier products are always placed on the bottom of the pallet and lighter products on the top. This procedure helps to prevent

damage to the goods, as well as the dangerous overturning of the pallet during transport or manipulation with a forklift. After loading the products onto the pallet, the entire pallet is secured with stretch film, which is wrapped around the goods several times, ensuring that the packaging remains stable and that the individual products do not move. The stretch film also protects the goods from moisture, dust and other external influences that could cause damage. The company uses different types of pallets for shipping, depending on the nature of the transported goods. It most often uses wooden pallets, which are strong, affordable and suitable for transporting most products. In some cases, especially for specific types of goods, the company also uses plastic pallets and metal pallets. Plastic pallets are valued mainly for their low weight, high resistance to moisture, fungi and chemicals, as well as dimensional accuracy, which is important in automated warehouse systems. Their disadvantage is their higher purchase price. Metal pallets are approximately three times more expensive than wooden ones, but they excel in exceptional durability, precise dimensions and high load capacity. They are used primarily for very heavy or special products, where extraordinary strength and stability are required. In addition, their solid construction and long service life make them suitable for repeated use in logistics cycles with high loads. Each customer pays for the pallet on which the goods are delivered as part of the order. The company does not subsequently deal with further collection of pallets, so their disposal or reuse remains the responsibility of the customer. Strict adherence to these procedures ensures that the goods reach customers in an intact condition, thereby reducing complaints and the associated costs. In addition to protecting the goods themselves, effective packaging and palletization also contribute to optimizing transportation, allowing for better use of space in vehicles, reducing the time required for handling goods and increasing safety during their transportation. An overview of the total number of complaints in the individual years 2022-2024 is provided in Figure 2. In 2022, 642 complaints were recorded, in 2023 slightly fewer 635 complaints, and in 2024 the number of complaints decreased to 571. This trend indicates that the number of complaints has a decreasing tendency, which can be a positive signal if it is caused by improved product quality or more efficient complaint handling. On the other hand, the decline may also be influenced by changes in the number of products sold.

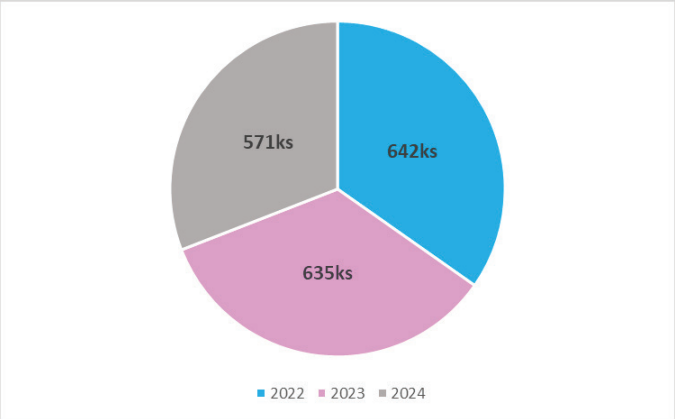

Figure 2. Share of complaints in 2022-2024. Own processing based on company data

The development of the number of returns in 2022-2024 is shown in Figure 2, which shows significant differences that can be influenced by several factors. In 2022, 298 returns were recorded, which represents the lowest value within the monitored period. This year was characterized by the impact of the COVID-19 pandemic, which changed the system in which customers purchased goods but also the number of projects and orders that customers created. However, in the following year, 2023, the number of returns increased sharply to 799. This increase was also due to the fact that customers were returning to normal operations after the pandemic and trying to quickly complete projects and also ordering goods that they would have in stock in case of unexpected problems in projects. In 2024, 498 returns were recorded. Based on the analysis of the processing of complaints and returns in the company AK158, s. r. o. for the period from 2022 to 2024, we have identified several weaknesses that cause unnecessary financial burden. One of the biggest burdens for the company is the costs associated with transporting the claimed goods for expert examination and also transporting the returns to the central warehouse in Hungary. The transportation itself would not be such a significant problem if each case of complaint or return was justified, i.e. in accordance with the terms of the warranty and business rules.

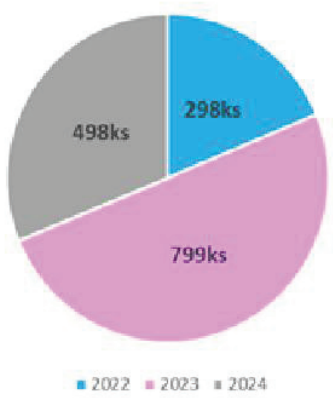

Figure 3. Number of returns in 2022-2024. Own processing based on company data

We found that the most significant problems are unjustified complaints, returns of goods after the warranty period or the specified period has expired, as well as damage to goods by the customer, which makes it impossible to re-sell them. These shortcomings are not only financially demanding, but also have a logistical and environmental impact due to unnecessary transport and material waste. In addition, it turned out that some processes are unnecessarily lengthy, are repeated manually or are not digitized, which slows down the company's reaction time to the customer.

Based on the results, we formulated proposals for solutions that are adapted to the structure and capabilities of a particular company. Key recommendations include the introduction of rules for invoicing costs for unjustified complaints or returns, for example, in cases where the goods are out of warranty, damaged, or when checked, they are found to contain no defect. This would reduce the number of unnecessarily processed complaints and at the same time strengthen customer responsibility. It is equally important to introduce regular transport schedules, such as weekly or biweekly collections, which would allow for better consolidation of shipments and reduce the number of trips. From quantitative data, we found that the annual carbon footprint resulting from individual transport of returns and complaints between the Slovak headquarters and the Hungarian warehouse is in the order of several tons of CO_2, including unnecessary routes caused by incorrectly filed complaints or uncoordinated shipments. This environmental impact points to the need to optimize these processes not only in terms of costs, but also from a climate responsibility perspective. This proposal is directly related to the company's efforts to reduce its carbon footprint, which in the case of regular transport between Slovakia and the Hungarian warehouse reaches several tons of CO_2 per year.

Other suggestions concern the use of modern technologies, for example, the introduction of an online system for tracking the status of complaints and returns, where the customer could obtain information about the progress of the processing in real time. This step would reduce the number of telephone or e-mail inquiries and improve the customer experience. In accordance with the principles of the circular economy, it is also recommended to consider buying back older products after the warranty has expired, and their subsequent remanufacturing or recycling. This could reduce the volume of waste and at the same time create new opportunities for offering remanufactured products at a lower price.

that reverse logistics has long been no longer just a support process, but a strategic element that has the potential to influence the overall performance of the company, its ecological profile and customer relations. Proper management of complaints and returns, supported by accurate data, automation and clear rules, can contribute to reducing operating costs, improving product quality and increasing competitiveness.

At the same time, the work provides space for further research in the field of intelligent reverse logistics systems, for example, the use of artificial intelligence in predicting the most common reasons for complaints, optimizing product collection routes or designing ecological distribution and collection models. An important direction for the future is also the connection of logistics with ESG criteria (environmental, social and governance factors), which will be increasingly important in evaluating companies from the perspective of investors and the public.

The company AK158, s. r. o., has created a good foundation for the development of effective reverse logistics. The result of the diploma thesis is a practical guide to further steps that will not only reduce operating costs and increase customer satisfaction, but also meet the goals of sustainable development. At the same time, it represents a benefit that can be generalized and applied in other industrial companies operating in related areas,

while offering inspiration for the introduction of effective and environmentally responsible solutions in the field of reverse logistics.

Conclusion

The methodological part of the thesis was based on a review of professional literature, analysis and synthesis of knowledge, and practical process analysis of the selected company. The practical part includes a detailed description of the complaint and return processes, their statistical evaluation, and the identification of problems. The analysis resulted in specific proposals for process improvement. We achieved the objective of the thesis by identifying specific weaknesses and proposing feasible solutions. At the same time, we pointed out that reverse logistics can significantly contribute to the economic and environmental performance of a company. The thesis provides a basis for further research in the field of reverse logistics optimization in industry and its connection with modern digital and ecological approaches. The implementation of these recommendations should not only increase the efficiency of reverse logistics processes, but also support the principles of the circular economy and contribute to reducing the environmental burden. The results of this work will provide valuable insights for the company and help it achieve higher levels of sustainability and efficiency.

The logistics industry, integral to economic and everyday activities, significantly contributes to environmental degradation and resource consumption. The sector faces increasingly stringent environmental regulations due to its impacts on traffic congestion, safety, and pollution, alongside a growing demand for sustainable logistics solutions. Con-sequently, companies are adopting Green Logistics strategies to meet these demands.

Reverse logistics is no longer just a supporting process, but a strategic element with the potential to influence the overall performance of the company, its environmental profile, and customer relationships. Proper management of complaints and returns, supported by accurate data, automation and clear rules, can contribute to reducing operating costs, improving product quality and increasing competitiveness. At the same time, the work provides space for further research in the field of intelligent reverse logistics systems, for example, the use of artificial intelligence in predicting the most common reasons for complaints, optimizing product collection routes or designing ecological distribution and collection models. An important direction for the future is also the connection of logistics with ESG criteria (environmental, social and governance factors), which will be increasingly important in evaluating companies from the perspective of investors and the public.

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CONSUMPTION OF ENERGY DRINKS BY CZECH GENERATION Z AND Y IN THE CONTEXT OF SOCIAL RESPONSIBILITY

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Abstract

Consumption of energy drinks has increased significantly in recent years, whereas the key consumer group is in particular constituted by young people. The trend towards excessive consumption of energy drinks raises concerns not only in terms of public health, but also with regard to environmental and social responsibility as a whole. Although alternatives such as organic and sugar-free options do exist, the factors influencing choice of these drinks have not as yet been sufficiently investigated. While some studies suggest that increased education and awareness regarding the issue can lead to reduced consumption of energy drinks, the reality of consumer behaviour is often different. The aim of this study is to analyse and evaluate the consumption and preferences of energy drink consumers from Czech Generation Z and Y in the context of social responsibility. Attention is focused on identification of key demographic factors influencing preferences among respondents for various energy drink alternatives. Quantitative research was conducted via an online questionnaire survey on a sample of 1,013 respondents from the Czech National Panel. The data were analysed using frequency analysis and statistical hypothesis testing to identify significant differences in consumer behaviour based on gender, age, and education. The findings of this study can be used by energy drink manufacturers and creators of health policy.

Introduction

Consumption of energy drinks has increased significantly in recent years, whereas the primary consumers are adolescents and young adults[1,2]. This trend is supported by strong marketing communication and promotion[2,3], which presents these drinks as an easily accessible and portable source of energy and stimulation, which is particularly attractive to people with busy lifestyles or people who travel frequently[4]. Increased consumption of energy drinks is also reinforced by their prevalence at social events, festivals and within the setting of sports teams[3,5], where the impression is created that consumption of these drinks is not only normal but even desirable[3]. Another factor may be the belief that these drinks, containing mainly caffeine and taurine, have positive effects on enhancing athletic performance[4,6].

However, increased consumption of energy drinks brings with it a number of health risks, particularly cardiovascular, gastrointestinal, neurological and kidney problems due to the high content of caffeine and other stimulants[4,5]. Apart from the individual aspect, this problem is also significant from a societal point of view. The rising prevalence of obesity, type 2 diabetes mellitus and cardiovascular disease is driving up healthcare costs, increasing the burden on the healthcare system and placing increased demands on public finances[7,8,9]. Besides the health impacts associated with consumption of energy drinks, the environmental impacts must also not be overlooked. The production and consumption of energy drinks are associated mainly with high consumption of plastic packaging, aluminium cans and other materials, creating an increased environmental burden[7,10]. For the given reasons, pressure for more sustainable alternatives to energy drinks is increasing[7].

One way to reduce the health risks associated with energy drink consumption is to promote alternatives such as organic energy drinks and products without any added sugar (zero-sugar or sugar-free)[7]. Organic energy drinks are made from organic ingredients and do not contain synthetic additives, meaning that they are perceived as a healthier and more environmentally friendly alternative[11]. Drinks which do not contain any added sugar allow consumers to avoid the negative effects of excessive sugar consumption, such as obesity or metabolic disorders[11,12,13].

From the perspective of social responsibility [14] this trend can be understood to be a combination of promoting a healthy lifestyle and environmental responsibility[7,11]. The reality is that consumers are increasingly looking for products with lower sugar content, natural ingredients and an environmentally friendly approach to production and packaging[7,15].

Studies focused on energy drink consumption confirm that adolescents and young adults are the most frequent consumers, with marketing, the social environment and perceived benefits of these products playing a key role[1,3,5,6]. Research also indicates that there are some positive effects in the form of a short-term increase in energy and concentration, although long-term consumption brings with it health risks[1,4,6]. On the contrary,

studies on organic and sugar-free options suggest lower health risks associated with their consumption, although consumption of these alternatives is still relatively low[7,13,15].

The aim of this study is to analyse and evaluate the consumption and preferences of Czech Generation Z and Y energy drink consumers in the context of social responsibility. Attention is focused on the influence of demographic factors which affect consumer attitudes towards the consumption of energy drinks, including organic and sugar-free alternatives, on the Czech market.

This study contributes to a better understanding of consumer behaviour in the field of energy drinks and offers recommendations for energy drink producers and policy makers in the context of promoting healthier and more sustainable alternatives. The findings of the study could contribute to increasing the effectiveness of public awareness campaigns promoting a healthy lifestyle and environmental responsibility.

Research methodology

Quantitative research was conducted as part of this study in the form of a questionnaire survey. The questionnaire was designed on the basis of a literature search and consisted of two parts. The first part contained closed-ended questions regarding preferences and amounts of energy drinks consumed, while the second part identified the demographic characteristics of respondents (see Table I). The questionnaire survey was conducted in November 2024 using the CAWI method[16]. Respondents were selected from the Czech National Panel, which specialises in consumer and public opinion surveys.

The research focused on the Czech Generation Z (aged 18-28) and Generation Y (aged 29-43) population[17]. Respondents were randomly selected to participate in the study according to set quotas. The quotas used were gender (2 categories), age (2 categories), education (4 categories), region (14 categories) and size of place of residence (5 categories). A total of 1,104 respondents completed the questionnaire. 91 questionnaires were discarded during processing. This means that data from a total of 1,013 respondents, i.e. 92%, were analysed.

Table I
Descriptive statistics

Demographics/ characteristics	Specifications	Counts	Proportion	Overall Czech population
	Total	1013	100%	
Gender	Male	510	50.3%	51.7%
	Female	503	49.7%	48.3%
Education (4 cat.)	Primary school	106	10.5%	11.1%
	Trained	238	23.5%	23.1%
	High school with graduation	374	36.9%	37.0%
	High school, vocational school	295	29.1%	28.8%
Generation	18 - 28 years – Generation Z	332	32.8%	32.5%
	29 - 43 years – Generation Y	681	67.2%	67.5%
Gross income amount	≤ 20 000 CZK	243	24.0%	—
	20 001 - 40 000 CZK	366	36.1%	—
	40 001 - 60 000 CZK	193	19.1%	—
	≥ 60 000 CZK	61	6.0%	—
	I don't want to answer	150	14.8%	—

Source: Own.

Data were statistically processed using IMB SPSS Statistics software and Microsoft Excel. Consumer behavior was evaluated based on the frequency distribution of responses to selected questionnaire items. To validate differences according to demographic characteristics, the chi-square test was applied at a significance level of 0.05. Post hoc paired testing enabled the identification of significant differences among respondent groups.

Analysis of results

First, an analysis of consumption behaviour was conducted for the entire target population (see Table II), and the results show that the majority of respondents consume energy drinks occasionally rather than regularly. Men more frequently consume energy drinks than women *(χ^2= 64,534, df=4, sig<0.05)*, with 57% of men consuming energy drinks every day or at least once a month. A statistically significant difference is also evident in average weekly consumption, where it is again confirmed that men consume more energy drinks than women *(χ^2= 6.308,*

df=4, sig>0.05). 43.1% of women say they never consume energy drinks, while 67.6% of men say they consume 1ml - 1,000ml of these drinks per week. On the other hand, more women (22.6%) than men (15.9%) prefer energy drinks labelled organic (χ^2= 4.391, df= 1, sig<0.05). However, a higher average consumption of organic energy drinks was reported by men *(χ^2= 6.308, df= 4, sig>0.05)*, with 29.2% of men claiming to consume 1ml - 1,000ml of organic energy drinks per week. A statistically significant difference can also be observed in the consumption of zero-sugar or sugar-free energy drinks *(χ^2= 8.970, df= 4, sig>0.05)*, with 11.7% of men responding that they consume 501ml - 3l of zero-sugar/sugar free energy drinks per week.

Table II
Consumption and preferences of energy drinks by gender

Characteristics		Total	Gender	
			Male[A]	Female[B]
Energy drink consumption	Total respondents	1013	510	503
	daily	3.9%	[B]6.1%	[A]1.8%
	at least once a week	13.5%	[B]18.4%	[A]8.5%
	at least once a month	14.0%	[B]18.0%	[A]9.9%
	a few times a year/ occasionally	35.6%	[B]32.5%	[A]38.8%
	never	32.9%	[B]24.9%	[A]41.0%
Average weekly consumption of energy drinks	Total respondents	680	383	297
	0ml	32.4%	[B]24.0%	[A]43.1%
	1ml - 500ml	49.7%	52.2%	46.5%
	501ml - 1000ml	12.4%	[B]15.4%	[A]8.4%
	1001ml - 3l	4.4%	[B]7.0%	[A]1.0%
	more than 3l	1.2%	1.3%	1.0%
Preference of energy drinks with the label bio	Total respondents	680	383	297
	YES	18.8%	[B]15.9%	[A]22.6%
	NO	81.2%	[B]84.1%	[A]77.4%
Average weekly consumption of energy drinks labeled bio	Total respondents	680	383	297
	0 ml	71.2%	[B]68.1%	[A]75.1%
	1ml - 500ml	22.1%	23.5%	20.2%
	501ml - 1000ml	4.7%	5.7%	3.4%
	1001ml - 3l	1.5%	2.1%	0.7%
	more than 3l	0.6%	0.5%	0.7%
Preference for energy drinks labeled zero or sugar free	Total respondents	680	383	297
	YES	40.1%	37.3%	43.8%
	NO	59.9%	62.7%	56.2%
Average weekly consumption of energy drinks labeled zero or sugar free	Total respondents	680	383	297
	0ml	58.5%	55.9%	62.0%
	1ml - 500ml	31.9%	31.9%	32.0%
	501ml - 1000ml	6.2%	[B]7.8%	[A]4.0%
	1001ml - 3l	2.8%	[B]3.9%	[A]1.3%
	more than 3l	0.6%	0.5%	0.7%

[A]The value significantly differs to the value of group A.
[B]The value significantly differs to the value of group B.
Source: Own.

Furthermore, statistically significant differences were found from a generational perspective (see Table III). The results showed that Generation Z drinks energy drinks more often *(χ^2= 2.505, df=4, sig>0.05)*, with 38.6% of respondents from Generation Z drinking energy drinks every day, at least once a week or once a month. No statistically significant difference was noted in the other areas of the investigation.

Table III
Consumption and preferences of energy drinks by age

Characteristics		Total	Generation	
			Z[A]	Y[B]
Energy drink consumption	Total respondents	1013	332	681
	daily	3.9%	[B]5.7%	[A]3.1%
	at least once a week	13.5%	15.4%	12.6%
	at least once a month	14.0%	[B]17.5%	[A]12.3%
	a few times a year/ occasionally	35.6%	34.9%	36.0%
	never	32.9%	[B]26.5%	[A]36.0%
Average weekly consumption of energy drinks	Total respondents	680	244	436
	0ml	32.4%	29.5%	33.9%
	1ml - 500ml	49.7%	51.6%	48.6%
	501ml - 1000ml	12.4%	13.9%	11.5%
	1001ml - 3l	4.4%	4.1%	4.6%
	more than 3l	1.2%	0.8%	1.4%
Preference of energy drinks with the label bio	Total respondents	680	244	436
	YES	18.8%	20.5%	17.9%
	NO	81.2%	79.5%	82.1%
Average weekly consumption of energy drinks labeled bio	Total respondents	680	244	436
	0ml	71.2%	69.3%	72.2%
	1ml - 500 ml	22.1%	23.4%	21.3%
	501ml - 1000ml	4.7%	5.7%	4.1%
	1001ml - 3l	1.5%	1.2%	1.6%
	more than 3l	0.6%	0.4%	0.7%
Preference for energy drinks labeled zero or sugar free	Total respondents	680	244	436
	YES	40.1%	41.4%	39.4%
	NO	59.9%	58.6%	60.6%
Average weekly consumption of energy drinks labeled zero or sugar free	Total respondents	680	244	436
	0ml	58.5%	54.9%	60.6%
	1ml - 500ml	31.9%	34.8%	30.3%
	501ml - 1000ml	6.2%	7.0%	5.7%
	1001ml - 3l	2.8%	2.5%	3.0%
	more than 3l	0.6%	0.8%	0.5%

[A]The value significantly differs to the value of group A.
[B]The value significantly differs to the value of group B.
Source: Own.

Lastly, consumer behaviour in the field of energy drink consumption was examined from the perspective of respondents' education (see Table IV). It is evident that 29.0% of respondents who have completed vocational training consume energy drinks every day or at least once a week, compared to 83.4% of respondents with a university education who reported that they consume energy drinks only occasionally or never *(χ^2= 70.125, df= 12, sig<0.05)*. Respondents with a university education are also the largest group whose average weekly energy drink consumption is 0ml (46.5%). On the contrary, 75% of respondents with only a basic level of education answered that their weekly consumption is 1ml - 1,000ml *(χ^2= 35.240, df= 12, sig<0.05)*. A statistically significant difference can also be observed in the weekly consumption of organic energy drinks *(χ^2= 14.943, df= 12, sig>0.05)*, where 13.9% of respondents with a basic level of education stated that their weekly consumption of organic energy drinks is more than 501ml.

Table IV
Consumption and preference of energy drinks in terms of education

Characteristics		Education			
		Primary school[A]	Trained [B]	High school with graduation[C]	High school, vocational school[D]
Energy drink consumption	Total respondents	106	238	374	295
	daily	[D]6.6%	[CD]7.6%	[B]3.2%	[AB]1.0%
	at least once a week	[D]17.9%	[CD]21.4%	[B]11.8%	[AB]7.8%
	at least once a month	[D]17,9%	[D]16.4%	[D]16.3%	[ABC]7.8%
	a few times a year/ occasionally	[CD]25.5%	[D]31.5%	[A]36.4%	[AB]41.7%
	never	32.1%	[CD]23.1%	[BD]32.4%	[BC]41.7%
Average weekly consumption of energy drinks	Total respondents	72	183	253	172
	0ml	[CD]18.1%	[CD]23.5%	[ABD]33.2%	[ABC]46.5%
	1ml - 500ml	[D]58.3%	[D]54.1%	49.4%	[AB]41.9%
	501ml - 1000ml	[D]16.7%	[D]16.9%	11.9%	[AB]6.4%
	1001ml - 3l	6.9%	4.4%	4.0%	4.1%
	more than 3l	0.0%	1.1%	1.6%	1.2%
Preference of energy drinks with the label bio	Total respondents	72	183	253	172
	YES	12.5%	15.8%	20.6%	22.1%
	NO	87.5%	84.2%	79.4%	77.9%
Average weekly consumption of energy drinks labeled bio	Total respondents	72	183	253	172
	0 ml	68.1%	[D]66.1%	72.3%	[B]76.2%
	1ml - 500 ml	18.1%	26.8%	22.1%	18.6%
	501 ml - 1000 ml	[D]9.7%	4.9%	4.0%	[A]3.5%
	1001 ml - 3l	2.8%	2.2%	1.2%	0.6%
	more than 3l	1.4%	0.0%	0.4%	1.2%
Preference for energy drinks labeled zero or sugar free	Total respondents	72	183	253	172
	YES	36.1%	37.7%	41.1%	43.0%
	NO	63.9%	62.3%	58.9%	57.0%
Average weekly consumption of energy drinks labeled zero or sugar free	Total respondents	72	183	253	172
	0ml	58.3%	56.3%	56.1%	64.5%
	1ml - 500ml	27.8%	34.4%	34.8%	26.7%
	501ml - 1000ml	8.3%	7.7%	5.5%	4.7%
	1001ml - 3l	5.6%	1.6%	2.4%	3.5%
	more than 3l	0.0%	0.0%	1.2%	0.6%

[A]The value significantly differs to the value of group A.
[B]The value significantly differs to the value of group B.
[C]The value significantly differs to the value of group C.
[D]The value significantly differs to the value of group D.
Source: Own.

Discussion

The results confirm that the younger generation (Generation Z) consumes energy drinks more frequently than Generation Y, a fact which is consistent with previous studies[1,3]. However, preferences for organic and sugar-free options are lower than would be expected, given the increasing emphasis on healthy living in the population. Whereas the theory suggests[7,8,11] that increased education and awareness of health risks lead to reduced consumption, the results show that even university-educated individuals consume energy drinks relatively frequently, although more on an occasional basis.

Implications

The findings of this study can be used by energy drink manufacturers and creators of health policy. Manufacturers can better target their marketing campaigns to groups with a higher preference for healthier alternatives. At the same time, educational campaigns aimed at raising awareness of health risks should be strengthened. The results

may also be useful for public institutions focused on regulating the sale of these products, especially in the setting of schools and sports centres.

Limits

The main limitation of this study is the fact that the data was obtained through a questionnaire survey, which is dependent on the subjective perceptions of the respondents. Another limitation is the focus only on the Czech Republic, which limits the possibility of generalising the results to other geographic areas. A possible bias may also have arisen from a sample that included only people from the Czech National Panel.

Directions for future research

Further research should focus on a more detailed analysis of consumer motivations for choosing specific types of energy drink, for example using qualitative methods. It would also be beneficial to extend the research to include other age groups and to make international comparisons. Analysis of the impact of marketing strategies on consumer preferences is also an important direction for future studies, especially in view of the growing trend towards sustainable products.

Acknowledgement

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MATERIALS ENGINEERING

FREEZE-THAW DURABILITY OF CEMENT MORTARS WITH CO-COMBUSTION MUNICIPAL WASTE ASH

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Abstract

The aim of this research was to investigate the possible use of ash produced from the co-combustion of coal with sorted municipal waste and limestone as a material with potential hydraulic properties. The obtained municipal FBC bottom ash (MFBC bottom ash) was treated by grinding in a ball mill. The research focused on the preparation and durability of mixed cement mortars to freeze-thaw. Specifically, the corrosion behavior of mortars prepared with different percentages of cement replacement by MFBC bottom ash (10, 20, 30%) was monitored in the environment of frost, moisture and deicing salts. The results showed that bodies prepared from a mixture of MFBC bottom ash and cement displayed, according to the ČSN EN 72 1326, Z1 standard, better resistance to alternating freezing and thawing both in water and 3% NaCl environments compared to the reference Portland cement. Even with a high water to binder ratio w=0.5, the mixed mortars had an undisturbed or slightly disturbed surface after 100 freeze-thaw cycles. These results are very positive from the point of view of the use of MFBC bottom ash in construction, because data from literature indicate significantly worse results even with a lower substitution of similar ash for cement.

Introduction

In order to reduce CO_2 emissions in the construction industry, it is necessary to investigate new possible admixtures for cement. Coal power plants are gradually being closed down and the combustion of fossil fuels, which produces high amounts of CO_2 emissions, is being abandoned as well. Alternatives, especially to high-temperature fly ash, are increasingly being sought, which could replace it in the future. It is important that admixtures have pozzolanic or latent hydraulic properties and are able to react with cement to form stable and durable hydration products while reducing the % of Portland cement. Industrial waste and energy by-products (CCP) are currently used as common admixtures in cement; blast furnace granulated slag, fly ash or silica fume[1,2]. The possibilities of using less conventional admixtures, such as lower-quality calcined clays, which are deposited in large quantities in landfills in the form of overburden or insufficiently suitable raw materials for the ceramic industry, are being investigated[3]. Other sources of pozzolans can be, e.g. rice husk ash, biomass ash, sewage sludge ash, residues from bauxite production, sugarcane bagasse ash, cement kiln dust, and even municipal solid waste (MSW)[1,4,5,6].

However, in order for admixtures to be suitable for usage in cement, their composition and subsequent effect on mechanical and corrosion properties, including freeze-thaw (FT) resistance, must be investigated in detail, as FT resistance is required for outdoor construction applications. Due to the moisture present, water-soaked mortar or concrete is damaged by freezing due to the conversion of water into ice, which is accompanied by a volume increase of about ca 9%[7]. Another influence on FT resistance is exerted by chemical de-icing agents, typically in the form of de-icing salts. The resistance of concrete to FT can be improved by reducing the water to binder ratio (*w*) or by controlled aeration. The chemical composition and particle size of the system also affect FT resistance[7,8].

The use and FT resistance of MSW ash in construction is currently being investigated in several academic works. For example, Gao et al. found that FT ecological concrete pavement bricks prepared with the addition of municipal solid waste incineration fly ash (MSWIFA) showed high FT resistance[9]. For clay bricks, a positive effect of the addition of municipal waste on FT was attested as well, for example, in the research of Voišnienė et al.[10]. Yan et al. investigated cement-stabilized macadam, which is utilized as a base course material, and found that increasing MSW ash addition has a negative effect on compressive strength and FT (they recommended a maximum ash replacement in the binder of 25%); contrastively, they noted that ash addition results in significant reduction of dry shrinkage deformation[11]. Lu et al. claim that the addition of municipal solid waste incinerator bottom ash (MSWIBA) leads to increased porosity and reduced density during FT cycles, which leads to lower

strengths and FT durability of concrete. However, the authors' observation is not entirely accurate, because with an increasing number of FT cycles (especially above 30 cycles with a temperature minimum of -10 °C and a maximum of +10 °C), according to the results, an increase in strength was noted in almost all concretes containing MSWIBA compared to reference cement[12].

In our work, a set of mortars with cement replacement (10, 20, 30%) by MFBC bottom ash prepared from co-incineration of 60% coal, 30 municipal waste and 10% limestone was prepared and subsequently the corrosion behavior of FT in water or de-icing salts environment was studied according to the standard ČSN EN 73 1326, Z1[13]. The results were compared with a reference Portland cement mortar.

Materials and methods

Raw materials

For the preparation of three mixed mortars, ground MFBC bottom ash (marked LP VRŠ IV) produced by co-incineration of sorted municipal waste with coal and limestone was used, specifically 60% coal (coal mine Vršany, CZ) + 30% municipal waste = plastics, wood, textiles, biomass (OZO Ostrava, CZ) + 10% limestone was burned. After combustion, the ash was ground in an amount of 5 kg of ash in a ball mill OM (Brio Hranice, CZ), speed 45 rpm, milling time 40 min. Furthermore, Portland cement CEM 42.5 R from the Mokrá cement plant (Heidelberg materials, CZ) was used for the preparation of reference bodies. Tap water at laboratory temperature and three different fractions of standardized sand in a ratio of 1:1:1 were used to mix the mortars so that a smooth granulometric curve was maintained (grain sizes according to EN 196-1)[14].

Figure 1. Photographs of sorted municipal waste (left), burned MFBC bottom ash (center), and ground MFBC bottom ash LP VRŠ IV (right)

The phase composition (XRD), oxide composition (XRF) and particle size distribution (PSD) of the raw materials are given in the following Tabs. I-IV. XRD was measured on an X'Pert3 powder diffractometer (PANanalytical, NL) with Rietveld method evaluation using HighScore Plus 5 software (PANanalytical, NL). Amorphous content was determined with an internal ZnO standard. XRF was measured on a Performix X-ray spectrometer (Thermo Scientific ARL, CH), evaluated using UNIQUANT software. PSD was measured with a Bettersizer ST laser particle size analyzer (Dandong Bettersize Instruments, CN).

Table I
LP VRŠ IV phase composition, XRD [wt.%]

Material	Amorph. phase	Quartz	Mullite	Anhydrite	Lime	Hematite	Portlandite	Anatase
LP VRŠ IV	60	23	6	4	3	2	1	1

Table II
Cement phase composition, XRD [wt.%]

Material	Amorph. phase	Hatrurite	Larnite	Brownmillerite	Calcite	Portlandite	Gypsum	Bassanite
CEM	23	47	16	5	4	2	2	1

Table III
Oxide composition, XRF [wt.%]

Material	Al_2O_3	SiO_2	CaO	SO_3	TiO_2	Fe_2O_3	MgO	K_2O	Others
LP VRŠ IV	28.3	52.2	7.7	1.5	1.6	5.0	1.0	1.9	0.8
CEM	4.1	17.6	67.8	3.8	0.3	3.4	1.5	0.8	0.7

Table IV
Particle size distribution quantiles [μm]

Material	D10	D50	D90
LP VRŠ IV	1.41	11.06	67.77
CEM	2.19	13.45	41.69

Preparation of samples

A total number of 4 mortar samples were prepared, one cement reference and three mixed mortars with increasing replacement of MFBC bottom ash according to Tab. V. The mortars were prepared with 3 parts of silica sand fractions and one part of binder with a constant water to binder ratio w=0.5. Mixing in a laboratory mixer took a total of 3 minutes. Immediately after mixing, cylindrical bodies were formed from the mixture using polypropylene tubes with a diameter of 100 mm with a minimum mortar height of 50 mm. After proper vibration (2 min.), the bodies were stored in a humid environment of a humidity chamber (Beton System, CZ, RH>95%) for 28 days to ensure sufficient strength before FT cycling.

Table V
Composition of mortars

Mixture	Water to binder ratio (*w*)	Cement [g]	LP VRŠ IV [g]	Sand fractions [g]
LP VRŠ IV 10%	0.5	360	40	3*400
LP VRŠ IV 20%	0.5	320	80	3*400
LP VRŠ IV 30%	0.5	280	120	3*400
CEM	0.5	400	0	3*400

Freeze-thaw method

After 28 days of curing in the humidity chamber, the surface of the specimens was cleaned and then, the surface was covered with water for 24 hours. Subsequently, tap water or a 3% NaCl solution (simulation of the chemical de-icing agent) was poured onto the surface of the samples to a height of about 20 mm. The prepared samples were placed in a Memmert CTC256 (Memmert, DE) FT test chamber and automatic cycling was performed according to ČSN 73 1326, Z1 (method C)[13]. The temperature alternated from -18±2°C to 5±2°C with a residence time of 3 hours at each temperature extreme. At the end of each of the 25 FT cycles, the surface debris was collected, filtered, dried in a drying oven to constant weight and weighed. The amount of surface waste was recorded together with a visual assessment of the surface condition of the bodies. The respective surface solution was replaced with a new one and cycling continued. Cycling was carried out until 100 completed FT cycles. The evaluation was carried out according to the standard ČSN 73 1326, Z1, which states that up to 50 $g.m^{-2}$ the surface is undisturbed, up to 500 $g.m^{-2}$ the surface is slightly undisturbed, up to 1000 $g.m^{-2}$ the surface is disturbed, up to 3000 $g.m^{-2}$ the surface is severely disturbed and above 3000 $g.m^{-2}$ the surface is crumbled[13].

Results and Discussion

FT H_2O

Figure 2 shows the amount of cumulative surface waste after FT cycling for cement and mixed mortars in H_2O environment. It may be seen that the amount of waste generally increases with the increase in the number of FT cycles in water for all mortars. The results, obtained according to the ČSN EN 72 1326, Z1, showed that the resistance of mortars to FT increases with the increasing amount of replacement of MFBC bottom ash for cement. Although the waste gradually increases with freezing, the LP VRŠ 20% and LP VRŠ 30% mortars displayed undisturbed surface according to the standard even after 100 cycles with a waste amount of up to 50 $g.m^{-2}$. The LP VRŠ 10% mortar had 174 $g.m^{-2}$ after 100 cycles corresponding to a slightly disturbed surface. In contrast, the reference CEM mortar displayed the largest surface waste of 400 $g.m^{-2}$ after 100 cycles. A similarly positive effect of MSW ash addition on FT was found, for example, in the research of Voišnienė et. al. and Gao et al.[9,10].

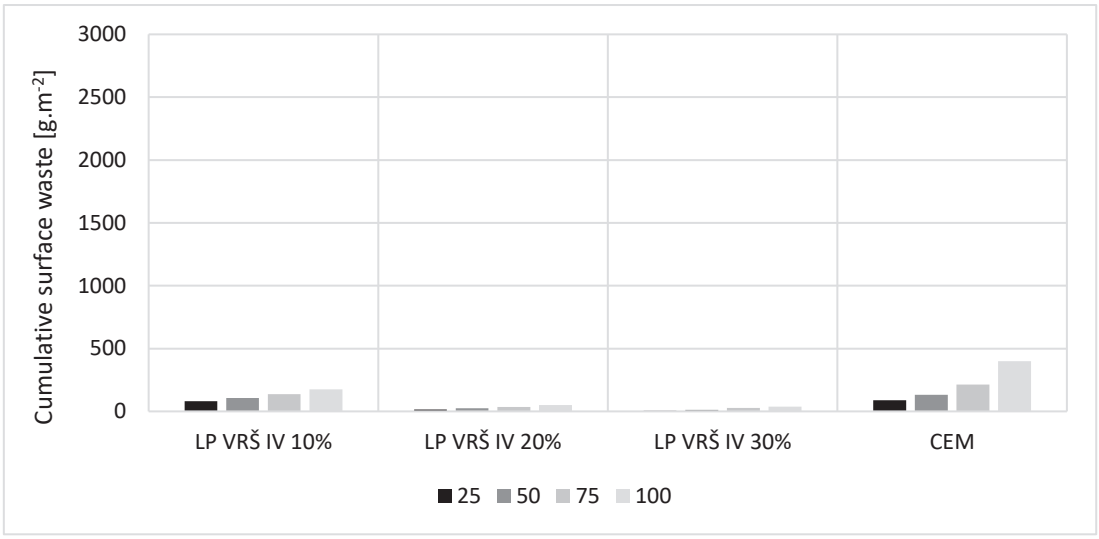

Figure 2. Cumulative surface waste with FT cycling after 25, 50, 75 and 100 cycles in H_2O

Photographs of the surfaces in Figure 3 after 100 FT cycles in H_2O show that for LP VRŠ 30% the surface was still smooth in character with a few peeled surface scales. For mortars LP VRŠ 10% and LP VRŠ 20% a greater surface disturbance can be seen. From the photograph of the cement reference mortar CEM large deeply peeled parts can be seen especially on the edges of the sample. The optical assessment corresponds to the gravimetric results.

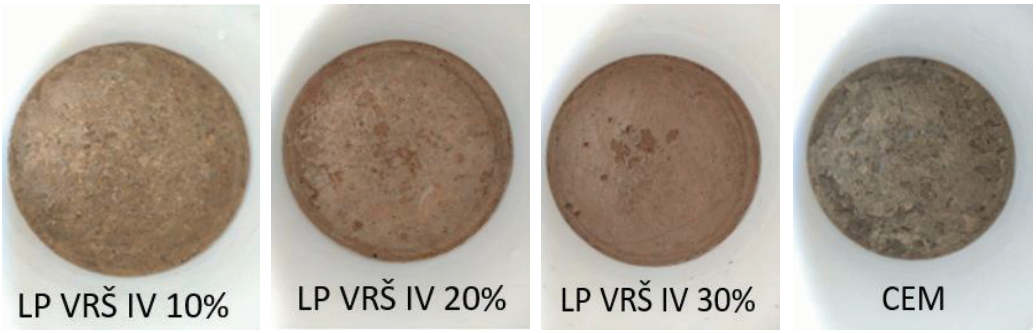

Figure 3. Photos of surfaces after 100 FT cycles in H_2O

FT NaCl

The following graph in Figure 4 shows the amount of surface waste after FT cycling of mortars in 3% NaCl solution. It can be seen that the amount of waste (as in H_2O environment) increases with the FT cycling for all mortars. Furthermore, it can be observed that the resistance in de-icing salt environment is significantly lower than in H_2O. The results, obtained according to the ČSN EN 72 1326, Z1, again showed that adding MFBC bottom ash to cement increases FT resistance in the NaCl environment. The difference between LP VRŠ 10%, LP VRŠ 20% and LP VRŠ 30% is not as conspicuous in the case of H_2O environment, but a significantly higher resistance of all mixed mortars compared to the reference CEM is still noticeable. Mortars LP VRŠ 10%, LP VRŠ 20% and LP VRŠ 30% had a strongly disturbed surface after 100 FT cycles (i.e. over 1000 $g.m^{-2}$), while the amount of waste was 1429 $g.m^{-2}$ for LP VRŠ 10%, 1604 $g.m^{-2}$ for LP VRŠ 20% and 1133 $g.m^{-2}$ for LP VRŠ 30%. In contrast, the reference cement mortar exceeded the 3000 $g.m^{-2}$ crumbled surface limit after 75 FT cycles (specifically 4610 $g.m^{-2}$ after 75 cycles and 7054 $g.m^{-2}$ after 100 cycles). The CEM waste after 100 cycles was therefore almost seven times higher than that of the most resistant sample LP VRŠ 30%. Comparable results for cement with MSW ash addition subjected to FT in the NaCl environment were not attested in literature.

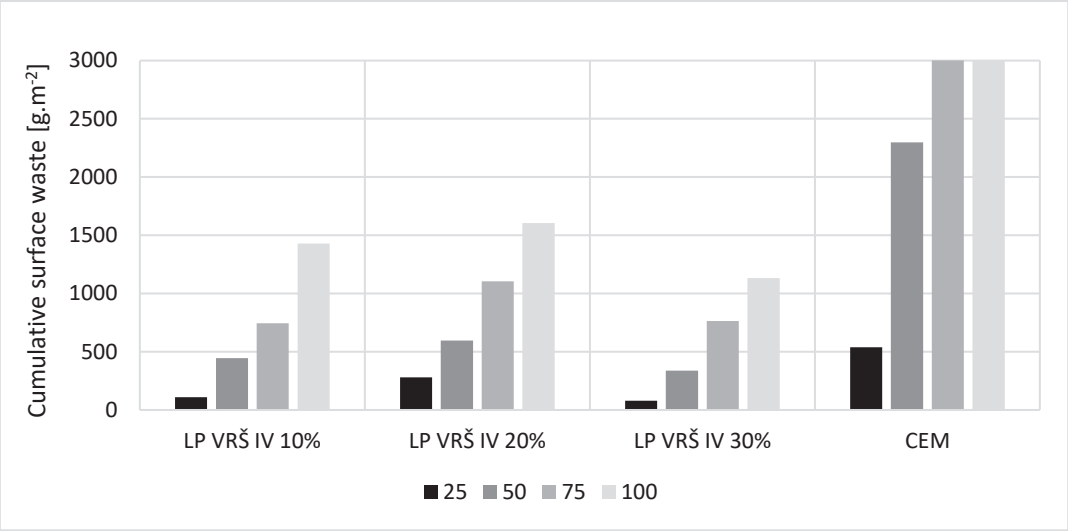

Figure 4. Cumulative surface waste with FT cycling after 25, 50, 75 and 100 cycles in 3% NaCl

Following photographs of the surfaces after 100 FT cycles in 3% NaCl in Figure 5, show that a similar degree of surface damage is visible in the mortars LP VRŠ 10%, LP VRŠ 20% and LP VRŠ 30%, with the upper layer still recognizable after mixing. However, from the photograph of the mortar CEM it is evident that the entire surface of the sample was peeled off during FT. The optical assessment again corresponds to the gravimetric results.

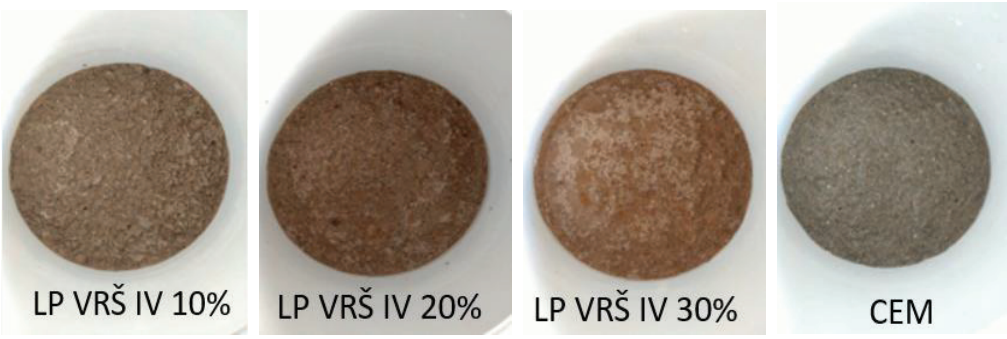

Figure 5. Photos of surfaces after 100 FT cycles in 3% NaCl

Conclusion

In general, it can be concluded that with an increasing number of freezing and thawing cycles, the surface damage increases as well as the cumulative amount of waste after cycling. Bodies prepared from a mixture of LP Vršany fly ash and cement displayed better results in terms of resistance to alternating freezing and thawing in water and 3% NaCl environments than the reference CEM. Although the mortars were mixed with a high water coefficient w=0.5, the mixed mortars showed an undisturbed or slightly disturbed surface due to the presence of water after 100 freezing cycles. The effect of a 3% NaCl solution had a negative effect on the resistance of the mortars and the mixed slurries showed a strongly disturbed surface according to the ČSN EN 72 1326, Z1. An increase in resistance could be achieved, for example, by reducing the water coefficient or using aeration additives. This result can be considered very positive in terms of data for the use of MSW fly ash in construction.

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BIOMASS ASH: A STUDY OF ITS LEACHABILITY

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Abstract

In recent years, the energy sector has been preparing for a transition from coal combustion to purely ecological green energy sources. This brings changes that have and will have a significant impact on the construction industry. One of these green energy sources is biomass (BMA). Biomass ashes generally have a high content of chlorides, sulphates and alkalis, which complicates their use in the construction industry. From a legislative perspective, BMA ash is classified as waste.
This study focuses on the leachability of 51 BMA ash samples from six locations in the Czech Republic, produced from grate and fluidized bed combustion of biomass and co-combustion of biomass with coal. The main emphasis was placed on the leachability of heavy metals and other potentially dangerous chemical substances. Simultaneously, pH, electrical conductivity (EC), total dissolved solids (TDS), soluble inorganic salts (SIS), and dissolved organic carbon (DOC) were measured. It was found that most of the BMA ashes exceed the limits for TDS, chlorides, fluorides, sulphates, chromium, molybdenum, and selenium. Additionally, most of the samples showed excessively high pH and electrical conductivity.

Introduction

Biomass combustion is the most traditional way of obtaining energy, and wood was the most traditional fuel until the Industrial Revolution. With the increasing energy demands of society, it was necessary to switch to an alternative fuel, which was coal. Although society's energy demands continue to rise, there is a greater emphasis on sustainable energy production. Currently, we cannot replace all energy sources that derive energy from coal combustion with "green energy." Therefore, there is currently a large-scale transition to biomass combustion or co-combustion. The CO2 emissions generated by burning biomass are roughly equivalent to the CO2 absorbed by the plants burned during their lifetime[1]. Because of this, biomass combustion can be considered a carbon-neutral energy source.[2,3,4]
Biomass is a natural material. Its origin can be either animal or, more commonly, plant. It is one of the most diverse sources of renewable energy and can be used to generate electricity and heat. The properties of biomass are crucial for its subsequent use. Like traditional fuel types, biomass also has basic indicators of its quality. These include humidity content, chemical composition of the fuel, ash content, volatile matter content, and calorific value[5]. The composition of biomass and its ash depends not only on the type of vegetation it comes from but also on subsequent storage and processing.[1,6]
There are many types of biomass combustion, and several types of ash are produced as a final product, which can be divided into two main groups – fly ash and bottom ash. The most common method is grate combustion[7]. Another method is fluidized bed combustion. This is a more modern method than grate combustion. Due to combustion at lower temperatures, it also reduces the emissions of NO_x and SO_x emitted during combustion [4,6,7]. Another option is biomass co-combustion with fossil fuels such as coal. This practice is becoming increasingly common in the energy sector and provides an efficient and transitional solution[1,8,9].
Ash can be added to concrete mixes for various purposes. Currently, the use of ash is permitted by European legislation only if it is fly ash from coal combustion or co-combustion[10]. The main problem encountered when using BMA ash in civil engineering is the instability of its composition. The main problems include high alkali and chloride content, which can have long-term effects on concrete corrosion[2,10]. Nevertheless, there is potential for utilizing ash produced from biomass combustion or co-combustion in the construction industry, which would make this product a valuable resource instead of waste, which is how biomass ash is currently classified under legislation. This is precisely the focus of this work, which aims to compare the leachability of biomass ash from the perspective of waste intended for landfilling and from the perspective of its potential use in the construction industry, by Technical Conditions 93: Design and Construction of Road Structures Using Fly Ash and Bottom Ash[11].

Materials and methods

Ash samples collected between 2021 and 2024 at six locations in the Czech Republic were selected as input materials for the analyses. These locations represent different types of combustion technologies – grate combustion of biomass, grate co-combustion of biomass with coal, and fluidised bed co-combustion (FBC) of coal with biomass. The combusted materials were bark, mixtures of hay and straw, wood chips, sawdust and coal. The output of these processes was bottom ash **(BA)**, fly ash **(FA)** or a combination of both **(FA+BA)**. Three representative samples were selected from each location according to the type of resulting ash. A total of 23 samples were analysed, and their specifications are described in Table I.

Table I: Overview of analysed samples

label	method of combustion	combusted material	type of ash	location
LBP_FA LBP_BA	grate combustion	bark	FA BA	Lenzing Biocel Paskov a.s **(LBP)**
JH_FA+BA	grate combustion	hay and straw in	FA+BA	Energeticke centrum s.r.o. Jindřichův Hradec **(JH)**
CZTL_BA	grate co-combustion	woodchips + coal	BA	CZT Litoměřice **(CZTL)**
CZTM_BA	grate co-combustion	woodchips and sawdust + coal	BA	CZT Mimoň **(CZTM)**
HO_FA HO_BA	FBC co-combustion	80 % coal + 20 % biomass	FA BA	power plant Hodonín **(HO)**
PO_FA PO_BA	FBC co-combustion	80 % coal + 20 % biomass	FA BA	power plant Poříčí **(PO)**

All samples were evaluated for environmental safety using leachability verification tests according to the standard EN 12457-4[12]. The sample was prepared in a ratio of material to distilled water of 1:10. Contrary to the standard, solidified samples were not used, but powder samples, i.e. 100 g of powdered material was weighed into plastic containers together with 1000 ml of distilled water. The container was sealed and placed in an overhead shaker for 24±0.5 hours, after which each mixture was filtered.

To evaluate the leachability of dangerous chemical substances, the strictest values were selected from TP ASVEP[13], TP 93[11] and Decree 273/2021 Sb.[14] with leachability classes I and IIa. Class I is defined for inert material – landfill S-IO (inert). Class IIa is defined for other waste S-OO1. The binding limits are set by Decree 273/2021 Sb., which specifies the maximum permissible values of dangerous chemical substances released in the case of waste disposal in landfills, and TP 93 in the case of material use for the design and construction of roads using fly ash and bottom ash. The TP ASVEP limits can only be considered as recommended values. Table II shows the limit values for leached substances. The colour-coded values in Tables III and IV do not meet the relevant evaluation criteria, and their colour coding corresponds to the header of Table II.

Table II: Limit values for leachates according to the relevant criteria, leachate values given in mg/l, electrical conductivity in $mS.m^{-1}$.

parametr	class I	class IIa	TP ASVEP	TP 93	parametr	class I	class IIa	TP ASVEP	TP 93
pH	≥6	-	6-9	-	Co	-	-	0,003	0,1
EC	-	-	125	-	Cd	0,004	0,5	0,0005	0,005
TDS	400	8000	-	-	Cr	0,05	7	0,05	0,1
SIS	-	-	-	-	Cu	0,2	10	0,014	1
DOC	50	80	10	-	Hg	0,001	0,2	0,0002	0,005
Cl^-	80	1500	-	-	Mo	0,05	3	0,005	-
F^-	1	30	-	-	Ni	0,04	4	0,02	0,1
SO_x	100	3000	-	-	Pb	0,05	5	0,005	0,1
Al	-	-	0,2	-	Sb	0,006	0,5	0,005	-
Ag	-	-	-	0,1	Se	0,01	0,7	0,01	0,05
As	0,05	2,5	0,01	0,1	Sn	-	-	0,025	1
B	-	-	0,3	-	V	-	-	0,018	0,2
Ba	2	30	0,05	1	Zn	0,4	20	0,15	3

Be	-	-	-	0,005	

The pH, electrical conductivity (EC), total dissolved solids (TDS) at 105 °C, soluble inorganic salts (SIS) and dissolved organic carbon (DOC) were measured in all samples. Trace elements were also measured using ICP: antimony, arsenic, barium, beryllium, boron, tin, aluminium, cadmium, chromium, cobalt, lead, copper, molybdenum, nickel, mercury, selenium, silver, vanadium and zinc. Finally, chlorides, fluorides and sulphates were monitored using ion liquid chromatography.

Results and discussion

Table III shows the measured values for pH, electrical conductivity, total dissolved solids, soluble inorganic salts and dissolved organic carbon for all samples. Colour coded values exceed limits according to the header of Table II. The measured values show that most samples exceed the values for total dissolved solids according to Decree 273/2021 Sb. class I (red font), regardless of the type of combustion. In samples from the grate combustion of pure biomass LBP and JH, this parameter is also exceeded according to class IIa of Decree 273/2021 Sb. (red highlighting). Furthermore, most samples from grate combustion exceed the values for pH and electrical conductivity according to TP ASVEP (blue highlighting). Some samples from this type of combustion and locations exceed the dissolved organic carbon parameter.

Based on these data, it is clear that none of the fly and the bottom ash from biomass combustion or co-combustion complies with Decree 237/2021 Sb. and is therefore not suitable for storage in S-other landfills as other waste S-OO1.

When compared with the results for coal ash[15], the analysed BMA samples, especially those from grate combustion of pure biomass, generally have a higher pH (coal ash pH 7.38 – 8.23), which indicates significant alkalinity, probably caused by a higher CaO content. All samples also show significantly higher electrical conductivity compared to coal ash (241 mS.m-1), which indicates a high degree of leachability of ions contained in the materials, as evidenced by another parameter, TDS, which is exceeded in all samples. When comparing BMA and coal ash (TDS 2220–2430 mg/l), the values for fly ash from grate combustion are visibly higher, up to fivefold higher. In some samples of fly and bottom ash from co-combustion, the values are slightly higher.

Table III: Ash leachability results – pH, EC, TDS, SIS and DOC: leachate values given in mg/l, electrical conductivity in $mS.m^{-1}$.

sample	pH	EC	TDS	SIS	DOC
LBP_FA_1	12.8	1510	7040	6500	5.02
LBP_FA_2	12.8	1760	8160	7580	6.06
LBP_FA_3	12.7	1360	5440	5090	5.54
LBP_BA_1	9.51	622	8240	6510	12.9
LBP_BA_2	8.0	439	5200	4100	17.8
LBP_BA_3	8.13	213	1960	1680	2.12
JH_FA+BA_1	9.96	879	5890	5660	2.54
JH_FA+BA_2	10.5	1440	11400	10700	15
JH_FA+BA_3	10.5	1440	11400	10700	15
CZTL_BA_1	8.29	67.1	504	455	1.9
CZTM_BA_1	8.49	152	1040	962	2.02
HO_FA_1	12.7	997	4190	3840	4.63
HO_FA_2	12.6	908	3990	3690	3.09
HO_FA_3	12.6	831	2830	2820	2.3
HO_BA_1	11.6	91.7	286	220	2.41
HO_BA_2	12.6	931	4340	4060	2.93
HO_BA_3	12.3	391	910	876	3.28
PO_FA_1	9.34	267	2310	1960	2.52
PO_FA_2	12.4	740	2720	2370	3.97
PO_FA_3	12.5	878	3170	2720	3.63
PO_BA_1	11.7	90.5	346	332	2.2
PO_BA_2	12.7	959	4250	3970	2.83
PO_BA_3	11.8	147	406	362	2.51

Table IV shows the results of trace element leachability, where the limit values were exceeded and this exceedance is color coded according to the table header II.
The results show that for most samples, regardless of the type of combustion, the limit for sulphates according to class I (red font) was exceeded. In samples from LBP grate combustion, this limit was also exceeded according to class IIa (red highlighting). In FBC biomass co-combustion, it can be seen that the limit is exceeded more significantly for fly ash than bottom ash.
Most fly ash samples exceeded the limits for chlorides according to class I (red font). Fly ash samples from Jindřichův Hradec (JH) also exceeded this limit according to class IIa (red highlighting). Several fly and bottom ash samples exceeded the limit for fluorides.
Furthermore, most samples did not comply with the molybdenum content, which was not exceeded in only two bottom ash samples. Other elements for which the samples did not meet the requirements were aluminium, boron, barium, mercury, lead, antimony, selenium and vanadium.
Samples from FBC co-combustion of biomass from Hodonín (HO) and Poříčí (PO) exceeded the chromium content limit. Samples from the grate combustion of pure biomass from Energeticke centrum s.r.o. Jindřichův Hradec exceeded the arsenic content limit.
When comparing BMA samples with coal ash[15], the limits for the same trace elements (As, B, Ba, Mo, Se, V and Al for fly ash) were exceeded. BMA samples from grate combustion show a higher sulphate content.

In general, according to Decree 273/2021 Sb., it can be stated that:
most input materials, regardless of the type of combustion and resulting ash, do not meet the definition of inert material (class I) in terms of total dissolved solids content. Samples from grate combustion of pure biomass from Lenzing Biocel Paskov a.s. and Energeticke centrum s.r.o. Jindřichův Hradec do not meet the definition of other waste (class IIa) in terms of total dissolved solids content. Furthermore, most samples, regardless of the type of combustion, do not meet the definition of inert material (class I) in terms of chloride, fluoride, sulphate, molybdenum and selenium content. Fly ash has worse results than bottom ash. Samples from FBC co-combustion from Hodonín and Poříčí do not comply in terms of chromium content. Samples from the grate combustion of pure biomass from Energeticke centrum s.r.o. Jindřichův Hradec have a higher arsenic content. Some samples from the grate combustion of pure biomass from the Lenzing Biocel Paskov a.s. and Energeticke centrum s.r.o. Jindřichův Hradec sites do not comply with the definition of other waste (class IIa) in terms of chloride and sulphate content.
According to Decree 273/2021 Sb., only bottom ash samples from FBC co-combustion of biomass with coal from the Hodonín and Poříčí would qualify as waste S-OO1 for landfilling. No sample would meet the requirements of a further evaluation according to the technical conditions of TP ASVEP, which are stricter than Decree 273/2021 Sb.
In terms of use in the construction industry, according to TP 93, the samples meet the parameters and are suitable materials. The exceptions are samples CZTL and CZTM from co-combustion, which exceed the limit for selenium and vanadium. One bottom ash sample from Hodonín and fly ash samples from Poříčí, i.e. samples from FBC co-combustion, exceed the limit for chromium.
It should be noted that the leachate samples were not prepared exactly by Decree 273/2021 Sb., where the leachate is made from a solidified sample, but a procedure was chosen to obtain the leachate directly from a powder sample. This procedure is the least favourable in terms of leachability results, but it shows the worst possible leachability values for the materials.

Table IV: Ash leachability results – trace elements: leachate values given in mg/l

sample	Cl^-	F^-	SO_x	Al	As	B	Ba	Cr	Hg	Mo	Pb	Sb	Se	V
LBP_FA_1	117	0.72	2080	<0.010	<0.001	0.184	0.23	0.011	0.00006	0.117	<0.001	<0.0010	0.007	<0.001
LBP_FA_2	145	<1.000	2780	<0.020	<0.002	0.317	0.217	0.015	0.00025	0.15	0.005	<0.0010	0.010	<0.001
LBP_FA_3	50	0.852	1710	<0.010	<0.001	0.238	0.218	0.012	0.00027	0.246	0.001	<0.0010	0.005	<0.001
LBP_BA_1	3.4	<0.200	5160	<0.010	<0.001	0.113	0.039	0.004	<0.0000	0.003	<0.001	0.0028	<0.005	<0.001
LBP_BA_2	1.31	<0.200	3320	<0.010	0.002	0.214	0.041	0.008	<0.0000	0.02	<0.001	0.0022	0.011	0.002
LBP_BA_3	1.06	0.232	1320	<0.010	0.002	0.155	0.043	0.003	<0.0000	0.008	<0.001	0.0015	0.006	0.002
JH_FA+BA_1	1310	<0.400	1140	<0.010	0.057	0.265	0.018	0.017	<0.0000	0.145	<0.001	0.0015	0.006	0.013
JH_FA+BA_2	1790	<0.500	2440	<0.010	0.051	0.55	0.007	0.004	0.00002	0.23	<0.001	0.0015	0.009	0.022
JH_FA+BA_3	1790	<0.500	2440	<0.010	0.051	0.55	0.007	0.004	0.00002	0.23	<0.001	0.0015	0.009	0.022
CZTL_BA_1	<1.00	1.36	314	0.016	0.031	4.22	0.076	0.001	<0.0000	0.024	<0.001	0.0011	0.080	0.21
CZTM_BA_1	<1.00	3.62	703	0.428	0.047	2.51	0.06	0.003	<0.0000	0.171	<0.001	0.0017	0.290	0.248
HO_FA_1	139	0.888	1280	<0.010	<0.001	0.068	0.189	0.057	0.00003	0.079	<0.001	<0.0010	0.010	<0.001
HO_FA_2	73.4	0.816	1580	<0.010	<0.001	<0.050	0.262	0.124	0.00001	0.086	<0.001	<0.0010	0.011	0.002
HO_FA_3	166	1.36	533	0.018	<0.001	<0.050	0.308	0.098	0.00002	0.084	0.008	<0.0010	0.005	<0.001
HO_BA_1	<1.00	<0.200	20.1	2.07	<0.001	0.185	0.188	0.003	0.00001	0.005	<0.001	0.0027	<0.005	0.011
HO_BA_2	<1.20	<0.400	1630	<0.010	<0.001	0.092	0.181	0.004	0.00006	0.048	<0.001	<0.0010	<0.005	<0.001
HO_BA_3	1.83	<0.200	<5.00	0.461	<0.001	<0.020	0.16	0.007	<0.0000	0.007	<0.001	0.0025	<0.005	0.005
PO_FA_1	181	0.601	1160	0.12	0.001	1.76	0.387	0.152	0.00002	0.041	<0.001	0.0052	0.012	0.016
PO_FA_2	5.8	3.27	864	0.011	<0.001	<0.050	0.533	0.17	0.00027	0.123	<0.001	<0.0010	0.021	0.008
PO_FA_3	128	0.836	901	<0.010	<0.001	<0.050	0.225	0.185	0.00001	0.104	0.003	<0.0010	0.007	<0.001
PO_BA_1	1.08	<0.200	11.4	0.669	<0.001	0.242	0.102	0.003	0.00001	0.006	<0.001	0.0043	<0.005	0.013
PO_BA_2	<1.20	<0.400	1700	<0.010	<0.001	<0.050	0.179	0.016	0.00002	0.045	<0.001	<0.0010	<0.005	<0.001
PO_BA_3	<1.00	<0.200	8.57	0.862	<0.001	0.198	0.123	0.004	<0.0000	0.008	<0.001	0.0039	<0.005	0.009

Conclusion

Based on the analyses performed, it can be stated that ash samples from biomass co-combustion show better results in terms of leachability compared to ash from biomass grate combustion. However, none of these ashes meet the conditions set by the waste decree for landfilling under Czech legislation. Nevertheless, it can be assumed that ash in a solidified form could comply with the legislation. The results obtained also indicate the potential for using ash from combustion and co-combustion of biomass in the construction industry, as stated in TP 93: Design and Construction of Road Structures Using Fly Ash and Bottom Ash, and could represent an environmentally and economically advantageous solution for their further material use.

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INFLUENCE OF THE ADDITION OF MUNICIPAL WASTE ASH ON THE CARBONATION IN CEMENT MORTARS

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Abstract

The effect of fly ash and bottom ash from the co-combustion of selected municipal waste with coal and limestone (MFBC ash) on the carbonation of mortar specimens were investigated. The reference samples were specimens containing standardized fly ash from a power plant and specimens containing Portland cement (PC) without admixtures. Mortars with binder, standardized sand and water to binder ratio of 0.35 were prepared. Carbonation of the mortar specimens took place in an incubator under conditions of 3% CO_2, a temperature of 30°C, and humidity of 60-65%. The depth of carbonation was measured directly using the phenolphthalein test (PT), and indirectly through compressive strength measurements. The samples were tested after 7, 14, and 28 days. The results showed that mortars with MFBC ash exhibited faster carbonation than the reference mortar with PC. The carbonation rate of mortars with MFBC ash did not exceed the carbonation rate of cement with standardized fly ash. In the mortars with ashes, carbonation was slowest in the sample of fly MFBC ash. The results from the compressive strength measurements did not conclusively demonstrate the effect of carbonation on the strength of the specimens.

Introduction

Carbonation is a chemical reaction in which atmospheric CO_2 reacts with calcium ions (Ca^{2+}) present in the cement binder. The reaction occurs mainly due to diffusion of CO_2 into the pore structure of the cement binder. Carbonation is described by three main phases: (i) dissolution of the portlandite, (ii) absorption of CO_2 and formation of carbonate ions, and (iii) precipitation of $CaCO_3$[1]. Carbonation results in the formation of calcium carbonate ($CaCO_3$), in various polymorphic forms such as calcite, vaterite, aragonite. Portlandite is the main phase in the cement binder that predominantly undergoes carbonation. Carbonation proceeds according to the following equation (1):

$$\mathbf{Ca(OH)_2 + CO_2 \rightarrow CaCO_3 + H_2O} \quad (1)^2$$

Another phase that undergoes carbonation on a smaller scale is the C-S-H phase, reacting with CO_2 according to the following reaction (2):

$$\mathbf{(CaO)\_x(SiO_2)(H_2O)\_z + xCO_2 \rightarrow xCaCO_3 + SiO_2\text{-}(H_2O)\_t + (z\text{-}t)H_2O} \quad (2)^3$$

Other minority phases in the cement binder, such as ettringite or non-hydrated clinker minerals (C3S, C2S etc.) may also undergo carbonation[4, 5].

The carbonation process is strongly dependent on both the environmental conditions and the composition of the cement binder. In terms of environmental conditions, the influencing factors are relative humidity, temperature and CO_2 concentration in the environment. The optimum humidity for carbonation is between 50-70 %. Lower humidity limits the dissolution of reactants, while higher humidity inhibits the diffusion of CO_2[6, 7]. Higher temperatures accelerate the chemical reactions of carbonation and promote diffusion of ions, but also reduce the solubility of CO_2 in water[6, 8]. At low concentrations, partial carbonation occurs, whereas at high concentrations (e.g., 100% CO_2), complete decalcification of the C-S-H phase can occur[9, 10]. In terms of cement binder type, in general, blended cements with the addition of pozzolans accelerate carbonation. The aluminosilicate component of the admixtures reacts with the resulting portlandite to form the C-S-H phase, thereby lowering the pH. The lower Ca:Si ratio then causes the sample to carbonate faster[11, 12]. The free CaO content is particularly important for fly ash. A higher amount increases the possibility of reaction with CO_2 to form $CaCO_3$, which reduces the porosity of the cement mixture and thus slows down carbonation[13].

Carbonation of cementitious binders brings with it both positive and negative impacts. The most significant problem of carbonation is the pH drop in the structure of reinforced concrete structures, which disrupts the passivation layer on the steel surface and leads to its corrosion[14, 15]. Among the positive phenomena can be included the reduction of the porosity of the cement binder due to the formation of $CaCO_3$, which can lead to higher strengths and hardnesses[16]. Last but not least, carbonation is seen as a way of CO_2 sequestration - or the permanent capture of CO_2 back into the solid phase[17].
The aim of the study was to investigate the effect of the addition of fly ash from the co-firing of sorted municipal waste with coal and limestone on the carbonation of mortar bodies. The degree of carbonation of the mortar bodies was evaluated by phenolphthalein test (PT). At the same time, the strengths of the mortar bodies were measured.

Materials and methods

Imput raw materials for preparing mortars were Portland cement CEM 42,5 R (PC) (Českomoravský cement, plant Mokrá), fluidised bottom ash (MFBC BA) and fluidised fly ash (MFBC FA) from co-combustion of municipal waste with coal and limestone (Experimental centrum Juliska, CTU Prague) and fly ash - FA (power plant Tušimice). All materials were sourced from the Czech Republic. Table I presents chemical composition, density, specific surface area and mean particle size of imput raw materials.

Table I
Chemical composition, density, specific surface area and mean particle size of input raw materials

XRF	PC	MFBC BA	MFBC FA	FA
SiO_2	17.6	52.2	43.0	51.3
Al_2O_3	4.1	28.3	24.1	33.2
Fe_2O_3	3.4	5.0	4.1	8.3
TiO_2	0.3	1.6	1.4	1.1
CaO	67.7	7.7	21.5	1.6
MgO	1.5	1.0	1.2	1.0
K_2O	0.8	1.9	1.7	1.8
SO_3	3.8	1.5	2.0	0.5
Other	0.8	0.8	1.1	1.2
Density [kg/m^3]	3412.0	2816.0	2766.0	2525.0
Specific Surface area [m^2/kg]	316.0	1382.3	1561.2	471.0
Mean Particle Size d50 [µm]	13.5	11.1	8.8	10.2

The measurement of chemical composition was performed on a sequential wave-dispersive X-ray spectrometer ARL 9400 XP with a Rh lamp. The evaluation was carried out in the Winxrf program using the UNIQUANT 4 software, where the spectral lines of the material were measured and analyzed without a standard, and the output was an elemental analysis in oxide form. The density measurement of all materials was carried out on a helium pycnometer (Pycnomatic ATC EVO) with accessories and temperature range of 14-40 °C. The specific surface of the materials was measured by an electronic Blaine device mod. 1.0210 (Testing Bluhm and Feuerherdt GmbH). The measurement of the particle size of the raw materials was carried out using a laser diffractometer (Dandong Bettersize Instruments Ltd.). X-ray diffraction analysis (XRD) was performed at room temperature on a θ-θ powder diffractometer X'Pert3 Powder (PANanalytical, Netherlands) using the wavelength of CuKα radiation (λ = 1.Qualitative and quantitative analysis was then performed by evaluation in HighScore Plus 4.0 (PANalytical, Netherlands). The amorphous content was determined by the indirect internal standard method. 10 % ZnO was added to the samples. The mineral composition of the materials PC, MFBC BA, MFBC FA, FA is given in Table II and Table III. The next Table IV shows the composition of the mortars.

Table II
Mineral composition of PC, wt. [%]

XRD	PC
Amorph.	29
hatrurite	43
larnite	15
brownmillerite	4
Bassanite	1
C3A	1
calcite	3
portlandite	2
gypsum	2
quartz	traces

Table III
Mineral composition of raw imput materials, wt. [%]

XRD	MFBC BA	MFBC FA	FA
Amorph.	60	52	58
anhydrite	4	4	0
quartz	23	17	10
mullit	6	2	29
calcite	0	10	0
lime	3	13	0
portlandite	1	0	0
hematite	2	1	1
magnetite	0	0	2
anatas	1	1	0

Table IV
Mortar mixtures

Labelled	Binder [part]		Sand [part]	w [to binder part]
	cement	admixture		
PC	1	0	3	0.35
MFBC BA				
MFBC FA	0.7	0.3	3	0.35
FA				

For the carbonation test, mortar prisms with dimensions 40x40x160 mm were created according to EN 196-1. After their production, they were stored for 28 days in a humidity cabinet and then subsequently for 14 days in air under laboratory conditions. After this time, the first PT and the compressive strength of the mortar prism was carried out. Subsequently, the prisms were stored in a CO_2 chamber under conditions of 3% CO_2, 65 ± 5% relative humidity and 30 ± 1 °C. Measurements of carbonation depth using the ftt test and strengths were taken after 7, 14 and 28 days of exposure in the CO_2 chamber. The measurements were carried out as follows:

- Breaking the prism in the middle
- Wetting the transverse fracture of the prism
- Application of Phenolphthalein solution to the transverse fracture of the prism
- Colour change of the ftt solution
    - Pink - pH ≥ 9 - non-carbonated part
    - Colourless - pH ≤ 9 - carbonated part
- Pressure measurement of 2 prism sections in a 40x40 mm press

Results

Table V shows the transverse fractures of mortar prisms treated with Phenolphthalein spray on different test days: 0D - before insertion into the CO_2 chamber; 7D - 7 days in the CO_2 chamber; 14D - 14 days in the CO_2 chamber; 28D - 28 days in the CO_2 chamber. Using image analysis, the percentage of carbonated area was evaluated in relation to the total area, which is elaborated and depicted in the graph (Figure 1a). The PT showed that all mortar prisms undergo carbonation in the CO_2 chamber environment, with the slowest carbonation observed in the unmodified samples, which is in agreement with the literature [11, 12]. In terms of the image analysis and its evaluation, the highest carbonation within the analyzed cross-fracture area after 28 days occurred in the MFBC BA (63.4%) and reference FA (59.8%) specimens. The MFBC FA specimen had the lowest carbonated area value after 28 days of testing at 43.3%. This is probably related to the higher amount of CaO in the admixture of MFBC FA, which is consistent with the findings in the literature [10].

Table V
Carbonated area of mortar mixtures by PT

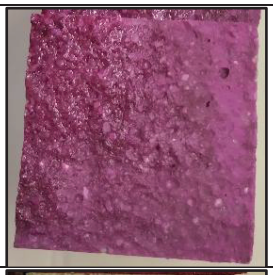
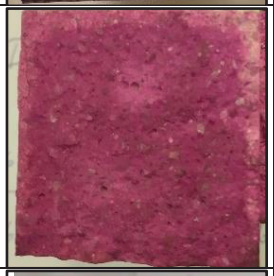
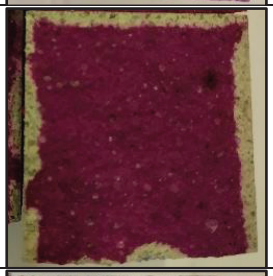
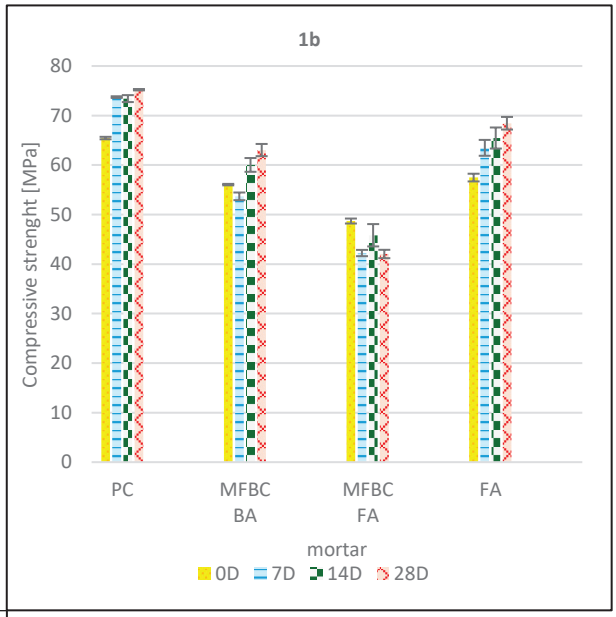
	PC	MFBC BA	MFBC FA	FA
0D				
7D				
14 D				
28 D				

Figure 1b shows the measured values of the compressive strengths of the prisms on different test days: 0D - before insertion into the CO_2 chamber; 7D - 7 days in the CO_2 chamber; 14D - 14 days in the CO_2 chamber; 28D - 28 days in the CO_2 chamber. The highest strengths were recorded for the mortar prepared from PC. On the other hand, the lowest strengths were measured for mortar prepared from MFBC FA, this FA contained a high proportion of CaO and the hydrated sample then probably contained the least C-S-H phase binder. Due to carbonation, the mortar samples from FA, PC, and MFBC BA showed an increase in strengths after 28 days in the CO_2 chamber, specifically by 19.1% for the FA sample, 14.9% for the PC sample, and 12.5% for the MFBC BA sample. The increase in strengths is probably related to the formation of $CaCO_3$ due to the carbonation reaction associated with pore filling and compaction of the structure. A decrease in strengths due to carbonation after 28 days in a CO_2 chamber was observed for sample MFBC FA, by 13.7 %. The cause of the decrease in strengths for this sample could not be determined, but is likely to be related to its phase composition. Further analyses would be required to explain the decrease in strengths.



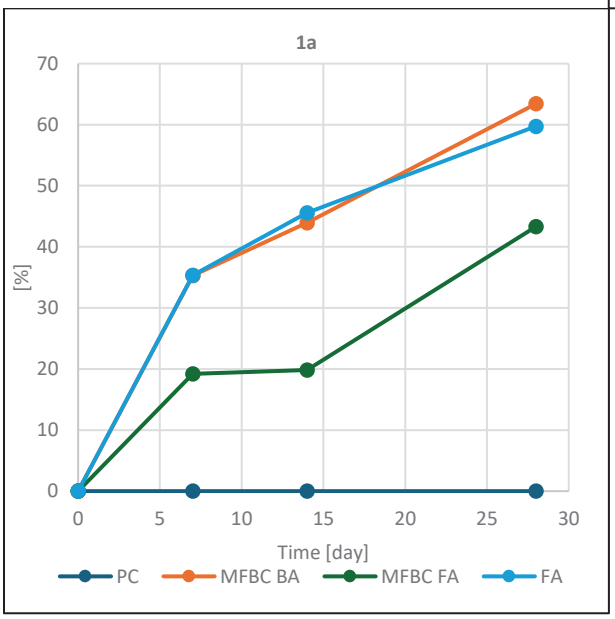


Figure 1a. Carbonated transverse fracture area of mortar prisms over time, measured by PT

Figure 1b. Compressive strengths of mortars at 0, 7, 14 and 28 days of exposure to 3% CO_2 environment

Conclusion:

This work investigated the effect of the addition of fly ash from the co-firing of sorted municipal waste with coal and limestone on the carbonation of mortar bodies. Based on the carbonation of a reference mortar with cement (PC), it was found that all three types of fly ash used accelerate the carbonation process. Fly ashes from co-incineration of municipal waste with coal and limestone (MFBC FA and MFBC BA) had a similar effect on carbonation as reference fly ash (FA). The fly ash mortar with the highest CaO content exhibited the lowest carbonation depth of the samples among the three ash mortars. The increase in strengths due to carbonation of mortar bodies was observed in FA, PC, MFBC BA samples. A decrease in strengths due to carbonation was measured for MFBC FA sample.

Acknowledgement:

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CORROSION RESISTANCE OF 10 425 CSN/ S185 DIN PRESTRESSING STEEL WITH BASALT COATINGS

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Abstract

Corrosion damage to conventional prestressing steel reinforcement stimulated by chloride anions has recently caused a critical reduction in the load-bearing capacity and subsequent collapse of several important bridges and footbridges. The use of suitable protective coatings on the surface of the prestressing reinforcement can ensure a significant extension of the service life of these structures. The paper evaluates the corrosion barrier protection of a coating formed from basalt, classified according to QAPF with a high proportion of forsterite and diopsite when hot-dipping on conventional prestressing reinforcement by evaluating the porosity of the coating and exposures in solutions of HCl and NaCl. The roughness and phase composition of two variants of applied basalt coatings, melted at 1260°C on a preheated steel substrate and surface-applied by plasma spraying technology on a cold substrate using a WSP-H 500 water-stabilized plasma torch, were also evaluated. The differences are particularly evident in the increase in the proportion of amorphous silica phases, which ensure almost zero coating porosity and high adhesion even to the plain surface of the metal substrate.

Introduction

The aim of creating ceramic coatings on steel surfaces is to increase both abrasion and corrosion resistance against moisture and aggresive ions. The corrosion of metallic materials by chloride ions not only causes huge economic losses, but also poses serious safety risks, especially in bridges and footbridges with steel reinforcement[1,2]. Electroplating (galvanic coatings) or cathodic protection is not optimal for use in bridges construction, but ceramic coating by phosphating, boriding and especially oxide ceramics has proven to be effective for concrete structures[3,4,5,6]. Increasing the resistance of the coating to abrasive wear requires, above all, a high surface hardness of the material and high degree of adhesion to the substrate respectively. Most ceramic materials, especially carbides, nitrides, borides or selected oxide compounds, meet the condition of higher hardness than that of low-alloy steels. Only the value of coating adhesion to steel surface is problematic, which depends on several factors. Coatings produced by CVD or PVD technology, which require a vacuum environment, are not suitable for coating large substrates for economic reasons. Thin-film ceramic coatings on large substrates can be produced by thermal or plasma spraying or by bake-in or melt coating. However, coatings prepared in this way tend to have a variable content of unmelted particles and open or closed pores and cracks, which reduces the effectiveness of this form of corrosion protection[7].

The adhesion of coatings have two critical parametres. In the first case, the strength of the ceramic-metal bond depends only on the roughness of the contact surfaces (parameters R_a R_q R_z). An example for the formation of coatings on a polished or roughened substrate surface is demonstrated in Figure 1. A screw substrate with a diameter of 20 mm from the Tira Test 2300 apparatus for tensile strength measurements was placed in a special mould made of ceramic hexagonal boron nitride and coated by plasma spraying using the WSP-H 500 plasmatron developed at IPP CAS Prague. In the case of the polished surface with Ra, Rq, Rz values < 0.06 µm, no melt fixation occurred on a large part of the surface and after placing this specimen in the tensile strength test apparatus, pull-off occurred with a force of only 50 N. From the image of the underside of the spray (Fig.1d), it is clear that no adhesion occurred.

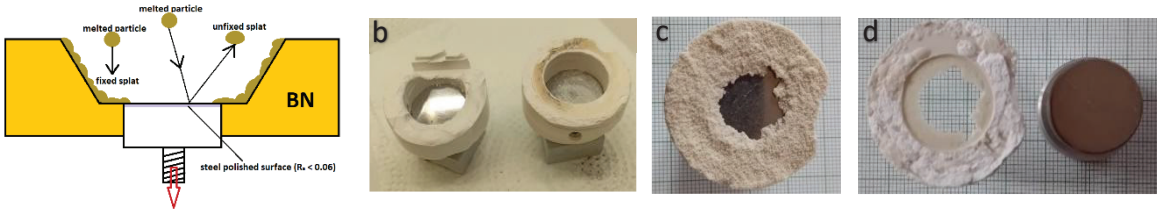
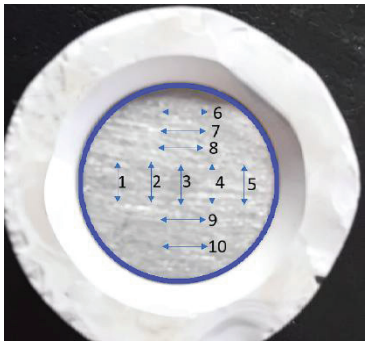


Figure 1. Boron nitride ceramic mold (a) with polished and roughened pull-off bolt-segment (b), plasma spraying of ceramics on polished substrate (c) and bottom part of ceramic coating after drop-off of polished steel substrate (d).

In the case of spraying on a test substrate with surface roughness with average values of R_a = 7.76 µm, R_q = 9.75 µm, R_z = 53.8 µm (see Table I), the tensile strength of this joint was measured at 27 MPa, which is within the limits of similar measurements for corundum or zirconium oxide sprays[8,9] .

Table I

Roughness measurement positions (Mitutoyo SJ-210)



position	1	2	3	4	5	mean
R_a (µm)	7.333	12.097	11.900	12.608	14.208	11.791
R_q (µm)	10.047	14.911	14.496	15.212	17.584	14.450
R_z (µm)	60.641	63.104	61.797	66.207	74.152	65.180

position	6	7	8	9	10	mean
R_a (µm)	6.598	4.382	6.568	7.975	7.571	7.764
R_q (µm)	8.863	5.824	8.396	10.470	7.666	9.757
R_z (µm)	45.45	31.81	41.49	49.318	44.45	53.83

In the second case, the ceramic-metal bond depends on the formation and mechanical properties of a new chemical compound formed during deposition. Examples are the deposition of calcium fluoride CaF_2 on steel (Figure 2a), where iron fluoride FeF_3 is formed at temperatures above 800°C, or the deposition of boron carbide B_4C, where a solid needle-like morphology feataures bonding of the FeB-Fe_2B phase is formed (Figure 2b). Both of these parameters have extreme opposite values in the case of thermal spraying or plasma spraying - short exposure time versus extreme high temperature.

Figure 2. Structure of plasma spray coating of CaF_2 with specific interlayer of FeF_3 (a) and structure of plasma spray B_4C with needle anchoring FeB and Fe_2B (b)

A promising option for large-sized substrates are coatings, but only from compounds that, in addition to the required hardness and chemical resistance, have a significantly lower melting point than the metal substrate, in our case reinforcing steel 10 425 CSN/ S185 DIN with a melting point of about 1470°C. One of the possible materials selected that meets most of the conditions outlined above is basalt, a natural mineral with a slightly different mineralogical composition of forsterite, augite and diopside depending on the geological location of occurrence, with a melting point in the range 1250-1350°C. However, the first experiments on the formation of basalt coatings from 2006 - 2011 [10,11,12] were mainly focused on monitoring the structural changes during the transition from crystalline to amorphous state at different stages of heat treatment and on the measurement of mechanical properties, mainly related to hardness and resistance to abrasion and mechanical changes. Only recently has there been an interest in corrosion issues of basalt in aggressive environments[13,14,15].

Experimental

For testing of corrosion performance of different variants of basalt coatings on reinforced steel 10 425 CSN/ S185 DIN a product of EUTIT s.r.o. was used[16]. Input parameters of powdered basalt are given in Table II.

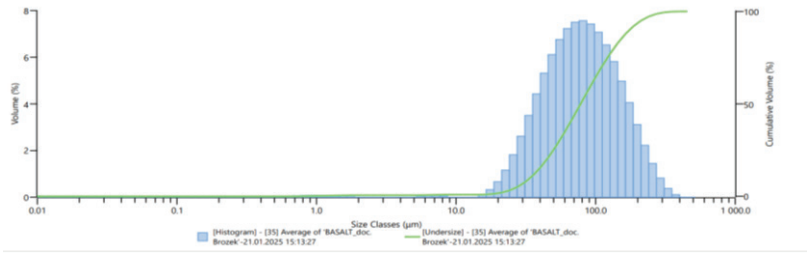
Table II

Basic specification of basalt – production EUTIT s.r.o. ®

XRF Analysis of Basalt Powder (wt.%)

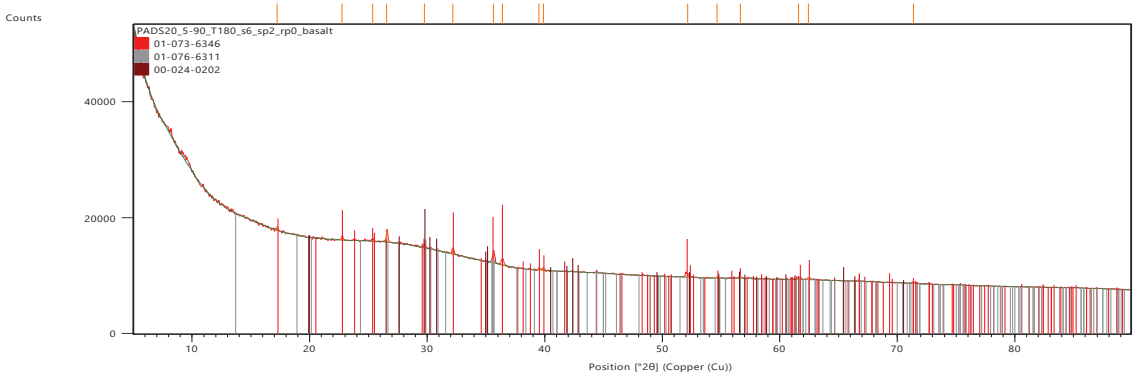
Na	Mg	Al	Si	P	S	Cl	K	Ca
3.01	9.27	8.95	33.16	0.52	0.01	0.08	1.49	16.17
Ti	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ba
3.72	0.10	0.37	21.99	0.04	0.07	0.03	0.04	0.21

Granulometry of Basalt Powder



D [3;2] 47.1 µm
D [4;3] 93.0 µm
Dv (6) 28.8 µm
Dv (10) 33.9 µm
Dv (50) 78.0 µm
Dv (90) 175 µm
Dv (97) 237 µm
Mode 79.1 µm

BET Surface area 0.294 sq.m/g, Correl.Coef. 0.9753 (Surface area report COULTER SA 3100)



Ref.code	Compound name	Mineral name	Chem. Formula
01-073-6346	Magnesium Iron Silicate	Forsterite	$(Mg_{1.7}Fe_{0.3})SiO_4$
01-076-6311	Calcium Magnesium Silicate	Diopside	$CaMgSi_2O_6$
00-024-0202	Calcium aluminium Iron manganes	Augite (Al^{3+} bearing)	$(CaNa)(MgFeTi)(Si,Al)_2O_6$

The amorphous proportion (SiO_2) predominates

In the first part of the experiments, the basalt coating was created using the WSP-H 500 plasma torch (Figure 3a) with deposition parameters of the spray distance SD = 380 mm, the feeding distance of the powder to the plasma FD = 65 mm, the current 500 A, the power of 145 kW. The structure and thickness of the created layer is shown in Figure 3b and Figure 3c. Hg-porosimetric measurements on AutoPore I Serial 437 found values of basal coating porosity of 1.46%, Median Pore 0.339 µm, Average Pore 0.122 µm.

Figure 3. Plasma torch in action indicating the location of substrates (a) and their SEM microstructure (b) cross section and (c) surface section

In the second part of the experiments, the basalt coating was formed by placing bars of 10 425 CSN/ S185 DIN steel into a backfill of powdered basalt and heated to 1260°C for 2 hrs. The resulting product (see Figure 4) with a basalt coating thickness of up to 1 mm is further described by microscopic analysis (Figure 4b - 4d)

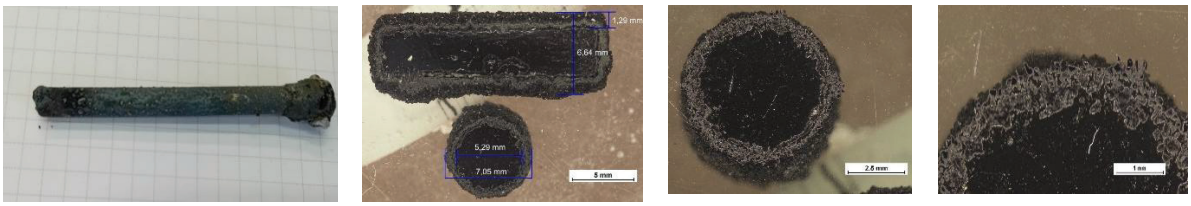


Figure 4. Coated bar reinforced steel 10 425 CSN and details of microscopic analysis of basalt coating

The third, only informative test of the reaction of basalt with steel at 1400°C confirmed the formation of new, structurally complex interconnected phases and the formation of a coherent joint of great thickness and great strength, so that the mechanical destruction of the ceramic sleeve of bornite ceramic occurred during the pull-off test, the toughness of which is given by the value of about 0.55 MPa.m$^{1/2}$ and the bonding strength of 48 MPa. The bond between the steel substrate and the basalt coating remained intact. A schematic representation is shown in Figure 5. The surface basalt layer (Fig.5a) retains its original crystallographic composition according to the X-ray diffraction analysis, but quantitative identification of the individual phases at the interface with the steel is problematic due to the high content of amorphous components, mainly SiO_2. The X-ray diffraction analysis only confirmed the differences between the structure of the plasma-deposited coating, i.e. with short-term heating of the fed spray powder in a plasma with a temperature of about 5000°C and ultrafast cooling versus gradual heating in a powder bed with a residence time of 2 hrs at a maximum temperature of 1260°C. Plasma spraying contains a larger proportion of the amorphous silica phase.

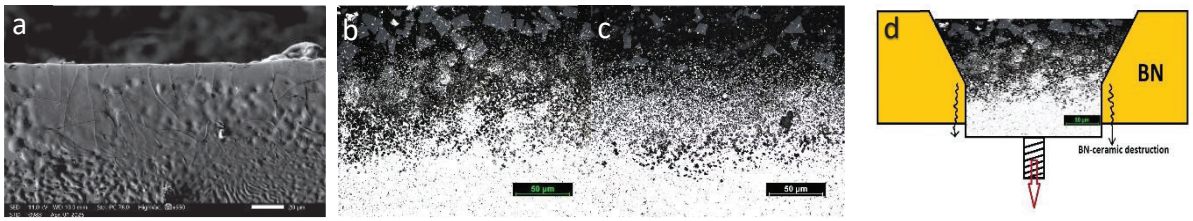


Figure 5. SEM microstructure of cross section structure of basalt coating melted at 1400°C a) smooth surface layer, b) and c) interface structure at the contact point of the steel substrate where the chemical reaction occurred, d) illustration of the technical design of the pull-off test with the destruction of a pull-off device made of BN-ceramic with a flexural strength of 48 MPa.

For both types of prepared basalt coatings - i.e. thermal plasma spray and backfill melting at 1260°C, corrosion performance tests were realised in a chloride environment. Samples with the same geometric surface area (3.14 cm^2) were dissolved in solutions of 1 M NaCl and 1 M HCl respectively for 24 hrs and 100 hrs at ambient temperature i.e. under the same conditions. The content of dissolved elements, mainly $Fe^{2+,}$ was analyzed by

AAS (Agilent 280FS AA Atomic Absorption Spectrometer with flame atomization technique). The measured values are given in Table III.

Table III

Results of the AAS surface etching analysis

Sample (reaction surface 3.14 cm^2)	Exposition 24 h in 1M NaCl	Exposition 100 hrs in 1 M NaCl	Exposition 24 h in 1 M HCl	Exposition 100 h in 1M HCl
OriginaL steel 10 425 CSN/ S185 DIN	Fe 81.7 mg/l	Fe 1300 mg/l	Not quantitatively analysed, reaction according to below: $Fe + 2\ HCl = FeCl_2 + H_2$	
Steel with plasma spray basalt coating 300 µm layer thickness	Fe 0.03 mg/l	Fe 0.107 mg/l	Fe 312 mg/l	not measured
Steel with basalt coating prepared at 1260°C	Fe 0.0 mg/l	Fe 0.0 mg/l	Fe 2150 mg/l	Fe 3620 mg/l

The first measurement of the solubility of the uncoated steel alone in 1 M HCl confirmed the expected results course of the reaction $Fe + 2\ HCl = FeCl_2 + H_2$, the rate of reaction being consistent with the size and initial surface quality of the sample examined, whereas only a minimal reaction occurred when this steel was reacted in 1 M NaCl solution, but this continued slightly with increasing etched surface size.

In the case of the basalt coating applied by plasma spraying, there was only minimal corrosion of the steel substrate in the NaCl solution, caused by the penetration of the corrosive medium into the open pores, the informative value of which measured by Hg-porosimetry was in the order of units by volume. By adjusting the plasma spraying conditions, these values can be optimized as needed.

In the case of the basalt coating melted in the backfill at 1260°C, corrosion process in the NaCl solution was practically negligible. In HCl solution, however the basalt reacted in an uneven manner, with time-selective dissolution of individual residual crystalline moieties. Elements from the augite moiety were preferentially transferred to the chloride solution, increasing the amorphous silica content of the solid surface layer. The solution obtained by intermittent etching of the basalt layer after 100 hrs was dried in a graphite crucible and the powder subjected to XRF analysis. Stoichiometric recalculation of the result after subtraction of the chloride compounds confirmed that, on the contrary, the ratio of the disolved fractions with silicon content was lower in the solution, i.e., that selective etching was indeed occurring. The values found are given in Table IV.

Table IV.

Corrosion etching of molten basalt coating (wt.%)

	Na	Mg	Al	**Si**	K	Ca	Ti	**Fe**	*0.1 – 0.4*	*0.04-0.07*
Orig. Basalt powder	3.01	9.27	8.95	**33.16**	1.49	16.17	3.72	**21.99**	*P,Cr,Mn*	*S,Cl,Ni,Cu*
*	3.52	9.75	8.56	**35.24**	0.94	15.8	3.54	**20.72**	*P,K,Mn,Ce*	*Cl,Ni,Zn,Zr*
**	0.35	4.56	4.72	**46.49**	0.56	12.7	1.54	**20.07**	*Mn,Sr,Ce*	*P,Ba,Zr*
***	0.19	0.78	1.13	**66.73**	0.68	9.33	3.40	**16.19**	*Mn*	*P,Cr,S,*
****	2.4	3.3	5.40	**17.00**	0.90	8.3	2.0	**18.6**	**Cl 40.02**	*Ni, Cu, Zn*
*	Molten basalt surface									
**	Surface layer after 24 hrs etching									
***	Surface layer after 100 hrs etching									
****	Chloride leachate after 100 hrs etching									

Conclusions

The deposition rate of basalt coatings is mainly influenced by the ratio of crystalline and amorphous phases, which in the next part influence the formation of a porous-free structure or the adhesion properties of the

coating. According to a kinetic studies [17,18], our results also confirm that the complex crystallographic structure of basalt coatings changes with variations in temperature conditions, suggesting the possibility of categorizing the results as high entropy ceramic coatings. Plasma spraying, characterized by an initial very high temperature of molten powder particles followed by a relatively rapid cooling below the melting temperature, produces a coating with a predominantly amorphous structure. However, the formation of micropores and microcracks cannot be prevented. The amorphous structure of the coating with a predominance of SiO_2 is, on the other hand, suitable for slowing down the dissolution in HCl.

Basalt coatings prepared by plasma spraying technology had a lower protective effect in terms of corrosion resistance compared to coatings prepared by conventional melting, but the different thickness of the coatings prepared in this way did not allow quantitative evaluation. In all cases, however, it was confirmed that corrosion by chloride ions from neutral NaCl solution is zero in the case of fused coatings, minimal in the case of plasma deposited coatings and, according to all secondary indicators, is only enabled by the higher porosity and low coating thickness. This "temporarily" inefficient phenomenon can be easily corrected by changing the plasma deposition parameters and, of course by creating protective layers of greater thickness. The aim of the presented experiments of corrosion measurements caused by 1 M HCl solution with pH = 0 was to investigate how the phase composition of basalt coating changes in terms of transition of a larger proportion of silicate components to the amorphous state. The amorphous SiO_2 present in the coating layer is insoluble in acidic environments and its transition from molten to amorphous state upon cooling of the melt produces a coating without pores and cracks, which is a positive factor for increasing the corrosion performance of basalt-coated steel substrates.

Acknowledgement

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MICROSTRUCTURE AND PROPERTIES OF NITINOL ALLOY REINFORCED WITH Ni-Ti INTERMETALLICS AND CARBIDES

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Abstract

Nitinol is well known for its unique properties, such as the shape memory effect and superelasticity. It is widely used in stents, bone fixations, joining elements, temperature sensors, actuators, and vibration dampers. The aim of this study is to investigate the effect of reinforcing intermetallic particles and carbides on the hardness, wear resistance, and microstructure of Nitinol. The samples were fabricated using direct energy deposition (DED) from powder feedstock. A pre-alloyed NiTi powder with the addition of nickel, a Ni79Ti21 (wt.%) powder mixture, and tungsten carbides (WC) was used as the feedstock material. The Ni_3Ti intermetallic phase were formed in situ during the 3D printing process, while carbide particles were added separately. No defects such as cracks or pores were observed in microstructures of the carbides-reinforcement samples and the same time, the wear resistance of these samples increased significantly. On the contrary, cracks were found in samples rich in the Ni_3Ti phase. The hardness of samples containing the Ni_3Ti phase increased, while the hardness of the NiTi matrix in WC-reinforced samples remained unchanged.

Introduction

Ni-Ti alloys with approximately equiatomic chemical composition called Nitinol, exhibit unique functional properties such as shape memory effect and superelasticity. This chemical composition corresponds to the NiTi phase, occurring in the high-temperature structure (austenite) and low-temperature structure (martensite). The shape memory effect and superelastic behavior result from a reversible martensitic transformation between these two phases. These unique properties are widely utilized in applications including stents, medical wires, actuators, and vibration dampers[1,2].

Efforts to improve the wear resistance of Nitinol have led researchers to incorporate reinforcement particles into the matrix. Ceramic particles such as TiC, ZrO_2, α-Al_2O_3, SiC, TiN, B_4C have been employed, resulting in enhanced hardness and reduced wear rates compared to pure Nitinol[3,4]. Further studies focused on improving mechanical performance through the in-situ formation of intermetallic phases, particularly Ti_2Ni and Ni_3Ti, arising from the reaction between nickel and titanium[3,5]. These intermetallic phases are formed during the powder metallurgy methods such as reactive sintering, self-propagating high-temperature synthesis and spark plasma sintering as described in[6,7]. It was found out that both the Ti_2Ni and Ni_3Ti phases caused very strong increase in hardness above the value of 1000 HV, while mainly, the Ni_3Ti phase was responsible for increase in wear resistance[5]. However, certain powder chemical compositions have shown a tendency to form pores during processing.

In this work, the effects of the Ni_3Ti phase and WC reinforcement particles on the properties of Nitinol was investigated. The samples were fabricated using the Directed Energy Deposition (DED) method, and their properties were assessed by evaluating hardness and wear resistance.

Experiment

Ni-Ti samples reinforced with the Ni_3Ti and WC particles were fabricated using the DED method (INSSTEK MX-600 system, Daejeon, Korea). The Direct Metal Tooling mode was used to ensure a consistent layer height throughout the deposition process. An atomized NiTi powder (55.8 wt.% of Ni) was used as powder feedstock. To this powder, a Ni79Ti21 (wt.%) mixture and tungsten carbide (WC) particles were added. Initially, a graded sample was deposited with increasing content of the Ni79Ti21 powder mixture in successive layers. Each layer contained a 12.5% incremental increase in the Ni79Ti21 content, starting from pure atomized NiTi up to a 50:50 mixture (in wt.%) of NiTi and Ni79Ti21. As a result, the overall nickel content increased from 55.8 wt.% in the first layer to approximately 67 wt.% in the final layer. Based on the results of hardness measurements and microstructural observations, a composition with 37.5 wt.% Ni79Ti21 was selected for further experiments. In the second phase of the experiment, WC particles (10 wt.%) were added to the atomized NiTi powder, and samples were fabricated using the same DED process. Cubic samples with dimensions of 20x20x20 mm were produced for both the NiTi + 37.5% $Ni_{79}Ti_{21}$ composition and the NiTi + 10% WC composition. The microstructure was observed using a light (Carl Zeiss Axio Observer Z1m) and scanning electron microscopes (SEM, JEOL IT 500

HR). Hardness (HV10) was measured by an automatic Vickers hardness tester (Struers DuraScan 50) and the abrasive wear resistance was evaluated by using a pin on disc method (CSM Instruments) with a Al_2O_3 ball and a load of 15 N.

Results and Discussion

The as-polished microstructure of the NiTi-Ni79Ti21 graduated sample is shown in Figure 1. Low porosity was observed, and cracking was noted only in the final deposited layer composed of 50% NiTi and 50% $Ni_{79}Ti_{21}$. The hardness profile (Figure 2) indicates that the first deposited layer—deposited solely from atomized NiTi powder—exhibits a relatively high hardness due to the formation of a Ti_2Ni intermetallic phase that resulted from the reaction between the atomized NiTi powder, and the titanium substrate. Within this layer the hardness subsequently dropped to approximately 200 HV10. In the subsequent layers, hardness increases again as the volume fraction of the Ni_3Ti phase grew, corresponding with increasing nickel content in the powder feedstock. The highest hardness was recorded in the layer deposited from a mixture of NiTi + 37.5 wt % Ni79Ti21 and a slight decrease in hardness was observed in the immediately subsequent layer with the highest content of nickel.

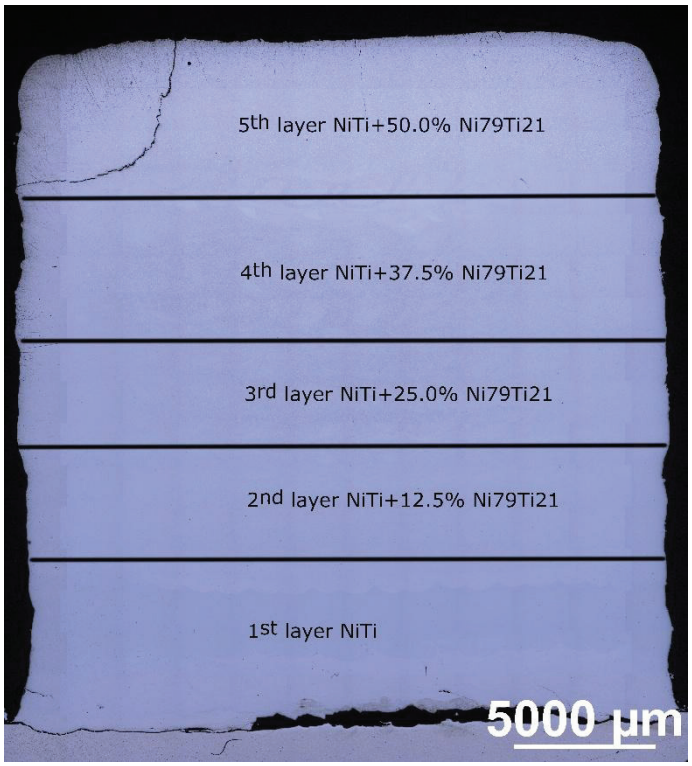

Figure 1. Macrostructure of the sample with graduated Ni79Ti21 (in wt.%) content.

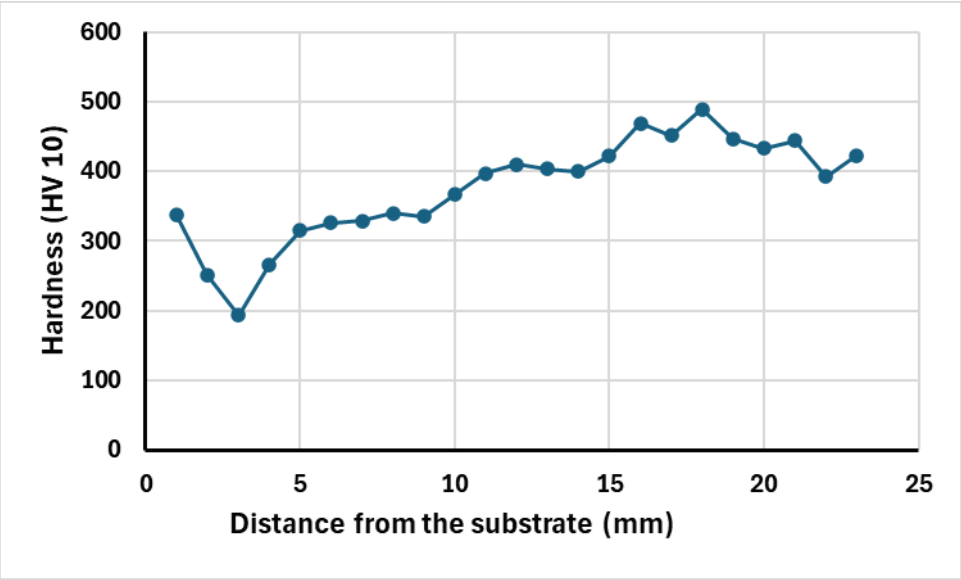

Figure 2. Hardness profile measured on the cube with graduated Ni79Ti21 (in wt.%) content.

The microstructure of the NiTi + 37.5% Ni79Ti21 sample consisted of a NiTi matrix and a significant amount of the Ni_3Ti phase (Figure 3). The area fraction of the Ni_3Ti phase was approximately 42.6% and a small amount of the Ti_2Ni phase was also observed in the microstructure. Due to its thermodynamic stability, the Ti_2Ni phase is often formed during the reaction between nickel and titanium powders[6].

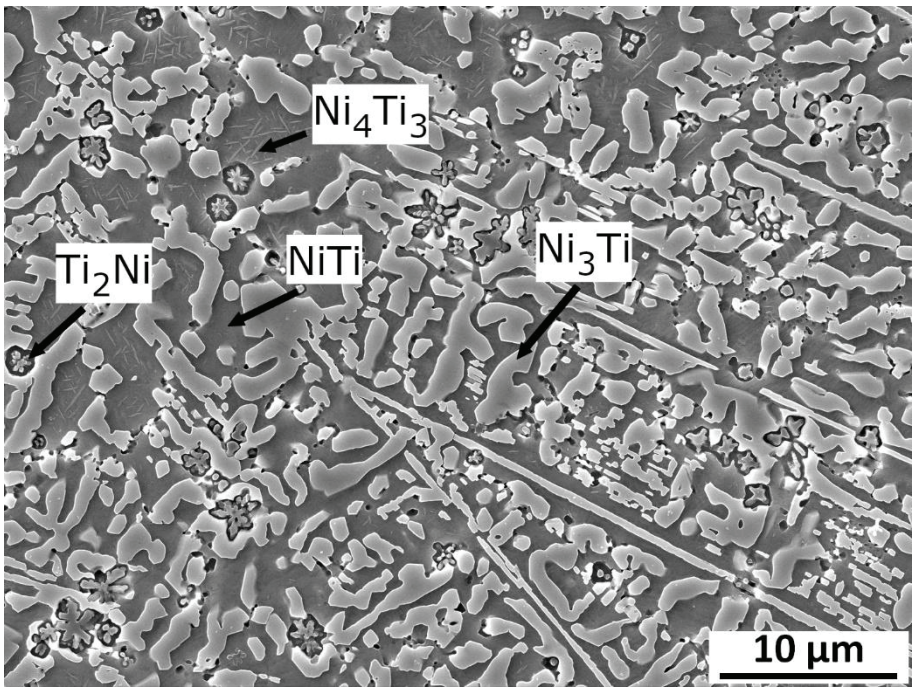

Figure 3. SEM micrographs of the sample NiTi + 37.5% Ni79Ti21.

The microstructure of the NiTi + 10% WC sample was composed of a NiTi matrix, a minor fraction of the Ti_2Ni phase, and WC reinforced particles (Figure 4). The area fraction of the reinforcing WC phase was approximately 8.2%.

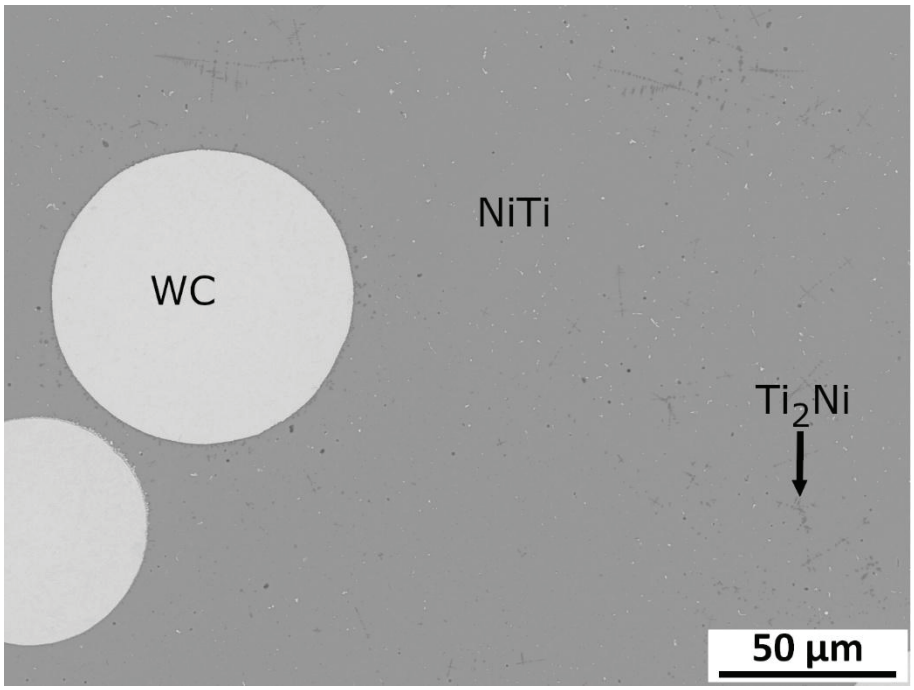

Figure 4. SEM micrographs of the sample NiTi + 10% WC.

The two reinforcing phases, Ni_3Ti and WC, exhibit significantly different area fractions and distinctly affect both hardness and wear resistance. The presence of Ni_3Ti significantly increased hardness, reaching up to 430 HV10, whereas the NiTi alloy reinforced with WC particles exhibited a lower hardness of approximately 360 HV10. This difference can be attributed to the fact that Ni_3Ti precipitates finely and is distributed homogeneously throughout the NiTi matrix, while WC particles remain distinct, exhibit lower area fraction, and do not affect the matrix hardness.

An opposite trend was observed in the results of the wear resistance test. The sample reinforced with WC particles demonstrated substantially higher wear resistance, with a wear rate of approximately 15×10^{-6} mm^3/Nm, compared to the NiTi + 37.5% Ni79Ti21 sample (wear rate of about 150×10^{-6} mm^3/Nm). This indicates that the addition of WC particles is more effective in enhancing wear resistance than the formation of the Ni_3Ti phase.

Conlusions

The study demonstrated that reinforcing NiTi alloys with Ni_3Ti intermetallic phase and WC particles significantly affects its mechanical properties. While the presence of the Ni_3Ti phase leads to a considerable increase in hardness (up to 430 HV10), the WC particles improve wear resistance more effectively, reaching a wear rate approximately 10 times lower than that of the Ni_3Ti-reinforced sample.

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OIL GAS COAL

Alternative raw materials, new technologies, biorefineries, fuels, biofuels

MODELING AND FEASIBILITY OF VARIOUS ANAEROBIC DIGESTION PLANT DESIGNS

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Abstract

Anaerobic digestion offers effective and green alternative to treat various types of organic waste. The process takes place in batch or continual reactors, in which organic substrates are transformed into biogas and digestate. There are two technological approaches that differs in total solids content in feedstock – wet (<15%), dry (>20%). Produced biogas is composed of ~55% methane, ~40% carbon dioxide, nitrogen, oxygen and hydrogen sulphide. Aim of this paper is to develop a model of each available technology (continual, dry batch, wet batch) as well as unit for biogas to biomethane purification and evaluate the potential of building a new plant in Slovakia. Both dynamic and steady – state behavior of the reactor is studied. Feedstock analysis, energy integration and usability evaluation of all products are also part of the paper.

Introduction

Anaerobic digestion (AD) offers effective and green alternative to treat various types of organic waste. The process takes place in batch or continual reactors, in which organic substrates are transformed into biogas and digestate. Generally, AD is a biochemical process which can be divided into four stages: hydrolysis, acidogenesis, acetogenesis and methanogenesis. There are two technological approaches that differs in total solids content in feedstock – wet (<15%), dry (>20%)[1]. On average, biogas is composed of ~55% methane, ~40% carbon dioxide, nitrogen, oxygen and hydrogen sulphide. Biogas yield is significantly influenced by feedstock composition, with energy crops such as maize silage and sugar beet achieving yields of 200-400 m^3 CH_4/ton volatile solids (VS), while agricultural residues typically produce 150-250 m^3 CH_4/ton VS. Organic waste streams, including food waste and sewage sludge, demonstrate variable methane potentials ranging from 100-350 m^3 CH_4/ton VS, depending on their organic content and biodegradability. Geographic location affects biogas plant performance through ambient temperature variations, with northern European facilities requiring additional heating systems compared to Mediterranean installations, consequently impacting overall energy balance and economic viability. Co-digestion of multiple feedstock types has proven effective in optimizing biogas yield, with mixtures of agricultural residues and energy crops often achieving 15-25% higher methane production compared to mono-digestion systems. Seasonal variations in feedstock availability necessitate strategic planning and storage solutions, particularly for agricultural-based biogas plants that rely on harvest-dependent materials.
Later, produced biogas can be used for combined heat and power generation or biomethane production although, then it requires further treatment[2,3]. Different kinds of separation techniques are available; however, membrane separation is on the rise, mainly due to their efficiency[4]. Water scrubbing represents the most widely deployed upgrading technology, utilizing the differential solubility of CO_2 and CH_4 in water under pressure, achieving methane purities of 96-98% with relatively low energy consumption. Pressure swing adsorption (PSA) systems employ molecular sieves to selectively adsorb CO_2 while allowing methane to pass through, offering high purity levels (>99%) but requiring higher capital investment and energy input. There are three categories of membrane materials used for gas separation – polymer, inorganic and mixed matrix membranes. Predominantly used are polymer membranes, especially due to their low cost and high stability even at higher operating pressures[5,6].
Currently, there are only two biomethane plants in Slovakia, however Slovakia has potential to replace 10 % of its natural gas consumption by biomethane. Therefore, there is a demand on the market and AD could offer an effective way of biomethane production[7]. As Slovakia is dependent on natural gas import, development of biomethane production and market could contribute to the resilience of domestic industry in terms of energy supply. Cost-effectiveness of converting biogas stations to biomethane producers strongly depends on the market price of biomethane certificates.

Aims of this study

Given the results of the literature survey, the study focused on several partial aims which together will serve for better understanding of AD applicability in Slovakia in our further research. These comprise:

- Evaluate and compare biogas production from biowaste under different conditions
- Calculate amount of heat required for each approach.
- Achieve at least 95% purity of biomethane using membrane separation technique.

Mathematical modeling

Mathematical modelling is essential in the process of designing AD plant. Over the years, there have been proposed numerous models to estimate biogas production. However, only Anaerobic Digestion Model 1 (ADM1) is universally suitable for all biogas simulations. On the other hand, its complexity and need of multiple input parameters is often problematic. For this reason, simplified ADM1 model is used, which considers 13 components and its concentrations, stoichiometric coefficients and kinetics. Disintegration, biomass decay and hydrolysis are modeled trough first order kinetics, other reactions as well as microbial growth using Michaelis-Menten and Monod kinetics. Firstly, the model is implemented on basic model of CSTR (Continuous stirred tank reactor) for both dry (20% TS) and wet (10% TS) digestion processes. Selected input parameters for mathematical model are displayed below in Table I.

Table I
Selected input parameters for mathematical models. $V_{reactor}$ – Volume of reactor, $\dot{m}_{in}$ – Mass flow of the feedstock, HRT – Hydraulic retention time, ρ_{waste} - biowaste density, TS – Total solids, $T_{inwaste}$- Temperature of incoming biowaste

	Input parameters	
	dry	wet
$V_{reactor}$, m^3	800	800
$\dot{m}_{in}$, kg d^{-1}	25000	15000
HRT, d	18	30
ρ_{waste}, kg m^{-3}	750	750
TS, %	20	10
$T_{inwaste}$, °C	15	15

Mass variation due to biogas production is neglected, also it is assumed that input waste flow rate is equal to digestate output and that waste volume remains constant. Secondly, thermal model is calculated for each approach[8]. Lastly, biogas to biomethane purification is modelled, using two membrane modules connected in series with compression of gas to 0.8 MPa only before first module, pressure drop in between modules is considered to be 1 bar. We assume biogas composition in the feed to be 60% CH_4 and 40% CO_2 with molar flow of 10 mol/s[4].

Results and discussion

In Figures 1. and 2., a comparison of the mathematical model results is displayed under different conditions. The double exponential trend of biogas production is caused by activity of two bacteria families at different time. Firstly, hydrogenotrophic methanogenesis occurs, followed by acetate consumption.
Heat duty depending on ambient temperature under different conditions is displayed in Figure 3. As anticipated, thermophilic operational regimes necessitated more intensive heating requirements compared to mesophilic conditions. The relationships presented in Figure 3 demonstrate that dry anaerobic digestion (AD) systems require greater heating intensity, which can be attributed to their capacity to process larger quantities of biowaste due to their reduced hydraulic retention time (HRT).

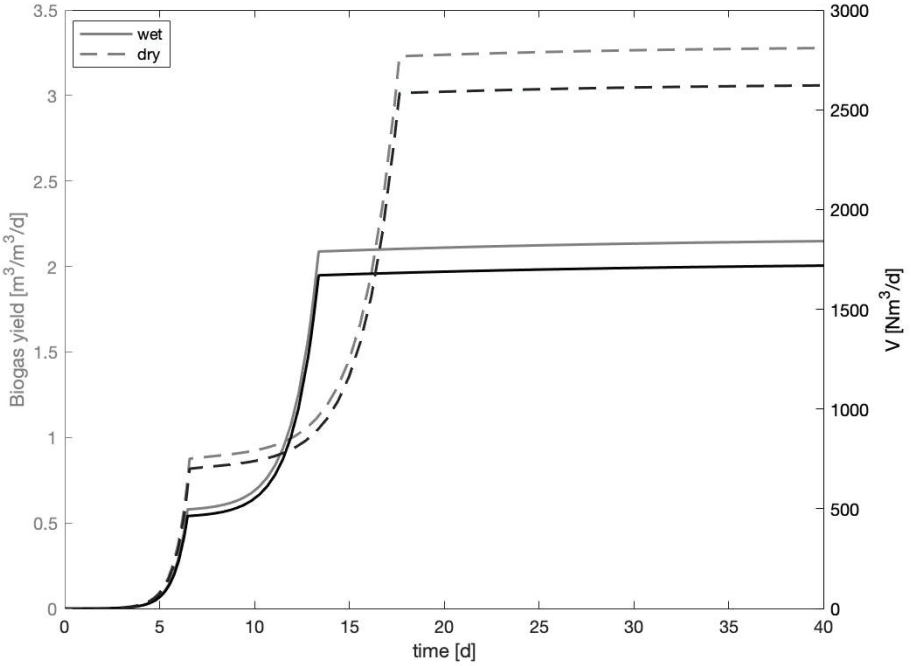

Figure 1. Biogas production and yield under termophilic conditions. V – Biogas volumetric production, wet – Wet AD, dry – Dry AD.

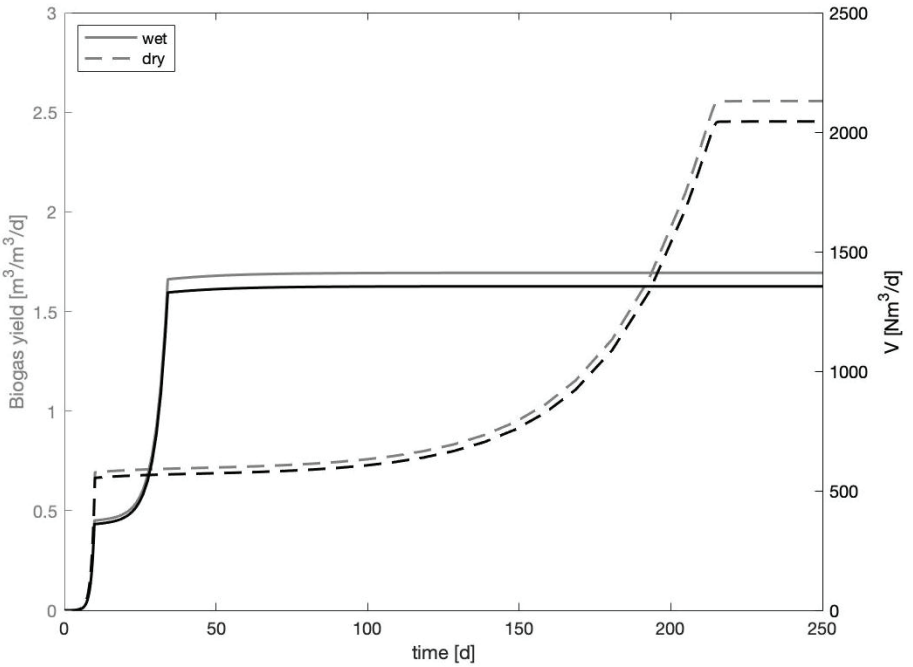

Figure 2. Biogas production and yield under mesophilic conditions. V – Biogas volumetric production, wet – Wet AD, dry – Dry AD.

The results presented in Table II indicate that in addition to biogas production, substantial quantities of digestate are generated. Several commercial options exist for digestate utilization, including application as fertilizer in agricultural operations, pellet manufacturing, and feedstock for composting facilities. However, all utilization pathways necessitate additional digestate processing.

Results of biogas purification are displayed in Figure 4. Only polyimide membrane shows results with required level of purity under selected conditions. However, as the CH_4 purity rises the amount of retentate declines. It is possible to reach higher CH_4 purity by increasing feed pressure. On the other hand, it also means increased compressor duty.

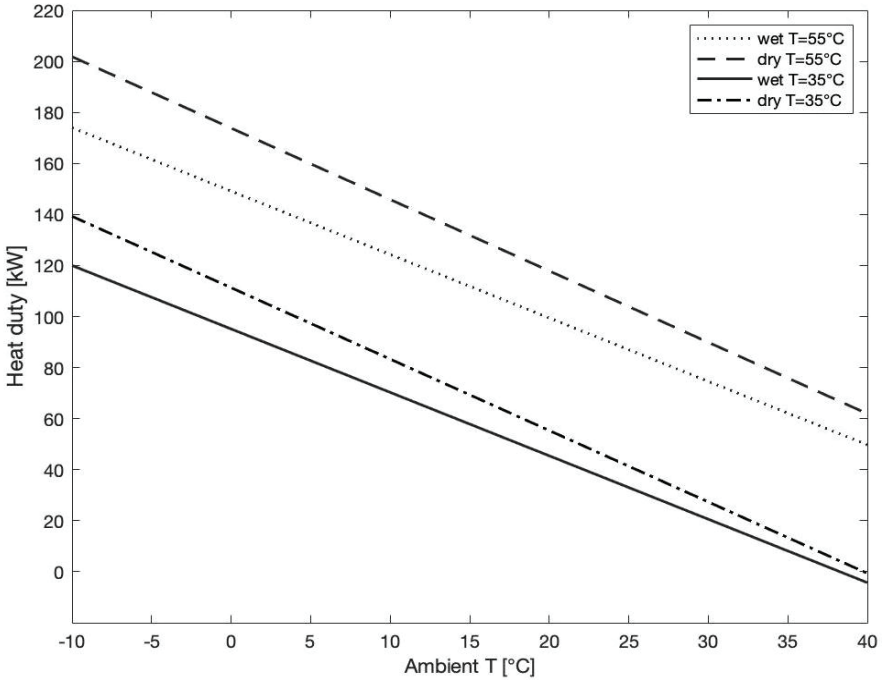

Figure 3. Required amount of heat depending on ambient temperature under mesophilic conditions. wet – Wet AD, dry – Dry AD.

Table II
Mass balance of the digester for each technological regime. m_{in} - incoming mass flow of biowaste, m_b - mass flow of produced biogas, m_d – digestate mass flow

	m_{in}, kg/d	m_b, kg/d	m_d, kg/d
Dry 55°C	25000	3172	21828
Dry 35°C	25000	2474	22526
Wet 55°C	15000	2070	12930
Wet 35°C	15000	1640	13360

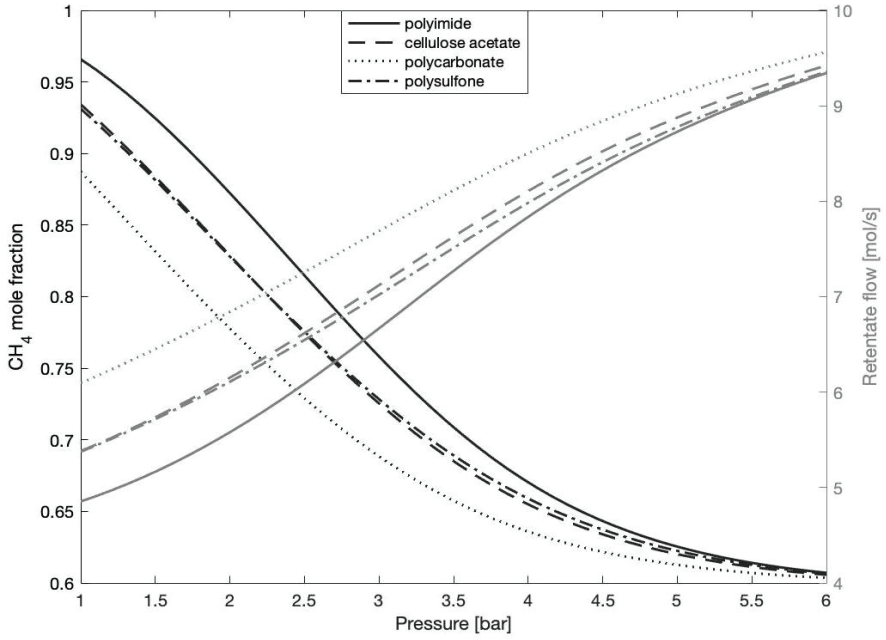

Figure 4. Methane purity and retentate flow depending on permeate pressure for various membrane materials.

Conclusions

It is evident, that dry AD, under thermophilic conditions is most advantageous from biogas generation and yield perspective. It is mainly caused due to lower HRT, which enables higher biowaste processing rate. On the other hand, it requires a more extensive heating, that can be seen in Figure 3. Heating requirements can be reduced by insulating the digester. Biogas production also depends on quality of incoming biowaste, a fact that will be included in future modeling. Mass balance for each technological regime showed, that digestate makes up a large part of product stream. Therefore, digestate post-treatment could play an essential role in economic viability of the AD plant. Under selected conditions for biogas to biomethane separation, polyimide membrane showed most advantageous results. Findings and results of this work are going to be further investigated using multicriteria decision analysis to determine a possibility of building an AD plant in Slovakia.

Acknowledgments

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CO-PROCESSING OF CNSL ON BGHT7 IN SLOVNAFT REFINERY

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Abstract

In September 2024, a test run for co-processing of cashew nut shell liquid (CNSL) was carried out on Bratislava - Gasoil Hydrotreating unit 7 (BGHT7). The test run was conducted at 80 to 98 % of the design capacity, with the biocomponent representing 2.3 % of the total processing. The aim of the test run was to monitor the impact of biocomponent on selected process parameters and yield structure, evaluate the low-temperature properties of the hydrotreated gas oil, and confirm the conversion products of the bio-component using GC-MS, as well as its total content in the final product using the carbon-14 method. CNSL proved to be an excellent feedstock for co-processing. Its processing resulted in only negligible changes in the BGHT7 product yield structure, and the CNSL-derived products had no negative impact on the low-temperature properties of the produced diesel. GC-MS analysis qualitatively confirmed hydrogenation products of the bio-component and its total content in the hydrotreated gas oil was verified by the ^{14}C isotope measurement method.
Key words: co-processing, CNSL

Introduction

Gasoil Hydrotreating unit 7 (BGHT7) was commissioned at the Slovnaft refinery in 2004, based on patent from Haldor Topsoe[1]. The unit processes intermediate products from various production units, including straight-run kerosenes and gas oils from distillation units, as well as gas oils generated by cracking processes within the refinery. The maximum daily processing capacity is 245 t/d.

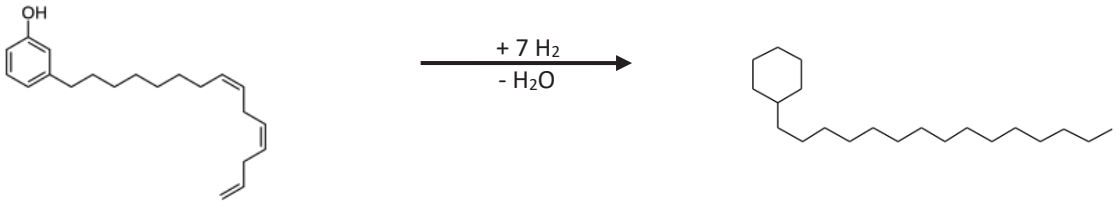
The MOL Group, which includes the Slovnaft refinery, has committed in its strategy[2] to reduce greenhouse gas emissions by 25 % by 2030 and to achieve carbon neutrality by 2050. In line with this strategy, a co-processing project for bio-components is being prepared for the BGHT7. However, the processing of bio-components brings various risks[3], such as increased corrosion due to the formation of HCl and H_2CO_3, higher hydrogen consumption, catalyst deactivation caused by the presence of catalytic poisons such as phosphorus, alkali metals, and alkaline earth metals, as well as deterioration of the low-temperature properties of the produced diesel due to the formation of n-paraffins during the hydrogenation of triglycerides.

To identify potential bottlenecks in the BGHT7 technology, the first test run for the co-processing of rapeseed oil was carried out back in 2019. The test was conducted at a feed rate of 125–130 t/h, with the bio-component accounting for 6 wt. % of the total feed. The rapeseed oil addition had an impact on the product yield structure – the yield of hydrotreated gas oil decreased by 0.8 – 1.2 wt.%, the yield of low-pressure gases increased by 0.1 – 0.2 wt.%, and the off-gas volume sent to the PSA unit increased by 0.1 wt. %. As a result of hydrogenation, 0.4 – 0.7 wt.% of water was released, and the gasoline yield increased by 0.1 – 0.3 wt.%. Due to the high oxygen content in rapeseed oil (10 wt.%), a significant increase in reactor exothermicity was observed, along with a rise in hydrogen consumption from 9.8 – 10.6 kg/t of feedstock to 11.2 – 11.7 kg/t.

The initial test conducted in 2019 provided basic information on the technological changes associated with the co-processing of rapeseed oil; however, it was carried out at the end of the catalyst's lifecycle and at a minimal feed rate. To obtain additional data, a follow-up test was performed in 2024, this time using a fresh catalyst and a higher feed rate. Cashew nut shell liquid (CNSL) was selected as the bio-component. CNSL is a dark brown oil that is generated as a by-product from cashew nut shell processing. The composition of CNSL can vary depending on the extraction method.

Based on the study by Scaldaferri[4], it was expected that under the operating conditions of HRP7 — at a pressure of 6.1 – 6.2 MPa and reactor inlet temperatures of 325 – 330 °C — full hydrogenation and deoxygenation reactions of cardanol would predominate. These include hydrogenation of its phenolic –OH group, saturation of olefinic

bonds on the side chain, as well as saturation of the aromatic benzene ring, resulting in the formation of *n*-pentadecylbenzene, as shown in the following reaction:



Cardanol
$C_{21}H_{30}O$ MW=298.5 g/mol

n-pentadecyl cyclohexane
$C_{21}H_{42}$ MW=294.6 g/mol

Test run conditions

During the test run, diesel fuel with transitional quality between winter and summer grades was produced. The expected cloud point ranged from –3 °C to –1 °C, and the 95 % distillation point of the processed gas oil was adjusted accordingly to approximately 360 °C. The unit feed rate was set at 200 t/h. The temperature before and after the first hydrogenation reactor was 328/351 °C, and before and after the second reactor 346/354 °C. Fresh hydrogen consumption was maintained at 16 000 Nm³/h, with the circulating gas purity at 85 %. Under these standard conditions, the yield structure of the main products consisted of 91.6 % hydrogenate, 1.2 % heavy naphtha, 1.0 % light naphtha, and 0.5 % low-pressure sulphur-containing gases.

Under these conditions, the injection of the CNSL biocomponent into the discharge line of the feed pump was initiated at 9:30. The injection rate ranged from approximately 3.7 to 6.1 t/h over a period of 5.5 hours, during which the first tanker truck with the biocomponent was unloaded and the operating regime was stabilized. Subsequently, the second tanker truck was unloaded over 4.5 hours, during which the feed rate of the fossil feedstock was gradually increased to 220 t/h, while the biocomponent injection rate ranged from 4.5 to 5.1 t/h. The final CNSL tanker was emptied over 4 hours, during which the fossil feed rate was increased to 240 t/h, and the biocomponent injection rate ranged from 4.8 to 5.9 t/h. The overall course of the processing is illustrated in Fig. 1.

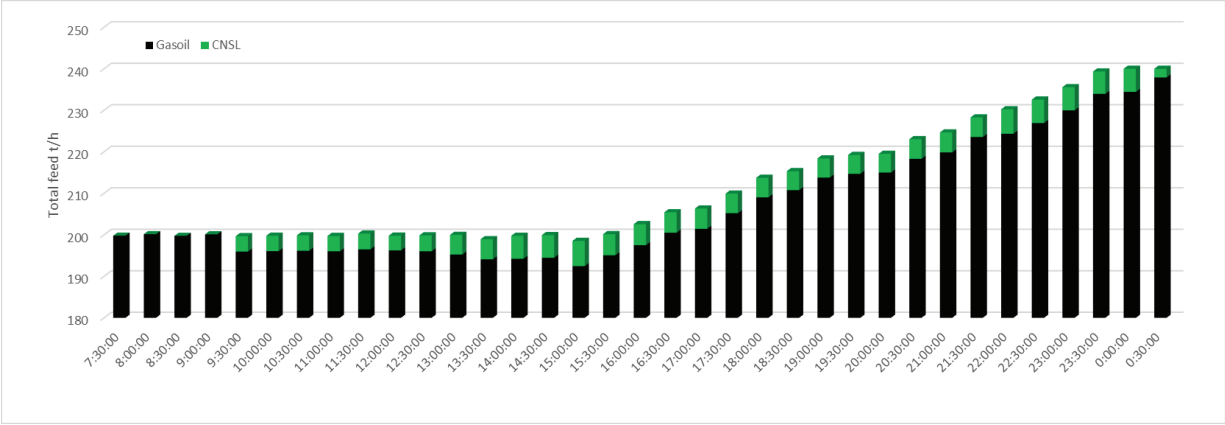


Figure 1 Co-processing test run total feed

During the test run, samples of the feedstock and individual products were collected at 8:00, 13:00, 18:00, and 23:00. Simultaneously, the control system monitored the product yield structure, exothermic reactions in the first and second hydrogenation reactors, fresh hydrogen consumption, and the purity of the circulating gas. Final diesel samples were taken for composition analysis using gas chromatography–mass spectrometry (GC-MS) and for determination of the ^{14}C isotope content. The composition of CNSL was also determined by GC-MS and is summarized in Table 1.

Table I GC-SM analysis of CNSL

Volatile component CNSL	wt %
Phenol, 3-C15 1x saturated (cardanol)	62.53
Phenol, 3-C15 2x saturated (cardanol)	18.92
Phenol, 3-pentadecyl- (cardanol)	5.04
Phenol, C17-	1.67
Cardoltriene	4.55
Cardoldiene	5.52
Benzenediol - C16	1.77

The total biocomponent content in the product is determined using ^{14}C isotope measurement by accelerated mass spectrometry, in accordance with ASTM D 6866-12 and EN 16640 standards. The resulting biocomponent content in the feedstock and products was determined according to the methodology developed by T. Varga[5].

Impact on technology

During the co-processing of the biocomponent, an increase in exothermic reactions is expected due to the higher content of oxygenates and unsaturated bonds. Prior to CNSL injection, the exothermic temperature rise across the first reactor was approximately 22 – 24 °C, mainly depending on the sulphur content of the gas oil. In the second reactor, the exothermic rise before CNSL injection was smaller, around 7 – 8 °C. The fluctuations in exotherms (and later also in other graphs, such as hydrogen consumption and hydrogenate yield) observed before 9:30 were due to a preventive temperature reduction before the reactor, as a sharp temperature increase was anticipated after CNSL injection. As shown in Fig. 2, the exothermic temperature rise in the first reactor was gradual and eventually stabilized at a level of 30 – 35 °C. This likely contributed to faster desulfurization of the fossil feedstock in the first reactor and thus reduced the exothermic temperature increase in the second reactor to 5 – 6 °C.

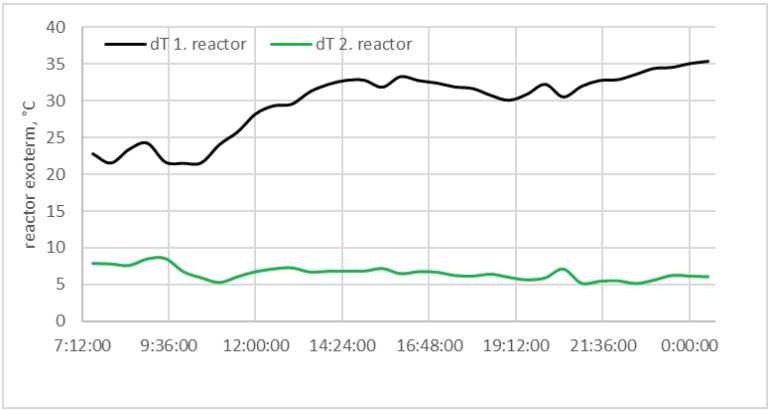


Figure 2 Reaction exoterms in 1st and 2nd reactor

Prior to the CNSL co-processing test run, the hydrogen content in the circulating gas was 85 vol. %, while the licensor recommends maintaining a minimum hydrogen content of 83 vol. % for proper operation of the hydrogenation catalyst. As a result of the hydrogenation of oxygenates and unsaturated bonds, fresh hydrogen consumption increases, while the purity of the circulating gas decreases due to the formation of CO, CO_2, and CH_4. This can be compensated by increasing the purge rate at the PSA unit.

Following CNSL injection, the fresh hydrogen feed per ton of feedstock gradually increased from 81 Nm^3/t to 100 Nm^3/t. This was progressively balanced by increasing the PSA purge from 1300 Nm^3/h to 1800 Nm^3/h, and the hydrogen consumption stabilized at approximately 90 Nm^3/t (Fig. 3). Despite this, the purity of the circulating gas slightly decreased to 83 vol. %, mainly due to the increase in CH_4 content from 8.5 to 9.4 vol. %.

A particularly positive outcome was that even at the maximum feed rate of 240 t/h, no capacity limits were reached—neither on the PSA unit, which operated at 95.5 % of its design capacity, nor on the make-up compressor, which was loaded to 91 %. It should also be noted that the CNSL co-processing test was conducted at the start of the catalyst's life cycle (SOR), when its elevated activity results in approximately 10 Nm^3/t higher hydrogen consumption compared to the end of the life cycle (EOR).

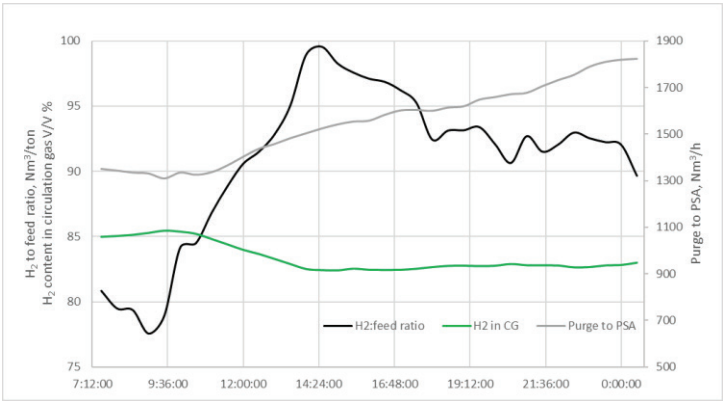


Figure 3 Hydrogen consumption, circulation gas purity and purge to PSA

In terms of yield structure, the addition of CNSL resulted in a slight decrease in the yield of hydrogenated gas oil from approximately 92.0 to 91.0 wt %. The hydrogenation and deoxygenation reactions of CNSL components were reflected in a slight increase in the yield of low-pressure gases and light gasoline—by approximately 0.1 wt % to 0.6 wt % for low-pressure gases, and to 1.1 wt % for light gasoline. The yield of heavy gasoline remained unchanged at around 1.2 wt % throughout the entire CNSL co-processing period.

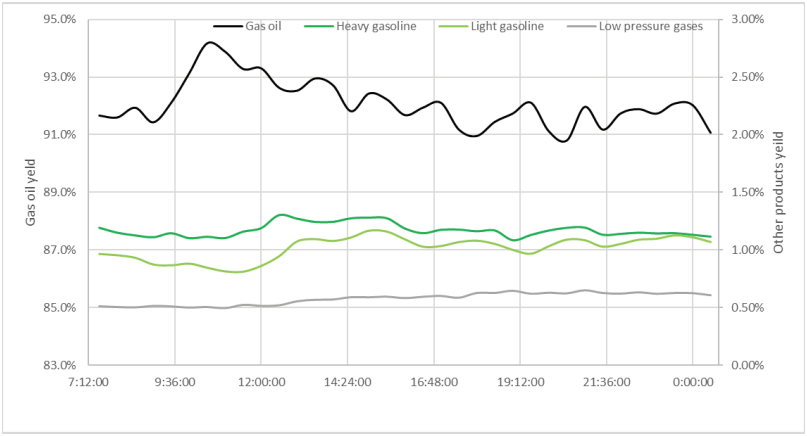


Figure 4 Yeld of BGHT7 main products during CNSL co-processing

Product analysis

Routine analyses of feedstocks and products were carried out by VÚRUP laboratories. A critical parameter in terms of the quality of the hydrogenated gas oil produced is the sulphur content. The biocomponent injection itself did not have a significant impact on this parameter; however, due to concerns about a potential excessive exothermic rise in the reactors, the temperature before the reactors was lowered prior to the CNSL injection, which subsequently had a negative effect on the sulphur content in the product. After the temperature was increased again, the sulphur content was suppressed to below 5 ppmw, while the typical specification limit is usually a maximum of 11 ppmw. This highlights the potential for optimizing injection temperatures for CNSL processing in the future, as operating the reactors at a sulphur threshold of up to 10 ppmw could have a positive effect on both heating gas consumption and hydrogen usage.

In co-processing, the impact on the low-temperature properties of the product, primarily represented by the cloud point, is closely monitored. The expected cloud point of hydrogenated gas oil is -1 °C for summer-grade and -3 °C for winter-grade fuel. During the operational trial, a transitional diesel fuel type was produced. The cloud point of the hydrogenated gas oil before the test-run was -2 °C and ranged between -1 °C and -2 °C throughout the test, indicating that the CNSL injection did not have a significant adverse effect on this key parameter.

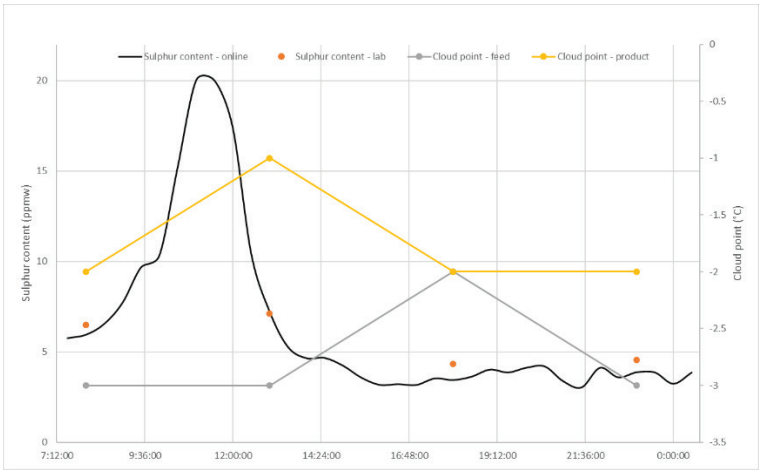


Figure 5 Key parameters – sulphur content, cloud point

In cooperation with the Department of Analytical Chemistry at the Faculty of Natural Sciences, Comenius University, the hydrogenation products of CNSL were analysed by GC-MS. The peak with a retention time of 20.33 minutes corresponds to n-pentadecylcyclohexane, which constitutes 1.2% of the sample. A minor but distinct peak at a retention time of 20.49 minutes was identified based on its mass spectrum as pentadecylbenzene, with a content of approximately 0.1%. Another minor peak eluting before the n-alkane C24 was identified as n-heptadecylcyclohexane, with a content of 0.06%. Phenolic components derived from cardanol were not detected.

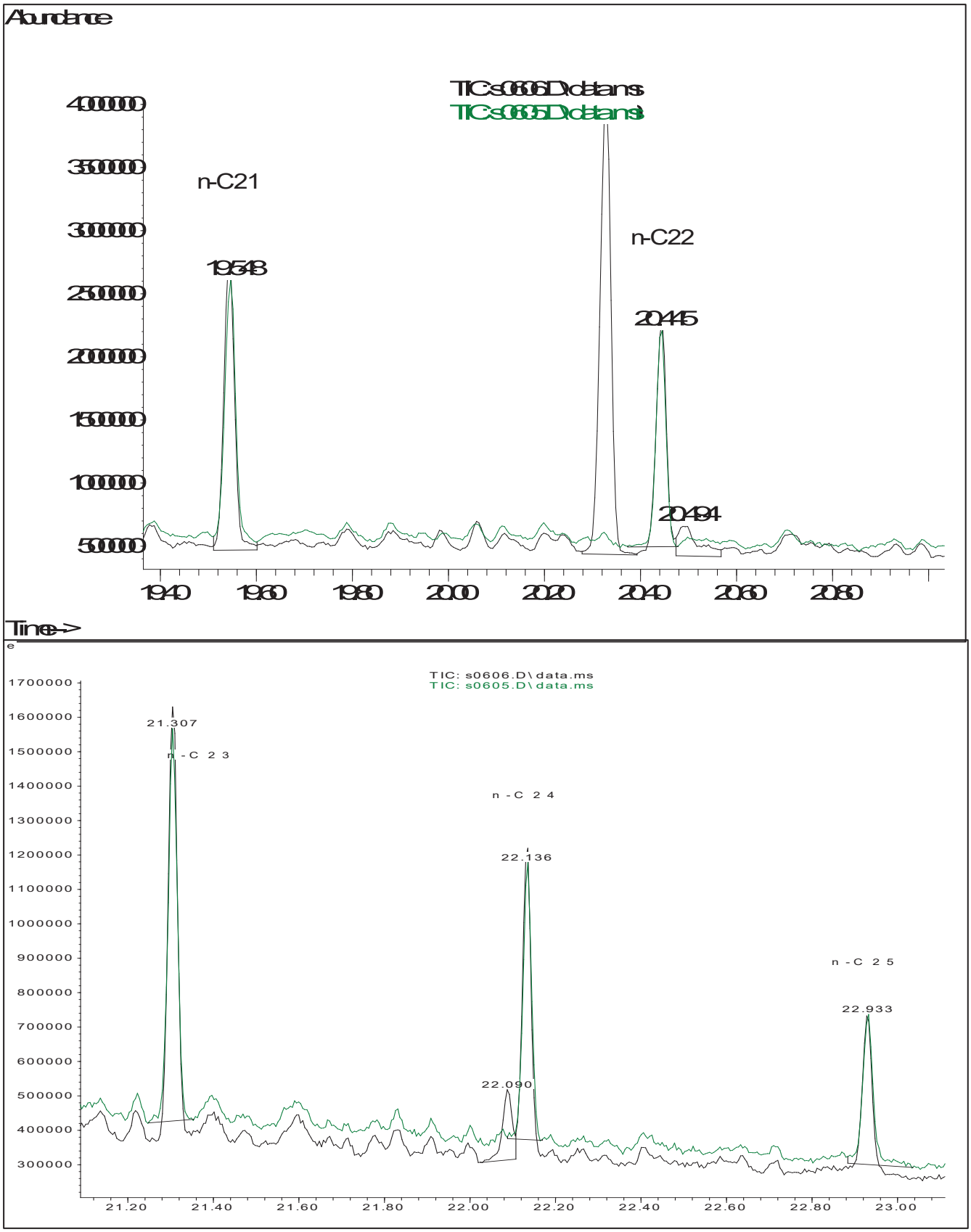


Figure 6 GC-MS analysis of gas oil with CNSL (green – feed, black - hydrotreated)

Samples of hydrogenated gas oil and naphtha were analysed for ^{14}C isotope content at the Izotoptech Zrt laboratory. The results are summarized in Table 2. In addition to these samples, non-hydrogenated gas oil was

also analysed using this method, showing a ^{14}C isotope content of approximately 0.2 %. The biocarbon content in the raw material could be attributed to the ongoing processing of slops in the distillation units, which are collected during the addition of biocomponents in the final production of motor fuels. Therefore, the average ^{14}C isotope value of 2.3 % measured in the CNSL-hydrogenated gas oil should be corrected by subtracting this baseline value.

Table II Isotope ^{14}C content analysis of gas oil

Sample time	^{14}C in gas oil (%)	^{14}C in Heavy naphtha (%)
3.9.2024 13:00	2.4	0.8
3.9.2024 18:00	2.5	1.5
3.9.2024 23:00	2.0	0.1
Average	2.3	0.8

Conclusion

The CNSL feedstock proved to be suitable for co-processing at the BGHT7 plant. The yield of hydrogenated gas oil decreased only slightly, from 92 % to 91 % wt. The addition of the biocomponent was reflected solely in the first hydrogenation reactor by an exothermic temperature increase of approximately 10 °C, with potential to reduce this temperature through optimized reactor heating in the future, considering the sulphur content. The purity of the circulating gas decreased minimally from 85.0 to 82.4 vol. %, while the purge capacity of the PSA unit was not fully utilized and the hydrogen make-up compressor did not reach its maximum output. During CNSL processing, there was no significant change in the low-temperature properties of the produced diesel; the cloud point ranged between -1 and -2 °C, and the biocomponent did not cause any increase. GC-MS analysis confirmed the presence of CNSL hydrogenation products, with n-pentadecyl cyclohexane constituting the largest portion at 1.2% wt. The ^{14}C isotope analysis confirmed the presence of 2.1% wt biocomponent in the produced gas oil.

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EVALUATION AND OPTIMIZATION OF THE WATER QUENCH COLUMN OF UNIPETROL'S STEAM CRACKER

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Abstract

The Water Quench Tower is a key part of steam cracker technology, cooling cracked gas before it enters the Cracked Gas Compressor (CGC). If cooling is insufficient, heavier hydrocarbons and excess steam can overload the CGC, increasing HP-steam consumption and operating costs. Elevated temperatures also promote polymer fouling, reducing heat transfer efficiency and causing higher pressure drops.

To address limited process data, a simulation of the hot section—including the Quench Tower and Primary Fractionator—was developed in Aspen HYSYS. This helped estimate the inlet stream composition of Water Quench Tower and better understand separation efficiency and process limitations.

The study focuses on optimizing operating conditions and implementing fouling prevention strategies. The main objective is to reduce HP-steam usage and CO_2 emissions by improving the reliability and performance of the quench tower, contributing to more sustainable ethylene production.

Introduction

Ethylene and propylene, two of the most widely used building blocks in the petrochemical industry, are primarily produced by steam cracking. Steam cracking, though well established, involves highly reactive intermediates and extreme operating conditions. Hydrocarbon feedstocks like naphtha or LPG are rapidly heated to temperatures over 800 °C to induce thermal decomposition. Once cracking occurs, the resulting cracked gas must be cooled to suppress unwanted secondary reactions, such as over cracking, polymerization or coke formation.

Immediate and controlled cooling of the cracked gas is critical. At Unipetrol's steam cracker in Litvinov, this initial rapid cooling is performed within the hot section of the unit, which includes two major process nodes: the Primary Fractionator, followed by the Water Quench Column (WQC). The Primary Fractionator inlet stream is the cracked gas directly from the pyrolysis section. Its role is to rapidly cool the gas and separate heavy hydrocarbons. The overhead vapor then flows into the Water quench column, located downstream, where the quench water is used to remove the remaining additional heat from the stream before it proceeds to compression node.

The performance of both columns is tightly linked. Together, they determine the thermal and phase behaviour of the cracked gas as it enters the compression node and the cold section of the unit. Even subtle inefficiencies in heat transfer, separation, or internal hydraulics can affect the downstream operation, such as overloading the Cracked Gas Compressor (CGC) or buildup of polymer deposits.

In early 2025, this study was initiated to evaluate and optimize the performance of the Water Quench Column, with particular attention to thermal efficiency. The modelling and simulation work was based on operational data and aimed to identify areas for improvement. However, early stages of the project were complicated by abnormalities in the behaviour of the Primary Fractionator, which showed signs of poor separation and heat transfer efficiency. At that time, the underlying causes of these divergencies were not fully understood. Later that year, during the scheduled turnaround, new information provided important context for interpreting these issues and raised further questions regarding the long-term condition of the unit. In particular, the possibility emerged that some of the malfunctions might be linked to the major fire in 2015, which had caused significant mechanical damage.

The objective of this paper is to evaluate and optimize the operation of the Water Quench Column, using both simulation results and new insights gained during the 2025 turnaround. The work aims to clarify the WQC's role in the system-wide performance and investigate previously unexplained operational behaviour.

Process Description

As mentioned, the hot section of Unipetrol's steam cracker is responsible for the rapid cooling of the cracked gas after it exits the pyrolysis section. The cracked gas first enters the primary Fractionator after passing through a set of transfer-line exchangers (TLEs), which recover part of the sensible heat.

Table I
Specification of Primary Fractionator and Quench Water Column

Column Configuration	Primary Fractionator	Quench Water Column
Height	37 m	35 m
Internals	15 valve and 7 chevron trays	3 structured packings
Temperature profile	200 – 100 °C	100 - 30 °C
Quench medium	Heavy pyrolysis gasoline recycle	Quench water

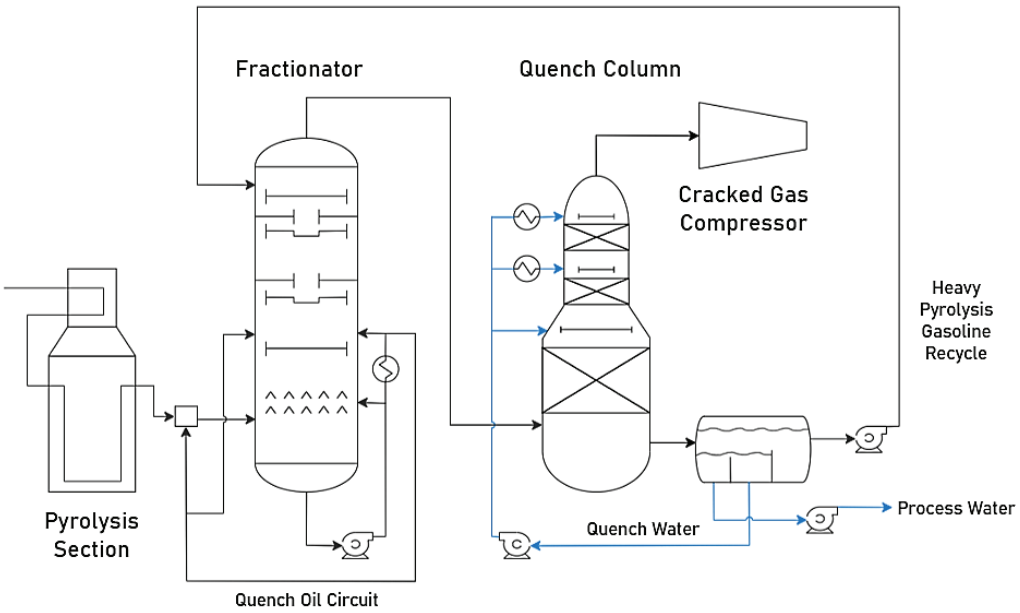

Figure 1. Process diagram

The cracked gas leaving the TLEs first enters the Primary Fractionator, where heavier components such as pyrolysis oils are partially separated. The remaining vapor then flows into the WQC, where it is directly cooled by circulating quench water. From the WQC, a portion of the condensed heavy pyrolysis gasoline is recovered and returned as a reflux to the Fractionator, supporting its separation efficiency and improving overall recovery. Additionally, the bottom section of the WQC provides heat to the reboiler of the propylene column, establishing a thermal and mass transfer link between the hot and cold sections of the ethylene unit.

Historical background: Impact of the 2015 fire

On August 13, 2015, a major accident occurred at Unipetrol's steam cracker unit, marking the largest petrochemical incident in the Czech Republic in over two decades. The explosion and fire originated in the cold section for propylene isolation, but the consequences affected multiple parts of the unit.

The incident was initiated by a loss of cooling to the condensers of the propylene column, resulting from the improperly executed pipeline switch during maintenance. This situation escalated into a loss of reflux, and shortly after, the pressure relief valves (PRVs) at the top of the column were activated. While the PRVs were designed to

handle emergency relief scenarios, chattering – a fast, cyclical opening and closing of the valve – triggered massive vibrations of the safety valves. These high frequency vibrations led to the mechanical failure of the flange connections at the inlet to one of the valves. The resulting loss of propylene vapor formed a flammable cloud, which ignited upon contact with a nearby high-pressure steam pipeline surface exceeding 500 °C, leading to a massive explosion and fire.

The explosion damaged critical utilities, including high-pressure steam and instrument air lines, leaving large parts of the unit uncontrollable. As a result, multiple pyrolysis heaters could not be safely shutdown. Under the conditions of emergency shutdown without controlled cooling, the radiant coils rupture on one of the pyrolysis heaters causing a localized fire that quickly spread to other heaters too.[2]

Relevance to the Present Study

Although the plant was fully repaired and restarted after the incident, the long-term process and mechanical impacts of the fire are still being uncovered. One of the known outcomes was the polymer fouling in the reboiler of the propylene column, likely caused by extended air exposure during post-incident repairs. During this time, residual higher hydrocarbons, referred to as ''yellow oil'', remained inside the equipment. When exposed to atmospheric oxygen, these unsaturated compounds likely underwent autooxidation and crosslinking, leading to the formation of a chemically and mechanically resistant polymer.

This polymeric layer is believed to have gradually blocked the inter-tubular space in the propylene column reboiler and therefore reducing heat transfer efficiency. Since this reboiler is heated using excess heat from the WQC, the system had to compensate for the reduced efficiency by raising the temperature on the WQC side. As a result, the WQC operated at higher temperature than originally intended.

Figure 2. Polymer deposit found in the inter-tubular space of propylene column reboiler

Methodology

The process modelling and evaluation work was performed using a steady-state simulation based on Aspen HYSYS. The simulation was constructed using the Peng-Robinson equation of state. Operational data were collected from the site's Control System and archived process databases. The datasets spanned regular operation periods in late 2023 and 2024. However, due to the limited number of sampling points along the columns, the available data were restricted to a small number of temperature and pressure readings.

To better understand the performance of the WQC and Primary Fractionator under different operational conditions, two separate steady-state simulation scenarios were developed. The first model assumed ideal behaviour. In contrast, the second model aimed to reflect more realistic conditions based on pre-turnaround data and observed operational issues. This included reduced tray efficiency due to fouling and possible mechanical damage, higher temperature in the WQC, and decrease in the quality of pyrolysis gasoline used as reflux.

Results and Discussion

Turnaround 2025 Observations

During the 2025 turnaround, several critical mechanical issues were identified across both the Primary Fractionator and the Water Quench Column. Visual inspection revealed polymer fouling on multiple trays inside the Primary Fractionator, with several trays showing signs of deformation or collapse. This kind of damage is consistent with gas bypassing and loss of vapor–liquid contact, which may explain the observed deviations from normal separation behaviour prior to the turnaround.

Figure 3. Polymer deposit found in the Primary Fractionator

In addition to the visual confirmation of fouling during the 2025 turnaround, further evidence of declining column performance is reflected in operational data recorded over the months preceding the outage. Figure 4 shows the combined trend of the overhead temperature, temperature at the sixth tray, and the total pressure drop across the Primary Fractionator between the September 2024 and March 2025.

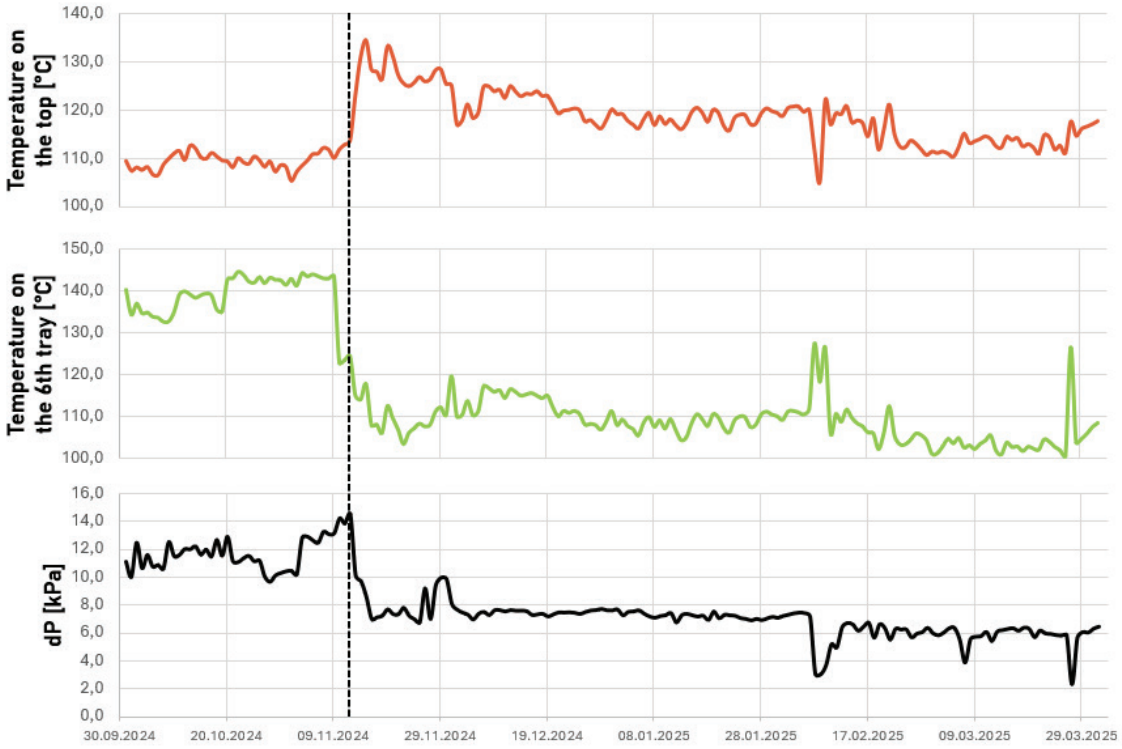

Figure 4. The temperature profile and pressure drop of Primary Fractionator

During the monitored period, a clear shift occurred in early November 2024. Initially, a gradual increase in pressure drop was observed, indicating rising hydraulic resistance likely caused by fouling and partial blockage of the trays. This was followed by sudden decrease in pressure drop, accompanied by fall in the 6th tray temperature and increase in overhead temperature. This combination suggests that the increased load may have damaged internal structure, leading to gas channeling, where vapor partially bypasses the flooded tray, further undermining the intended separation mechanism. These effects point to a gradual loss in efficiency that culminated in the need for a corrective action during the turnaround.

In addition to the degradation observed in the Primary Fractionator, further attention was given to the propylene column reboiler, which is thermally coupled with the bottom section of the WQC. The buildup of polymer in the reboiler likely impaired its heat transfer capacity, requiring higher operating temperature in the WQC to maintain sufficient heating duty. This temperature increase in the lower section of the WQC appears to have caused localized polymerization within the structured packing. The formation of polymer deposits in the WQC not only reduced the mass transfer efficiency but also compromised the quality of the recovered pyrolysis gasoline, which is used as reflux in the Primary Fractionator. This introduces a plausible pathway for early-stage polymer precursors to be carried back into the Primary Fractionator, where they have contributed to fouling. The resulting decline in separation efficiency then degrades the quality of cracked gas returning to the WQC, creating a self-reinforcing degradation loop.

Operational Impact of Polymerization

The simulation results revealed significant differences in stream composition between the ideal and non-ideal operating scenarios. One of the most notable findings was a marked increase in the concentration of aromatic compounds, especially heavier C9+ aromatics, observed in the Fractionator outlet stream. In realistic case, the total aromatic content increased by 2,7 %, while the concentration of heavy aromatics (C9+) rose by as much as 21 %. This substantial shift supports the hypothesis that poor separation efficiency and contaminated reflux allowed heavier, unsaturated components to migrate further downstream.

Under ideal conditions, these aromatics would be effectively retained in the lower sections of the Primary Fractionator. However, in the realistic case, tray inefficiency and reduced vapor-liquid contact allowed them to carry over into lighter product streams. This led to a measurable drop in product purity, which is consistent with plant observations in the period before the turnaround. The impact is illustrated in Figure 5, where the aromatic content is compared in the Fractionator overhead outlet stream. These findings highlight how even small mechanical and thermal imbalances can significantly influence the system's performance.

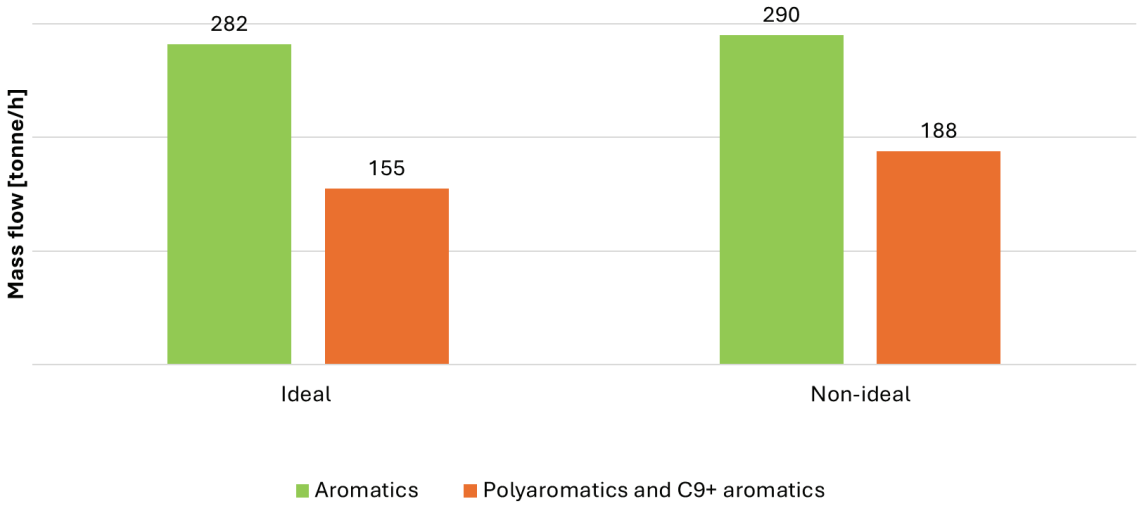

Figure 5. Changes in the composition of Fractionator outlet stream

Conclusion

The presented results demonstrate that mechanical degradation, particularly in the form of polymer fouling, can gradually undermine the performance of both the Primary Fractionator and the Water Quench Column. Observed shifts in temperature profiles and pressure drop, along with the marked increase in heavy aromatics content, support the hypothesis of a system-wide feedback loop, where heat transfer limitations in the propylene column reboiler led to inefficient operation, reflux contamination, and further fouling upstream. These insights highlight the importance of early detection and cross-linked diagnostics across units.

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IMPACT OF QUENCH TOWER MALFUNCTION ON STEAM CRACKER YIELDS AND PERFORMANCE

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Abstract

This paper deals with the analysis of the impact of primary fractionation column malfunction on the operation of steam cracker focusing on changes in the distillation profile, yields of key products and necessary changes in operating parameters. Damage to the column internals led to a reduced ability to separate pyrolysis products. Maintaining effective fractionation in the column required increased pyrolysis gasoline recycle. This change had a major impact on the composition of medium and heavy pyrolysis condensates.
The paper further describes the effect of pyrolysis gasoline recycle on the yields of light olefins (ethylene, propylene) and the increased formation of aromatics and carbon precipitates. During pyrolysis, naphtha containing a higher proportion of unsaturated hydrocarbons (C5 and C6 olefins) is cracked by a different mechanism than regular naphtha, which reduces the conversion to light olefins and promotes a higher coking rate in pyrolysis reactor. Other topics include changes in the temperature profile of the furnaces, reduced steam production and strategies to optimize operation under these conditions.
The results of this work are relevant not only for dealing with unplanned operational malfunctions, but also for predicting the impact of processing pyrolysis oils from waste plastics in steam crackers. Pyrolysis oil from waste plastics has a similar composition to recycled pyrolysis gasoline, which provides valuable insights for future integration of this feedstock into the steam cracking process.

Introduction

The global production and consumption of plastics continues to grow and is also one aspect of a country's economic maturity. Virtually all widely used types of plastics (polymers) are produced from monomers made from fossil sources. The most widely used raw materials for the production of these monomers worldwide include ethane, LPG and naphtha fractions. These groups of hydrocarbons are processed at steam crackers by pyrolysis. This process is the most widely used worldwide and is very energy demanding.
The most widely used feedstock for pyrolysis in Europe is naphtha. The pyrolysis of this fraction, in addition to the main products (ethylene and propylene), provides a range of by-products that can be used in the production of other polymers, dyes, solvents, pharmaceuticals and organic synthesis. In addition to the main operating parameters, the composition of the feedstock also has a major influence on the yields of the individual components in the product.
The aim of this paper is to introduce the reader to some of the complex relationships between the different sections of the steam cracker, focusing on the loss of separation ability at the primary fractionator and the fluctuating composition of the naphtha feedstock, which affects the overall efficiency of the steam cracker.

Process Overview

The investigated unit comprises of quench oil tower, quench water tower and associated separation and recovery systems. The quench oil tower is responsible for primary cooling and separation of heavy hydrocarbons (e.g., PGO, PFO), while the water tower enables further cooling and separation of cracked gas from dilution steam (water). Basic correlations are shown in a figure bellow.

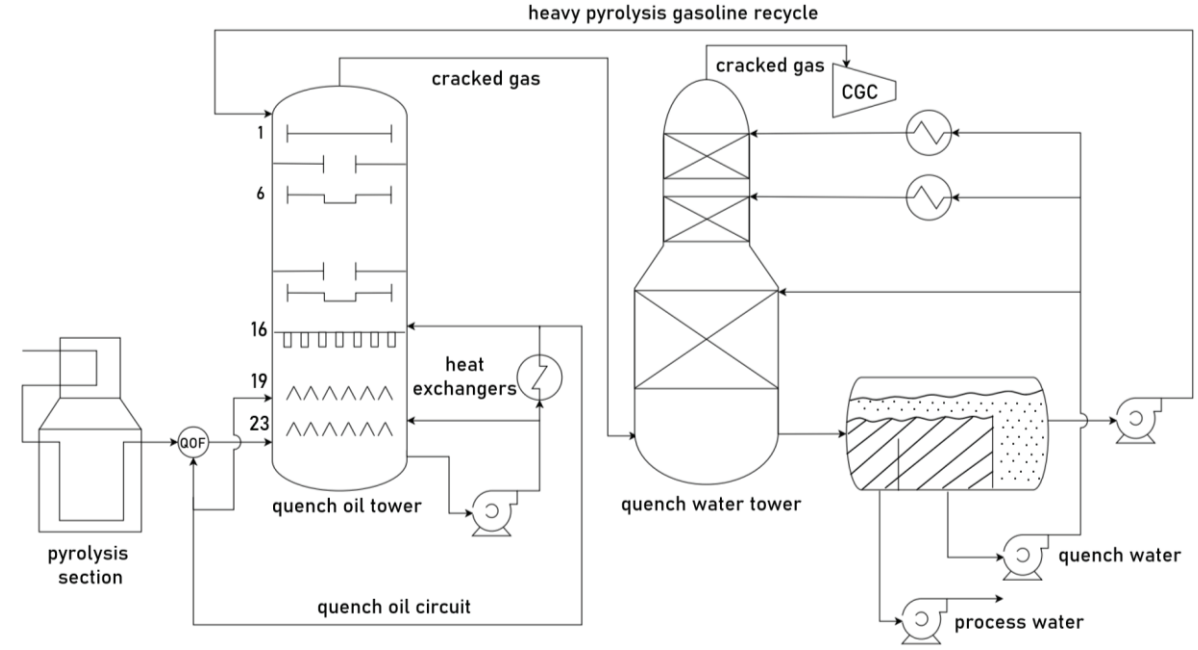

Figure 7: Basic chart of a hot section of a steam cracker

Event timeline

Beginning on 10th November 2024, initial signs of malfunction in the quench oil tower are detected. On 13th November 2024 increasing operational irregularities are observed (pressure drop, tray temperatures). Radionuclide scan of the whole tower is conducted, giving however no definitive answer on the cause. Most sings seem to lead to damaged trays. In figure 2, temperature at first and fifth tray on 9-15th November are showed.

11/8/2024 10:19:07 AM 11/15/2024 4:19:07 A

	Visible	Trace Color	Object Name	Object Description	Current Value	Ruler Value	Ruler Time	Low Range	High Range	Time Offset	Style	Mean Value	Min Value	Max Value	Extrapolate	Property	Log Name
1	X		1TI01277	DA101 5.P	107.20	136.71	11/10/2024 3:02:01 AM	99.61	176.17	00:00:00 00:00:00	Linear	116.58	110.30	145.00	Value	MEASURE_COMP	SEAMLESS
2	X		x1TI01277	DA101 5.P	107.04		11/10/2024 3:02:01 AM	0.00	250.00	00:00:00 00:00:00	Linear				Value	Measure	SEAMLESS
3	X		1tch01276	DA101 HLAVA	118.65	110.73	11/10/2024 3:02:01 AM	100.00	140.00	00:00:00 00:00:00	Linear	131.62	109.73	135.49	Value	MEASURE_COMP	SEAMLESS
4																	
5																	
6																	

Figure 2: Temperatures at respective trays of quench oil tower

Next, on November 23rd 2024 feedstock pumps at DPG unit catch on fire, only further disrupting steam cracker balance and prohibiting pyrolysis gasoline processing. The excess of pyrolysis gasoline that would accumulate during the shutdown of the DPG unit if it were not further processed would be enormous. The only reasonable processing option was to co-pyrolyse it with naphtha. Selected parameters of quench oil tower are shown in figure 3 below.

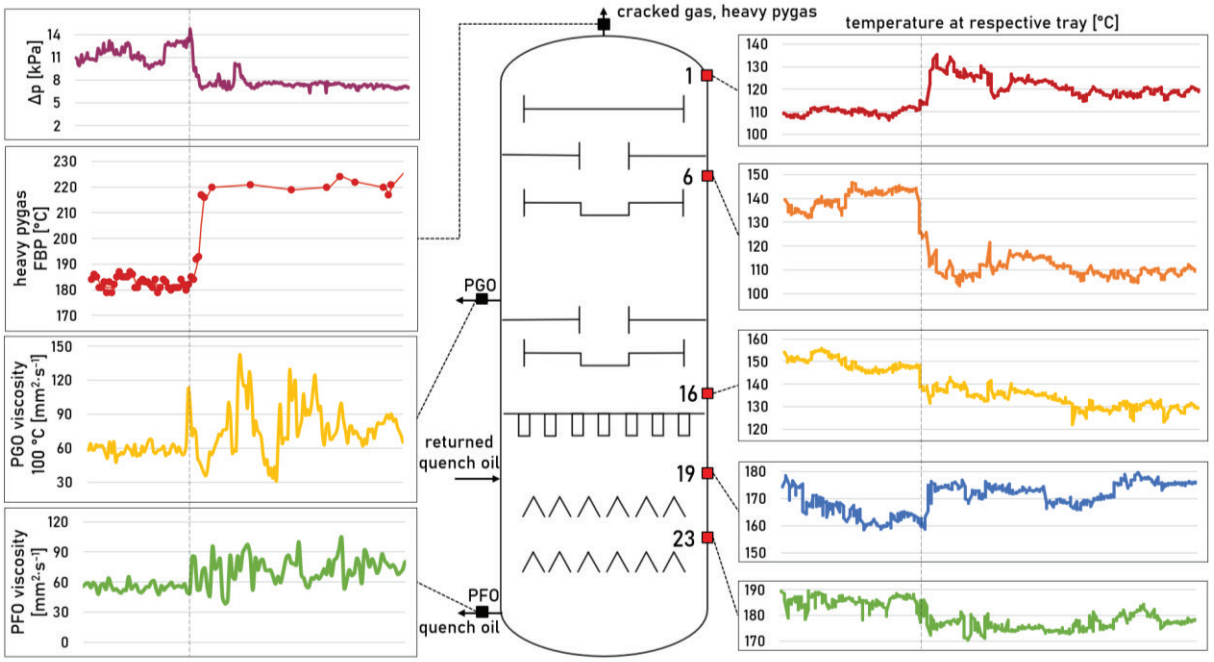

Figure 3: Quench oil tower parameters, dashed line indicates the turning date od 13th November

Experiment

The experimental part of the work was carried out to determine the effects of the co-pyrolysis of the pyrolysis gasoline. Due to pyrolysis gasoline having significantly higher aromatic and olefin content and higher density, than naphtha, severe effects on yields were to be expected. The experiment consisted of continuous monitoring of laboratory analyses of the properties of naphtha (PIONA). Sampling of hot pyrolysis products was carried out during the monitoring of the feedstock itself.

Analysis of feedstock

The samples of the feedstock and cracked gas were taken at the same time and immediately analysed by gas chromatography (GC). Analysis of the samples was performed on Agilent Technologies 7890A gas chromatographs. Typical raw material group compositions from hot cracked gas sampling are shown in table I.

Table I: Typical feedstock composition

Component [% wt.]	Typical naphtha	Blended naphtha
n-alkanes	26,7	23,3
i-alkanes	33,8	32,8
olefins	3,2	4,1
naphthenes	27,2	27,3
aromatics	8,3	11,3

Hot gas sampling

Method of hot gas sampling was conducted at pyrolysis heaters cracking feedstock. The method allows for getting qualitatively and quantitatively representative sample of hot pyrolysis products separated into three different fractions (PFO, pyrolysis gasoline, cracked gas). Quantitative results were obtained from mass balance based on amounts of liquid products and known volume and density of cracked gas. Qualitative composition was obtained by GC.[1]

Impact of malfunction on quench oil tower
Damage to internal trays led to severe maldistribution of the flow and gas channeling, compromising the separation efficiency. Notable observations included:

- Tray temperature anomalies: e.g., the first tray temperature increased from 110 °C to 125 °C, while the sixth tray dropped from 140 °C to 110 °C
- Reduced pressure drop across the tower (Δp = 7–9 kPa instead of normal 13–16 kPa)
- Heavy pygas density increased, suggesting uneffective separation ability

Impact of malfunction on quench water tower
As a consequnce of poor separation in the oil tower, the water tower experienced:

- Aromatic buildup in the water/pygas phase in separator
- Emulsion formation tendency due to a lower density difference of water/organic phase
- Higher temperature at the top, reducing separation efficiency and downstream cracked gas cooling

Adjustment of the process parameters of the quench oil tower
In order to stabilize the quench oil tower and therefore the steam cracker unit as a whole, several major operational interventions had to be made. Most important were:

- Plant load was lowered form 1480 t·day-1 to 1000 t·day-1 of ethylene
- Reflux maximization in order to lower the temperature at the top of the tower
- Compressor suction pressure was increased from 40 to 80 kPa

While turnaround, physical evaluation of the tower insides uncovered damaged (cracked, tilted) and in some cases missing trays, leading to gas channeling and poor tray flooding. Some oligomer deposit buildup was also found.

Table II: Yields of typical and blended naphtha respectively

Component [% wt.]	Typical naphtha	Blended naphtha
Hydrogen	0,84	0,66
Methane	13,35	10,93
Ethylene	25,96	20,60
Propylene	13,88	11,15
Buta-1,3-diene	4,24	3,49
Benzene	9,33	14,98
Toluene	4,94	7,90
Styrene	1,44	2,50
Naphthalene	0,91	1,94
C_{9+} aromatics	4,61	6,87
oil	4,49	6,65

The table II clearly shows the effect of raw material composition on yields. While keeping the same reaction

conditions (COT 830 °C, S/O 0,50, feed 26 $t \cdot h^{-1}$), the higher content of linear alkanes and isoalkanes in regular naphtha corresponds to higher yields of methane, ethylene and propylene. Naphthenic hydrocarbons, the content of which is similar in both types of gasoline and whose pyrolysis usually leads to the formation of dienes, correspond to a comparable content of buta-1,3-diene and other C4 and C5 dienes in the product. Conversely, because of the substantially increased content of olefins and aromatics, which tend to pass through the process either unchanged (in the case of aromatics) or condensed (olefins and aromatics) to form heavier hydrocarbons and coke, the blended gasoline shows a substantial increase in the heavier aromatic hydrocarbons in the yields, namely benzene, toluene and pyrolysis oil.
A total of 6 hot cracked gas samplings were carried out on pyrolysis furnaces equipped with GK6 reactors all of which were on furnaces with BAT layout (T.EN). The results of the sampling show a clear correlation between the change in the group composition of the primary gasoline and the change in the pyrolysis yields, even when the operating parameters of the pyrolysis furnace are kept the same.

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STUDY IN THE INFLUENCE OF FEEDSTOCK TYPE AND PROCESS PARAMETERS OF PYROLYSIS HEATERS ON THE FORMATION OF COKE DEPOSITS

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Abstract

The ORLEN Unipetrol's steam cracker has a total of eleven pyrolysis heaters fitted with three different types of pyrolysis reactors. The cracker can process five different hydrocarbon fractions (ethane, LPG, different naphtha fractions, atmospheric gas oil and hydrocracker residue). The variety of feed-stocks in combination with different design of pyrolysis heaters (configuration of reactors, arrangement of the individual tube bundles of the convection sections, TLEs) allows the deep investigation of the coke formation and deposition at different process conditions. The paper focuses on the quantitative aspect of coke formation for each type of feedstock. The compilation of the proper mass balance of the coke deposits is an essential condition enabling the description and understanding of the process of coke formation and deposition. The properly settled mass balance is capable to precisely quantify the amount of coke produced during the pyrolysis of individual feed-stocks. Taking into account that the proper mass balance has to cover both the amount of coke deposits carried in the stream of cracked gas and deposited on the surface of reactors tubes and TLEs. While the coke carried in the stream of cracked gas can be estimated only in limited way using the CRU situated at the quench oil loop, the amount of coke deposited in reactors and TLE can be precisely determined as the sum of the coke converted to carbon dioxide during decoking, remnants of coke remaining on the walls of TLE tubes and portion of coke released during the decoking and separated in the cyclone situated downstream the joint decoking line. The achieved results are presented for four different process cases, i.e. cracking of ethane (SMK reactors), LPG (SMK reactors), naphtha (GK6 reactors) and hydrocracker residue (SRT III reactors).
The comparison of the results enables to make general conclusions applicable to the coke deposits production at whole pyrolysis section of the steam cracker. The compilation of the balances brings an important benefit for the optimization of process parameters in case of different pyrolysis heaters, especially more precise estimation of the length of the operating cycle and decoking time. The better understanding of the coking rate makes more efficient the management of pyrolysis section, i.e. the determination of the appropriate timing of coils decoking and TLE cleaning.

Introduction

The pyrolysis section of ORLEN Unipetrol's steam cracker consists of eleven pyrolysis heaters fitted with three different types of pyrolysis reactor (SMK, GK6 and SRT III). Feedstocks processed are ethane, LPG, different naphtha fractions, atmospheric gas oil and hydrocracker residue. The aim of the research is the deep investigation of the coke formation and deposition at different process conditions is an essential condition enabling the description and understanding of the process of coke formation and deposition.
It can be distinguished two types of coke. The first is catalytic coke which is a hard type of coke, deposition especially in the pyrolysis coils and mainly produced by pyrolysis of naphtha fractions. The catalytic coke is shown in Figure 1.

Figure 1. Catalytic coke

The second one is pyrolytic coke which is a soft type of coke, deposition especially in the transfer line exchanger (TLE) and mainly produced by pyrolysis of hydrocracker residue.

Simulation and/or experiment

The experimental plan starts when the pyrolysis heater comes into routine repair - during this repair the waste heat boilers are cleaned. After inspection of the cleaned boilers and a general inspection of the heater, the furnace will start up into hot backup. The heater is fed on the feedstock with the appropriate process parameters, which are holding throughout the operating cycle. It is important to monitor the operation - regular pyrometric measurements of the surface temperatures of the coils, and sampling of hot cracked gas - to determine the yields of individual products. The decoking is carried out using an air compressor with water vapour, where the carbon is converted to CO_2, during the experiments the flue gases were taken after every twenty minutes and analysed on a gas chromatograph with results in % vol. CO_2. The decoking process was carried out through a cyclone (FC-101), which the separator ensures the capture of coke from the flue gases during decoking of pyrolysis heaters and then the cleaned flue gases are introduced into the stack. The cyclone is shown in Figure 2.

Figure 2. The cyclone

After the decoking process, nitrogen is fed into the cyclone as part of the drying and cooling of the coke. The coke was always discharged the day after decoking, the coke was dumped into a big bag and weighed. After weighing, about ten kilograms of coke was taken in a bag, which was put in storage and a one kilogram representative sample was taken, which was spread on a plate metal and given to the laboratory, where the plate with the coke was left to dry under laboratory conditions. Regular weighing was carried out to determine the water loss, if the weight was the same 3 times in a row, the coke plate was put into the dryer. In the drying room it was the same again 3 times in a row if the weight was the same, then the coke was considered dry and converted to total weight. After decoking pyrolysis heater swapped the connection from the decoking line DN 500 to the atmosphere exhaust DN 300 and the pyrolysis heater started ramp down fifty degrees celsius per hour the pyrolysis heater to cold backup. The day after the cold backup, the transfer line exchangers started to open. After the transfer line exchanger was opened, the coke layers were checked and measured. The coke from each transfer line exchanger was taken into sample tubes and the density was determined and after the tubes were measured and observed, the transfer line exchangers started to close. The process parameters of the

experiments are shown in Table I. The transfer line exchanger inspections before and after the experiment are shown in Figures 3 and 4.

Table I

Process parameters

Parameters	BA-106	BA-110	BA-102
Feedstocks	Hydrocracker residue	Naphtha fractions	Hydrocracker residue
Reactor	SRT III	GK6 (new)	SRT III
Feed, t/h	23.0	25.0	23.0
COT, °C (coil outlet temperature)	797	833	797
S/O ratio (feedstock/steam)	0.75	0.48	0.75
Number of days in operation	37.5	64.7	18.5

Figure 3. The transfer line exchanger inspections before and after the experiment - BA-106 (hydrocracker residue)

Figure 4. The transfer line exchanger inspections before and after the experiment – BA-110 (naphtha fractions)

Discussion and result analysis

So far three experiments have been completely evaluated, from hydrocracker feedstock and naphtha fractions at the following process parameters, which are shown in table I. The results gained by the evaluation of this process date are shown in Table II. The individual carbon deposits come from four different sources.

Table II
Results of carbon deposits

Carbon deposits	BA-106 Hydrocracker residue (kg)	BA-110 Naphtha fractions (kg)	BA-102 Hydrocracker residue (kg)
Carbon deposits accumulated from FC-101	107.9	749.4	205.5
Carbon deposits burnt during decoking	211.5	620.8	257.4
Carbon deposits leaving with the cracked gas	315.0	550.0	420.0
Transfer line exchanger	23.0	1.0	6.0
Total of carbon deposits	657.4	1921.2	888.9

At the pyrolysis heater BA-110 the amount of coke is less than two tons. The largest content of carbon deposits was from FC-101, unburnt coke from decoking. At the pyrolysis heaters BA-106 and BA-102 was the largest content of carbon deposits leaving with the cracked gas. These results confirmed that pyrolysis of naphtha fractions produces a hard (catalytic) coke, that are deposited on the inner surface of pyrolysis coils. on the contrary, pyrolysis of hydrocracker residue produces soft (pyrolytic) coke, which is entrained with the cracked gas.

Scanning electron microscopy images with elemental analysis were taken of individual carbon deposits, which are shown in figures 5 and 6. Figures are ten micrometers in size.

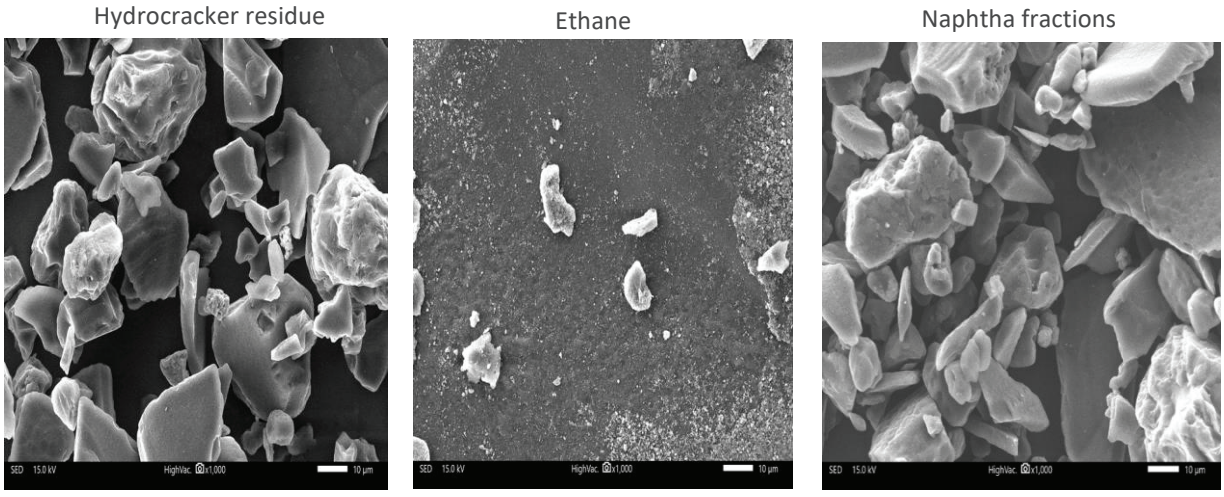

Figure 5. Differences of carbon deposits

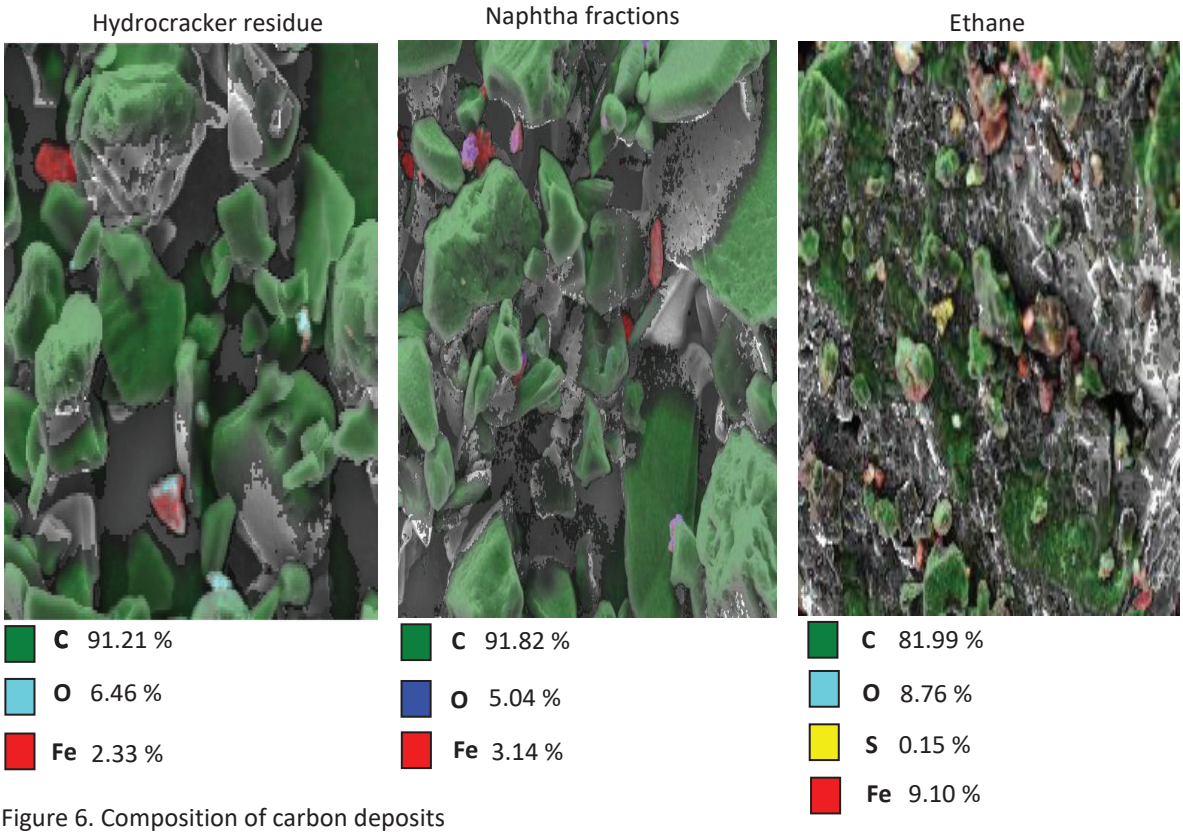

Figure 6. Composition of carbon deposits

Conclusion

So far we have an idea of how much coke is being produced and this work will lead to optimization of the control of the decoking of the heaters, so far are the so-called typical progress, as suitable, no longer. At least thirty experiments are needed for application. The formation of a carbon deposits balance sheet will be of great benefit for the control and optimization of the operation parameters of pyrolysis heaters

- Give a much more accurate estimate of the operating run length
- Time required for removal of carbon deposits
- Correct timing of transfer line exchangers cleaning
- Reducing emission permissions
- Better understanding of the coking rate

Acknowledgement

The author would like to thank ORLEN Unipetrol RPA for their support of this research.

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COKE BALANCE DURING THE DECOKING OF PYROLYSIS HEATERS

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Abstract

The pyrolysis section of ORLEN Unipetrol's steam cracker unit includes eleven heaters that process four different types of feedstock. The pyrolysis heaters operate in cycles. The operating cycle terminates with the removal of the carbon deposits (coke) produced during pyrolysis. The coke produced during the pyrolysis of hydrocarbons is a significant operational problem as its accumulation inside the reactors and transfer line exchangers reduces the efficiency of heat transfer and increases the pressure losses in the reactor. Regular decoking is necessary to maintain a stable operation of the unit.
The paper describes a methodology for quantification of combusted coke based on mass balance and flue gas composition analysis. The calculation model uses flue gas composition data at time intervals from experimental sampling and allows estimation of the total amount of removed coke.

Introduction

The pyrolysis heater is a critical component in the ethylene production process, used for the thermal cracking of hydrocarbons such as ethane, propane, naphtha, LPG, and hydrocracker residue (HCR). The main purpose of these heaters is to produce olefins — particularly ethylene and propylene — through the process of steam cracking. Pyrolysis is an endothermic reaction that requires significant heat input to break down complex hydrocarbons into simpler compounds.[1] This heat is provided by the heater burners, which heat the coils where the cracking reactions occur.
One of the major operational challenges in pyrolysis heaters is coke formation. Coke is an inevitable byproduct of pyrolysis, particularly in steam cracking reactors. During pyrolysis, complex hydrocarbons such as ethane, propane, naphtha, and LPG are cracked into lighter compounds like olefins (e.g. ethylene, propylene) and other gaseous hydrocarbons. However, some carbon from the feedstock does not fully react and instead forms coke, which deposits on the inner walls of the reactor coils. This coke buildup reduces heat transfer efficiency, increases pressure drop, and necessitates regular decoking.[2]
Coke can form through several mechanisms:
Catalytic Coke Formation: This reaction occurs when metal surfaces inside the reactor — typically iron and nickel — catalyse the dehydrogenation of hydrocarbons at high temperatures. The products of these reactions are often carbon-rich, leading to coke deposition on the reactor walls. This type of coke formation is more prominent with certain feedstocks, such as naphtha.[3]
Radical Coke Formation: In this mechanism, free radicals formed during pyrolysis can undergo polymerization reactions, resulting in coke deposits. These reactions are strongly influenced by the operating temperature and the chemical composition of the feedstock.[3]
Condensation of Heavy Aromatics: Heavy aromatics formed during the cracking of heavier hydrocarbons are prone to condensation reactions. These condensed species can accumulate and form coke deposits on the reactor walls.[3]
To mitigate coke formation, dimethyl disulfide (DMDS) is often added to the feedstock. DMDS acts as an effective coke inhibitor by preventing the formation of hard carbon deposits on the reactor coils. Additionally, modern reactors employ advanced alloys and surface coatings that resist coke buildup and extend the interval between decoking cycles.[2]
Decoking is a necessary maintenance process involving the removal of coke deposits from reactor coils. This is typically carried out by injecting of air and steam mixture under specific conditions into the pyrolysis reactor. Decoking is essential to restore the heater's heat transfer efficiency; however, it results in production downtime. The frequency of decoking is therefore a key factor in the overall economics of the pyrolysis process.

Experiment

The aim of the experimental part of this paper was to quantitatively determine the amount of coke removed during the decoking of selected pyrolysis heaters at the ethylene unit of ORLEN Unipetrol RPA. The experiment was carried out on heaters BA-102, BA-106, and BA-110 by collecting data and subsequently analysing the composition of flue gas during the final phase of the operational cycle, specifically during the decoking procedure.

Flue gas samples were taken at the outlet of each heater during decoking, a period characterized by the combustion of coke deposited on the inner walls of the pyrolysis reactor, associated heat transfer surfaces, and piping. Sampling was conducted manually at twenty-minute intervals. Each sample was subsequently analysed by gas chromatography (GC) to determine the volumetric concentration of carbon dioxide (CO_2) and carbon monoxide (CO). Based on the measured concentrations of CO and CO_2, a mass balance of the combusted carbon was calculated in MATLAB software. It was assumed that all detected CO and CO_2 originated from the oxidation of solid carbonaceous deposits.

```
%Iteration
n_out = zeros(size(n_air));
n_CO2 = zeros(size(n_air));
n_CO = zeros(size(n_air));
n_C = zeros(size(n_air));
for i = 1:length(n_air)
    n_out_i = n_air(i);
    for iter = 1:100
        n_CO2(i) = y_CO2(i) * n_out_i;
        n_CO(i) = y_CO(i) * n_out_i;
        n_O2_reacted = n_CO2(i) + 0.5 * n_CO(i);
        n_out_new = n_air(i) + n_CO(i) + n_CO2(i) - n_O2_reacted;
        if abs(n_out_new - n_out_i) < 1e-6
            break;
        end
        n_out_i = n_out_new;
    end
    n_out(i) = n_out_i;
    n_C(i) = n_CO2(i) + n_CO(i);
end
m_C = n_C * M_C;
%Integration
m_C_total = trapz(t_seconds, m_C);
m_C_total_kg = m_C_total/1000;
```

Figure 8. Used MATLAB script

For each manually sampled data point at 20-minute intervals, the script processed the input data, which included air flow rate [t/h], steam flow rate [t/h], and the volumetric concentrations of CO and CO_2. The script applied an iterative algorithm to estimate the total output flow, followed by a molar balance to calculate the amount of combusted coke based on the stoichiometric conversion of carbon to CO and CO_2. Finally, numerical integration was performed over the entire sampling period to obtain the cumulative mass of removed coke.

To illustrate the time-resolved development of flue gas composition during decoking, the following figures present the measured concentrations of carbon monoxide (CO) and carbon dioxide (CO_2), along with the corresponding air flow rate, for heaters BA-102, BA-106, and BA-110. These visualizations provide insight into the dynamics of coke combustion and support the reliability of the applied mass balance methodology. For the original heaters BA-102 and BA-106, the decoking procedure is divided into two distinct stages: decoking of the pyrolysis reactor coils and subsequent decoking of the transfer line exchangers (TLE).

Completion of the heater coil decoking is defined by a drop in CO_2 concentration in the flue gas below 0.2 vol. %, while decoking of the TLE is considered complete when the outlet temperature decreases below 440 °C or the temperature decline rate falls below 2 °C per hour. In contrast, the modern heater BA-110 undergoes decoking as a single, continuous process lasting 36 hours, following the procedure specified by the furnace manufacturer.

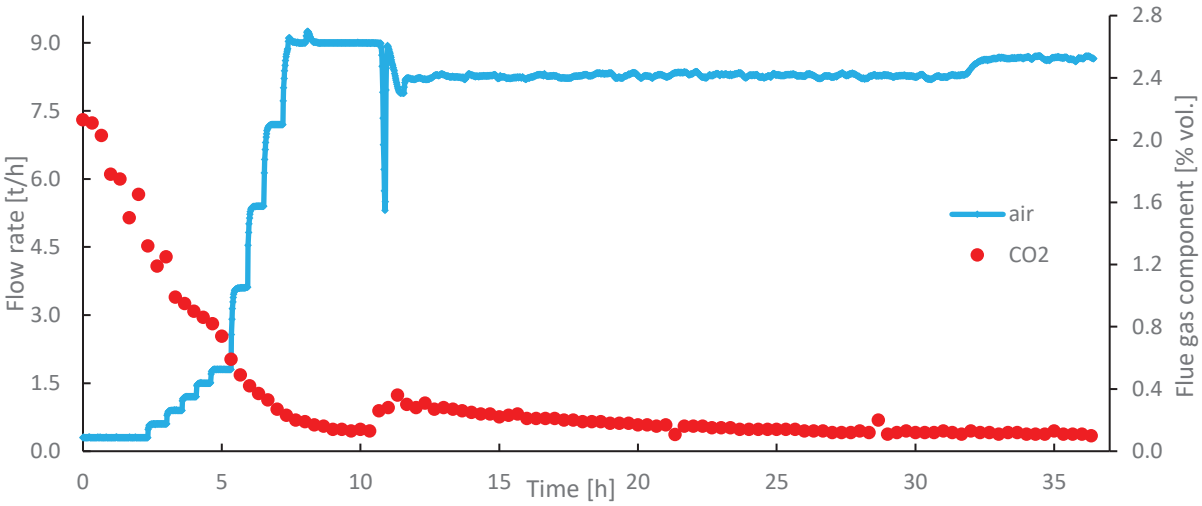

Figure 9. Flue gas composition and air flow rate during decoking of heater BA-106

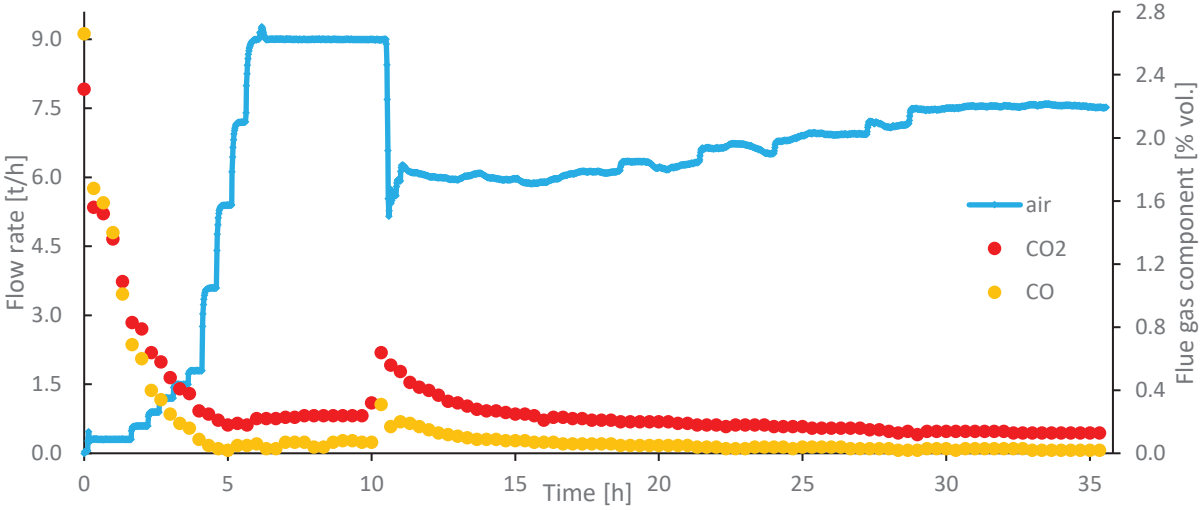

Figure 10. Flue gas composition and air flow rate during decoking of heater BA-102

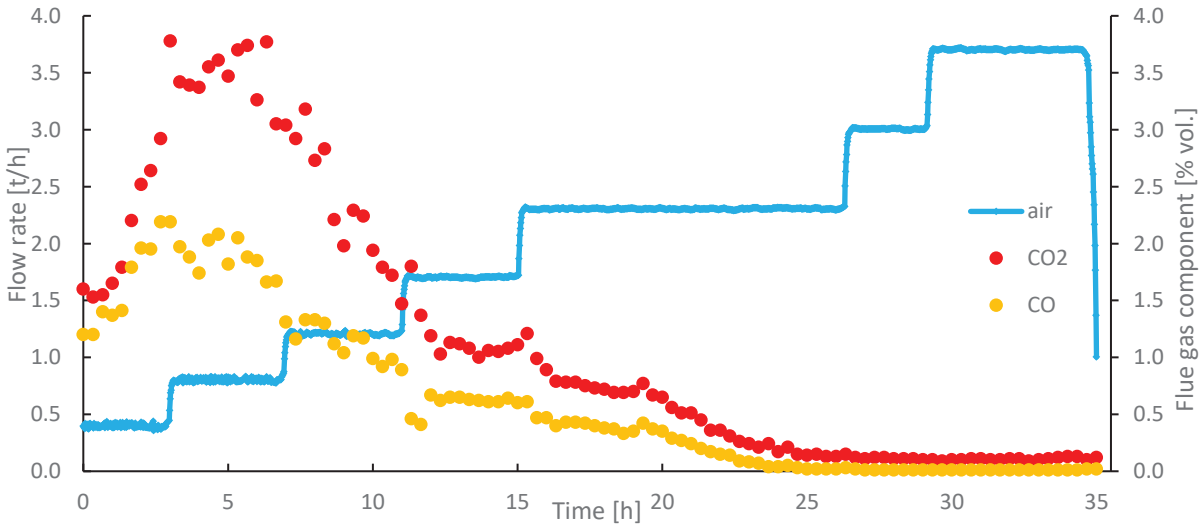

Figure 11. Flue gas composition and air flow rate during decoking of heater BA-110

However, complete conversion of coke to gaseous products does not occur during decoking. A portion of the residual carbon is carried by the flue gas as fine particulate matter and is subsequently separated in a cyclone separator. After decoking, this solid residue is discharged from the bottom of the cyclone and weighed. The measured mass is incorporated into the total coke balance.
In addition, a fraction of the coke remains in the TLE after decoking. These are opened and visually inspected following each decoking cycle. Based on the observed degree of fouling, the residual amount of coke is estimated by experienced operators. This estimated value is also included in the overall balance.

Results and discussion

The total mass of coke removed from each heater is therefore composed of three parts: the calculated amount of oxidized carbon (based on CO and CO_2 concentrations), the solid residue captured in the cyclone, and the estimated coke remaining in the TLE.
The results of CO and CO_2 concentrations, the calculated mass of combusted coke, the cyclone residue, and the estimated remaining coke in the TLE are summarized in the following table:

Table I. Comparison of combusted and dumped coke across different heater types

Heater	Feedstock	Reactor type	Cycle duration [days]	Combusted coke [kg]	Dumped coke [kg]
BA-102	HCR	SRT III	18.5	257.4	221.6
BA-106	HCR	SRT III	37.5	211.5	114.7
BA-110	Naphta	GK 6	64.7	620.8	796.4

During the decoking tests, heater BA-106 served as a pilot test, and therefore only CO_2 was monitored, while CO was not analysed. This limitation was accepted for the purposes of a simplified evaluation. In contrast, heater BA-102 exhibited a significantly higher amount of coke, which required more sensitive temperature control and a lower air flow rate to avoid thermal stress. The increased coke deposition was attributed to the fact that the reactor coils and TLE of BA-102 were brand new and had not yet undergone full operational conditioning.

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COMPATIBILITY OF CRUDE OILS AND THEIR PRODUCTS

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Abstract

The paper focuses on ensuring the compatibility of processed crude oils when changing the crude diet in a refinery. A set of suitable methods for assessing this problem was proposed, the results of which complement each other synergistically. Fourteen crude oils differing in origin and composition were examined. Using the selected methods, a total of 91 binary mixtures of these crude oils were evaluated in the form of compatibility cards. It was found that the compatibility of crude oils deteriorates with increasing API gravity. Based on the results, crude oils with an API gravity of 31 and below were identified as suitable carriers for other crude oils. The results can be used in practice to make strategic decisions on the optimal crude oil diet.

Introduction

Crude oil is an extremely complex mixture of compounds of varying composition. A change in the diet of the crude oil diet at a refinery always poses a challenge. It requires a skilful, comprehensive, and project-based approach to manage this change. Commercial, logistic, technological, balance sheet, and quality issues must be addressed[1]. In connection with the suspension of the operation of the Druzhba crude oil pipeline, which has supplied the Litvínov refinery with crude oil from the Urals region for the past 60 years[2], the question of a proper crude oil diet and related issues of miscibility and compatibility of various crude oils are gaining importance for refineries in the Czech Republic (CR). Most processed crude oil is transported to CR from the first half of 2025 via the Transalpine (TAL) crude oil pipeline and subsequently the Ingolstadt-Kralupy-Litvínov (IKL) pipeline, on which both refineries in CR processing crude oil are located, that is, Litvínov and Kralupy nad Vltavou. TAL connects the sea crude oil terminal in Trieste, Italy, with refineries in Austria, Germany, and also via IKL in CR. Since 2022, the TAL has been intensified in order to satisfy the CR needs after suspension of the operation of the Druzhba pipe line. The problem of this strategy is that both CR refineries are currently supplied by the same crude oil pipeline, while at the same time they are configured to process different types of crude oil. For these reasons, it is necessary to prevent unwanted contamination or incompatible mixtures, either in the pipeline itself during the transport of individual batches of the required crude oils, or during their storage, blending, and preparation in dedicated storage tanks. Taking into account the assets configuration of both CR refineries, it is expected to process two- or three-component crude oil blends. Another key factor is the limited storage capacity on the route and the time between the tanker docking at the Trieste terminal and processing at one of the two refineries. If crude oil from more distant locations (e.g., South America) is to be processed, a sufficient time window must also be allowed for from purchase to the tanker's arrival in Trieste. It follows from the above that any unpredictable change in quality due to incompatibility or contamination will result in technological difficulties and considerable financial losses; therefore, it is necessary to prevent it. For this reason, it was decided to select a series of different crude oils to subject them to mutual compatibility tests on a laboratory scale. The aim was also to develop a comprehensive methodology for the evaluation of blended samples utilizing a set of analytical indicators based on standard and newly developed analytical methods.

Materials and analytical methods

Fourteen commercially available crude oils, differing in their qualitative properties, especially API gravity, sulfur content, and yield structure were selected. Individual mixtures were prepared on the laboratory scale. Initial samples of crude oil were thoroughly homogenized in 5 liter canisters at laboratory temperature. The required amount of each crude oil was then weighted to prepare the resulting mixture, and the mixture of crude oils was shaken thoroughly for 15 minutes using a laboratory shaker. In the first step, two-component mixtures of individual crude oils were prepared in the screening series 0 – 25 – 50 – 75 – 100 and their mutual compatibility was assessed. In the case of a borderline tested ratio, subsequent mixing was focused on specific mixing ratios.
The mutual compatibility of the mixtures prepared in this way was investigated using the following analytical methods[3-6] (Table 1).

Table I:
Analytical methods and equipment used

Property	Standard	Equipment	Comments
Density	ASTM D4052	Eradens X device from Eralytics	Instrument with oscillating U-tube. Measurements at 15 and 50 °C, approx. 15 ml sample
Spot test	ASTM D4740	Herzog HVM 472 Manual	Cleanliness and compatibility test. A drop of the sample at 25 °C was applied to the filter paper, subsequently inserted into the dryer. The result was assessed using an empirical 5 stage scale (1-5).
Compatibility assessment	Proprietary method	Leica DM2500 LED + software LAS X	Optical microscopy, 10x zoom, sample drop
Group composition-saturates, aromatics, resins, and asphaltenes (SARA)	IP 469	NTS Iatroscan MK-6 analyzer	Thin layer chromatography (TLC) with flame ionization detector (FID). Sample 1µl. Alkenes were included in saturated hydrocarbons.
Sulfur	ASTM D5453	Thermo Scientific Flash 2000	Catalytic combustion of the sample (80 µl) in oxygen at 1200 °C and detection by ultraviolet fluorescence spectrometry. Range 1–1000 $mg \cdot kg^{-1}$ of S.

As a result of the compatibility assessment by microscopy analysis, the homogeneity and compatibility of the prepared crude oil mixtures were verified by optical microscopy on a Leica DM2500LED. The microscope was set to black-and-white mode and images were captured at 10x magnification. The resulting values of the total area of heterogeneous particles represent the average of ten measurements of the prepared microscopic preparation[7, 8]. The colloidal instability index (CII) was calculated on the basis of SARA results according to equation [1]

$$CII = \frac{saturates + asphaltenes}{resins + aromatics} \quad [1]$$

where saturates; asphaltenes; resins and aromatics are the total contents of individual groups in wt%.

Because the mixture of crude oils is a complex colloidal system, a comprehensive approach was chosen, in which not only one of the parameters was taken into account, but their combined results.

Results and discussion

Individual crude oils can be characterized and subsequently categorized using basic quality properties such as their API gravity, density, or sulfur content (Table 2). Crude oils with an API gravity parameter lower than 30 (heavy crude oils, mostly with a high sulfur content) were marked in green, those higher than 40 (light low-sulfur crude oils) are marked in red.

Table II:
Basic specification of the individual crude oils

Sample	Location	°API Gravity	Sulfur (wt%)	Density at 15 °C (g/cm^3)	SARA* (wt%)
1	Ural region	30.40	1.19	0.8704	29.7/50.6/12.9/6.8
2	Scandinavia	28.00	0.58	0.8854	30.7/46.5/17.3/5.5
3	Arabian Peninsula	28.58	2.14	0.8909	19.8/57.0/11.1/12.1
4	Arabian Peninsula	32.79	1.40	0.8589	26.5/60.1/7.9/5.5
5	South America	35.30	0.32	0.8546	44.8/41.1/10.0/4.1
6	Ural region	45.04	0.44	0.8089	58.7/34.8/3.9/2.6
7	North Africa	37.30	0.20	0.8434	46.1/42.4/7.5/4.0
8	Southwest Asia	38.09	0.12	0.8294	60.3/27.5/10.4/1.8
9	South America	32.00	0.43	0.8683	41./42.2/12.0/4.7
10	North Africa	42.42	0.18	0.8174	18.7/61.2/11.5/8.6
11	Arabian Peninsula	28.35	2.86	0.8846	29.1/52.4/11.5/7.0
12	Arabian Peninsula	31.00	2.10	0.8846	52.9/31.1/5.6/10.4
13	Arabian Peninsula	24.12	2.78	0.9109	14.7/58.1/14.1/13.1
14	North America	42.43	0.12	0.8079	64.3/31.5/3.5/0.7

*The order of results is *saturates/aromatics/resins/asphaltenes*

A compatibility card was created for each pair of crude oils (91 combinations), which lists the basic qualitative parameters of the resulting mixtures, especially the result of the spot test, optical microscopy, and the CII index. Significant differences were observed between the individual prepared mixtures, from completely compatible mixtures (Figure 1 and Table 3) to incompatible ones throughout the screening range (Figure 2 and Table 4).

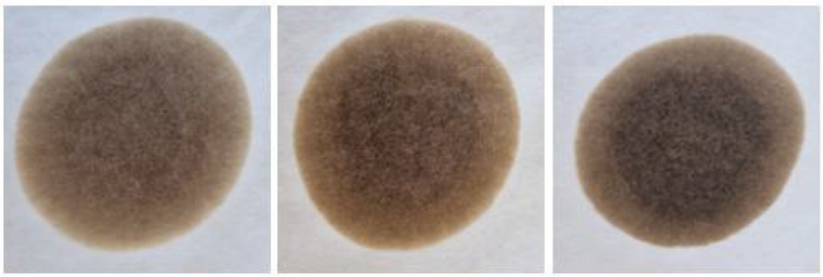

Figure 1. Spot test (25 °C) of mixtures of samples 3 and 4 in ratio (from left) 25:75; 50:50 and 75:25

Table III:
Evaluation of the screening ratios for mixture of samples 3 (°API 28.58) and 4 (°API 32.79)

Ratio sample 3 : sample 4 (wt%)	25:75	50:50	75:25
SARA (wt%) *sat/arom/res/asph*	25.2/59.7/7.0/8.1	22.7/59.4/8.2/9.7	20.6/59.3/9.0/11.1
CII	0.499	0.479	0.464
Optical microscopy – average area (μm^2)	1745.7	1027.7	2155.9
Spot test (25 °C)	2	2	3

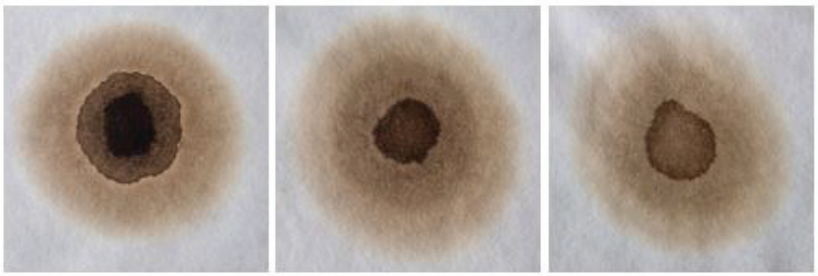

Figure 2. Spot test (25 °C) of mixtures of samples 6 and 7 in ratio (from left) 25:75; 50:50 and 75:25

Table IV:
Evaluation of the screening ratios for mixture of samples 6 (°API 45.04) and 7 (°API 37.30)

Ratio sample 6 : sample 7 (wt%)	25:75	50:50	75:25
SARA (wt%) *sat/arom/res/asph*	55.5/29.5/7.8/7.2	56.5/30.5/6.8/6.2	56.7/33.6/5.8/3.9
CII	1.681	1.681	1.538
Optical microscopy – average area (μm^2)	3778.8	2171.8	602.1
Spot test (25 °C)	5	4	4

The results for both oil blends were clearly different, but at the same time complemented each other very well when evaluating a specific blend. Based on the results obtained, the prepared dual mixtures were sorted to four groups: 1) compatible, 2) hint of incompatibility,3) tendency to be incompatible, and 4) incompatible (Table 5). Compatible mixtures are considered for trouble-free real processing.

Table V:
Explanation of the use of colour markings at the traffic lights and range of the selected parameters

Explanations		Spot test classes		CII	
	compatible	1. - 2.	compatible/stable	< 0.7	stable
	hint of incompatibility	3.	potentially incompatible	0.7 - 0.9	uncertain stability
	tendency to be incompatible	4. - 5.	incompatible/unstable	> 0.9	unstable
	incompatible				

The summary information including 24 mixtures was displayed graphically using the so-called “traffic lights”, which make it easy to identify the ideal ratio for the planned mixing of the crude oils delivered in terms of their mutual compatibility (Figures 3-5).

Compatible																						
1	(°API 30.40)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
2	(°API 28.00)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
3	(°API 28.58)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
4	(°API 32.79)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
2	(°API 28.00)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
3	(°API 28.58)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0

Figure 3. Compatible mixtures in the whole range

Incompatible																						
5	(°API 35.30)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
7	(°API 37.30)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
6	(°API 45.04)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
5	(°API 35.30)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
6	(°API 45.04)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
8	(°API 38.09)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
6	(°API 45.04)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
9	(°API 32.00)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
6	(°API 45.04)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
7	(°API 37.30)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
5	(°API 35.30)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
10	(°API 42.42)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0

Figure 4. Incompatible mixtures and mixtures with the tendency to be incompatible

5	(°API 35.30)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
11	(°API 28.35)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
5	(°API 35.30)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
2	(°API 28.00)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
5	(°API 35.30)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
12	(°API 31.00)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
1	(°API 30.40)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
5	(°API 35.30)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
1	(°API 30.40)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
10	(°API 42.42)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
9	(°API 32.00)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
11	(°API 28.35)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
9	(°API 32.00)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
3	(°API 28.58)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
9	(°API 32.00)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
2	(°API 28.00)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
13	(°API 24.12)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
2	(°API 28.00)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
13	(°API 24.12)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
9	(°API 32.00)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
14	(°API 42.43)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
2	(°API 28.00)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
5	(°API 35.30)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
3	(°API 28.58)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
5	(°API 35.30)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
4	(°API 32.79)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
6	(°API 45.04)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
4	(°API 32.79)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0
6	(°API 45.04)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100
13	(°API 24.12)	100	95	90	85	80	75	70	65	60	55	50	45	40	35	30	25	20	15	10	5	0

Figure 5. Mixtures with the optimal ratio found for mutual mixing

The overall results show that in, some cases, it really depends on the percentage units that must be observed in order for the resulting mixture to be in a safe area. Laboratory tests have shown that crude oils with a higher API gravity value, such as crude oils labelled 6 (°API 45.04); 7 (37.3); 8 (38.09); 10 (42.42) and 14 (42.43), are more prone to incompatibility. On the other hand, crude oils with lower API gravity parameter, such as 1 (°API 30.4); 2 (28.1); 3 (28.58); 4 (32.76); 11 (28.35); 12 (31.00) and 13 (24.12), seem to be a good candidate for the majority component of the processed mixture and, therefore, act as carriers of other oils. Generally, this trend can be explained by the fact that oils with higher API gravity values have a lower content of aromatics, which stabilizes the colloidal system of the crude oil. In contrast, oils with lower API gravity values and those defined as heavier contain a higher content of aromatics and the colloidal system of the crude oil is stabilized, which is also reflected

in a lower CII parameter. Crude oils 6 proved to be the most problematic in terms of compatibility, as it also showed the highest value of the API gravity parameter (45.04). For this crude oil (6), the recommended dosage is up to a maximum content of 40 wt% only together with crude oil with lower API gravity. It should be noted that only mutual compatibility is evaluated here, not the resulting value of sulfur content, yield structure, or other quality parameters.

Conclusion

Based on laboratory tests of compatibility of selected types of crude oil, it has been proven that when changing the crude oil diet of a refinery, such a procedure is necessary. A portfolio of suitable analytical methods was compiled and subsequently verified, with which mutual compatibility can be well and reliably monitored. Compatibility cards were used to describe the properties of 91 dual crude oil blends. The screening revealed suitable candidates for the so-called carrier crude oils, which will be the majority in the selected process mixtures. The laboratory test confirmed that these candidates could be crude oils with an API gravity value of 31 or less. During laboratory compatibility tests, optimal blend ratios were defined for subsequent processing. Critical parameters were defined that could cause a problem during further processing. The incompatibility of some crude oils was demonstrated, closely related to the blending ratio. These findings are directly applicable to refineries that process various crude oil diets. On their basis, it will be possible to prevent various outages, such as clogged pumps and filters, unwanted sedimentation in storage tanks, and off-spec products, thus, minimizing operating costs

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POLYMERS COMPOSITES

CHARACTERIZATION OF ELASTOMER DURABILITY: INSIGHT INTO COMPRESSION SET AND STRESS RELAXATION

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Abstract

This study investigates the thermal aging behaviour of EPDM rubber compounds cured with varying concentrations of peroxide. Mechanical properties such as hardness, tensile strength, elongation at break, compression set, and stress relaxation were evaluated before and after exposure to elevated temperatures. A key innovation of this research is the use of a newly developed testing apparatus for stress relaxation measurements, designed to enable discontinuous long-term testing under controlled deformation and environmental conditions. The device allowed monitoring of stress decay over time, providing deeper insight into the viscoelastic behaviour of rubber material during thermal exposure. Results showed that peroxide concentration significantly influences crosslink density and aging resistance, with optimal performance observed at intermediate peroxide levels. The findings highlight the importance of formulation design and introduce a novel methodology for evaluating long-term elastomer durability.

Introduction

Elastomeric materials, particularly ethylene-propylene-diene monomer (EPDM) rubbers, are extensively used in sealing and damping applications due to their excellent resistance to weathering, outstanding flexibility, and high thermal stability. However, their long-term functionality is critically dependent on their ability to preserve mechanical integrity and sealing performance under sustained deformation and environmental stress, especially at elevated temperatures.

One of the most common environmental stressors encountered during the service life of elastomer is the combined action of mechanical loading and thermal exposure in the presence of oxygen. This combination induces thermo-oxidative degradation, leading to gradual deterioration of the rubber network structure [1]. As aging progresses, rubber materials experience a loss of key mechanical properties, including elasticity and the ability to recover from deformation, which can ultimately result in sealing failure.

To evaluate and predict the long-term durability of rubber components under such conditions, accelerated aging tests are commonly employed. These tests subject the material to harsher environmental conditions—typically higher temperatures over shorter periods—than those experienced during normal use, thus enabling a more rapid estimation of material life [2].

The degradation behaviour of elastomers during thermal aging is closely associated with their viscoelastic characteristics, which can be assessed using standardized methods such as compression set and stress relaxation. These methodologies are extensively applied in both academic and industrial settings to quantify the time-dependent degradation of elastic recovery and residual stress [3–6]. These approaches provide valuable insights into the degradation kinetics and mechanical reliability of EPDM-based materials under aging conditions relevant to industrial applications such as nuclear power plants, automotive components, and long-term sealing systems.

Recent studies have demonstrated that crosslinking density, network architecture, and the composition of the curing system—particularly the type and concentration of organic peroxides—are critical factors influencing the aging behaviour and long-term durability of elastomers [7, 8]. Peroxide-cured EPDM compounds are known to offer improved thermal resistance in comparison to sulphur-cured systems [9]. However, the interplay between peroxide dosage, homogeneity of crosslink distribution, and resulting mechanical properties remains complex and requires further investigation.

Building upon these insights, the present study explores the influence of varying peroxide concentrations on the mechanical performance and thermal aging resistance of EPDM rubber formulations. A core innovation of this work is the implementation of a novel stress relaxation testing apparatus, specifically designed for long-term, intermittent measurements under defined thermal and mechanical conditions. This experimental setup enables precise monitoring of stress decay over extended periods, offering new insights into viscoelastic relaxation behaviour.

Experiment

Materials, compound and sample preparation

EPDM rubber (Nordel 4520, DOW), carbon black (N772, Cabot Corp.), paraffinic oil (AP/E Core 600, Exxon Mobil Corp.), zinc oxide (ZnO, SlovZink), antioxidant (Irganox 1035, BASF) and peroxide (Perkadox 14-40, Nouryon) were utilized for the preparation of rubber compounds.

All ingredients, except the peroxide, were initially mixed using a laboratory internal mixer (Everplast Machinery), with the total chamber volume of 1.8 l and fill factor of 0.72. The mixing was conducted at 50 rpm for 5 minutes. Two separate batches were prepared and subsequently combined using a two-roll mill (LabTech) for an additional 5 minutes. The resulting masterbatch was stored at room temperature overnight prior to peroxide incorporation. Final compounding was performed on a double roll mill (Farrel), where 400 g of the masterbatch was blended with 4-20 phr of peroxide for 5 minutes. The detailed formulation of the rubber compound is provided in Table I.

Table I
Rubber compounds composition

Raw material	Composition [phr]
EPDM	100
Carbon black	100
Paraffinic oil	50
ZnO	3
Antioxidant	2
Peroxide	4/8/12/16/20

The curing characteristics of the rubber compounds were evaluated using a Premiere MDR rheometer (Alpha Technologies) at 180 °C. Due to the use of peroxide as the curing agent, the scorch time (ts_1) and optimum cure time (t_{90}) were similar across all formulations, approximately 0.5 and 5.5 minutes, respectively. Nevertheless, a curing time of 12 minutes at 180 °C was selected to ensure complete vulcanization for samples with a thickness of 2 mm. For thicker samples (6.3 mm), the moulding time was extended by approximately 6 minutes. All specimens underwent a post-curing process at 150 °C for 2 hours to eliminate residual peroxide and stabilize the crosslinked network.

Test methods

Tensile testing was performed in accordance with ISO 37 using a Tensometer T10D (Alpha Technologies) at a crosshead speed of 500 mm/min. Six S2-type specimens were tested for each compound formulation.

Hardness test was measured according to ISO 48-4 using a Bareiss hardness tester. The compression set was evaluated following ISO 815-1, sample B, method A under a constant deformation 25 %.

Stress relaxation measurements were conducted in accordance with ISO 3384-1, method B, using an initial deformation of 25%. This test was carried out using a custom-designed apparatus developed by Tomas Bata University in collaboration with PolymerTest (Figure 1). The device enables discontinuous measurement of stress relaxation over extended periods. It features a pressure gauge driven by a stepper motor, integrated with a control system that records the applied force. The test specimen is clamped within a specialized cell at the required deformation. This cell can be exposed to various environments, including elevated or reduced temperatures, chemical media, and more. It can also be removed from the test environment and reinserted for repeated measurements at defined intervals.

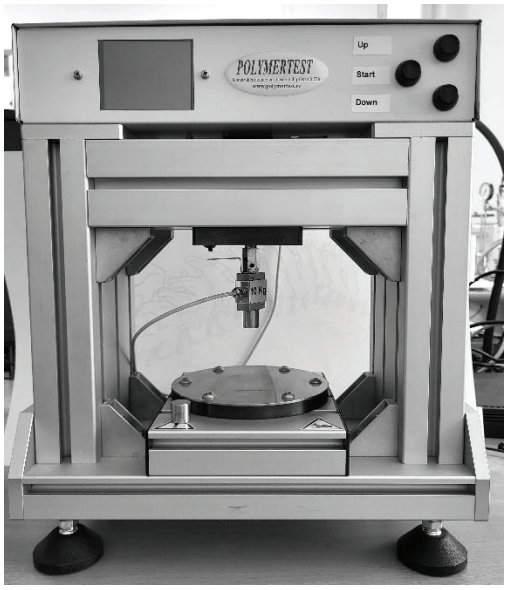

Figure 1

Discussion and results

In this study, the elevated temperature durability of EPDM compounds cured with varying concentration of peroxide was investigated through hardness, tensile strength, compression set and stress relaxation measurement. Tables II – IV present the hardness, stress at break and strain at break of EPDM samples with different peroxide concentrations before and after thermal exposure.

Table I displays the hardness values of EPDM samples. The data reveal a consistent increase in hardness with both peroxide concentration and exposure time at elevated temperature. The crosslink density increases with peroxide content, resulting in higher hardness values ranging from 45 ShA to 62 ShA for 4 to 20 phr of peroxide. Thermal aging further enhances hardness across all samples, with the most pronounced increase observed at the lowest peroxide concentration (13 ShA), compared to 7 ShA at the highest concentration. This behaviour is attributed to additional crosslinking during thermal exposure, leading to stiffer rubber matrices.

Table II
Hardness Development of EPDM Samples During Thermal Aging at 150 °C

Elevated temperature exposure [hours]	0	24	72	120	168
Peroxide concentration [phr]	Hardness [ShA]				
4	45 ± 1	48 ± 1	53 ± 1	55 ± 1	58 ± 1
8	50 ± 1	51 ± 1	55 ± 1	57 ± 1	59 ± 1
12	55 ± 1	56 ± 1	59 ± 1	62 ± 1	64 ± 1
16	58 ± 1	59 ± 1	62 ± 1	64 ± 1	65 ± 1
20	62 ± 1	63 ± 1	65 ± 1	67 ± 1	69 ± 1

Table II summarizes the tensile strength (stress at break) of EPDM samples exposed to 150 °C for 168 hours. The lowest tensile strength (6.4 MPa) was recorded for the 4 phr peroxide sample. Increasing the peroxide concentration resulted in tensile strength values around 10.5 MPa, indicating that beyond a certain peroxide level, no significant improvement in tensile strength occurs. Thermal exposure did not significantly alter tensile strength, despite the observed increase in hardness. This suggests ongoing network changes, likely due to post-curing or additional crosslinking, without substantial impact on tensile strength.

Table III
Effect of Elevated Temperature (150 °C) on Stress at Break

Elevated temperature exposure [hours]	0	24	72	120	168
Peroxide concentration (phr)	Stress at Break [MPa]				
4	6.4 ± 0.1	-	6.34 ± 0.21	-	7.09 ± 0.5
8	10.4 ± 0.5	10.93 ± 0.2	9.45 ± 1.1	9.58 ± 0.8	9.78 ± 0.5
12	10.9 ± 0.6	11.54 ± 0.3	10.58 ± 0.5	10.07 ± 0.7	9.64 ± 0.6
16	10.3 ± 1.2	10.3 ± 1.7	10.81 ± 0.9	10.85 ± 0.7	9.76 ± 1.2
20	10.4 ± 0.7	10.84 ± 0.8	10.77 ± 1.3	11.09 ± 0.5	10.1 ± 1.0

Table III presents the elongation at break. A clear decreasing trend is observed with increasing peroxide concentration. A similar decline is evident for samples subjected to elevated temperature. The sample with the lowest crosslink density showed the greatest deterioration, with a reduction of nearly 50 %. Samples with 8 to 20 phr of peroxide exhibited a decrease in elongation ranging from 36 % to 28 %, indicating greater thermal stability of the network. Nevertheless, the reduction in elongation reflects a loss of flexibility and increased brittleness, consistent with the formation of a denser crosslinked structure.

Table IV
Thermal Aging Impact on Strain at Break at 150 °C

Elevated temperature exposure [hours]	0	24	72	120	168
Peroxide concentration (phr)	Stress at Break [MPa]				
4	839 ± 9	-	676 ± 15	-	447 ± 19
8	562 ± 18	589 ± 12	466 ± 37	394 ± 24	360 ± 13
12	396 ± 16	421 ± 15	356 ± 8	306 ± 12	265 ± 12
16	307 ± 24	291 ± 29	284 ± 15	253 ± 12	206 ± 15
20	252 ± 11	259 ± 6	229 ± 17	210 ± 6	177 ± 11

Figure 2 illustrates the compression set (Figure 2a) and stress relaxation (Figure 2b) of samples exposed to 150 °C. These tests are critical for applications such as gaskets, O-rings, dampers, and tires, where dimensional stability under compression is essential. Lower values are desirable for sealing applications. The results show that higher peroxide concentrations yield lower compression set values, indicating improved elastic recovery. Samples with 16 and 20 phr of peroxide exhibited compression set values around 35 % after 168 hours, suggesting an optimal balance between crosslink density and elasticity in the range of 12 to 16 phr. In contrast, samples with lower peroxide content reached compression set values close to 90 %. These findings are corroborated by stress relaxation data in Figure 2b, where samples with higher peroxide content showed slower stress decay, indicating better resistance to stress relaxation. This behaviour is advantageous in dynamic applications requiring sustained mechanical performance. However, thermal exposure induces additional network changes, leading to material hardening. The most significant crosslinking changes were observed in samples with 4 and 8 phr of peroxide, where stress relaxation decreased over time.

Figure 3 presents compression set (Figure 3a) and stress relaxation (Figure 3b) data at a reduced aging temperature of 120 °C. Compared to the results at 150 °C, both compression set and stress relaxation values decreased significantly. Only the sample with 4 phr of peroxide showed undesirable increases in both tests. These results indicate that aging temperature strongly influences network stability and has a substantial impact on the long-term durability of the material.

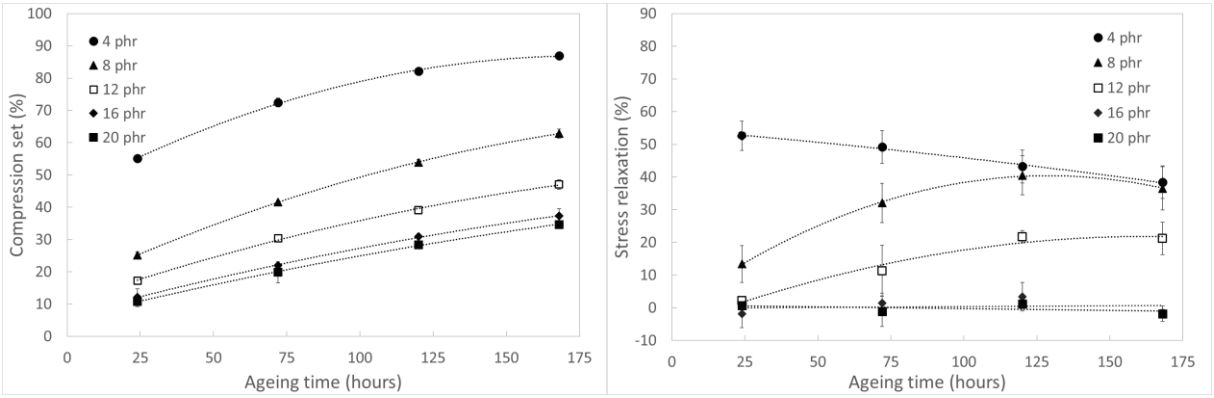

Figure 2. Compression set (a) and stress relaxation (b) dependence on ageing time at the temperature of 150 °C

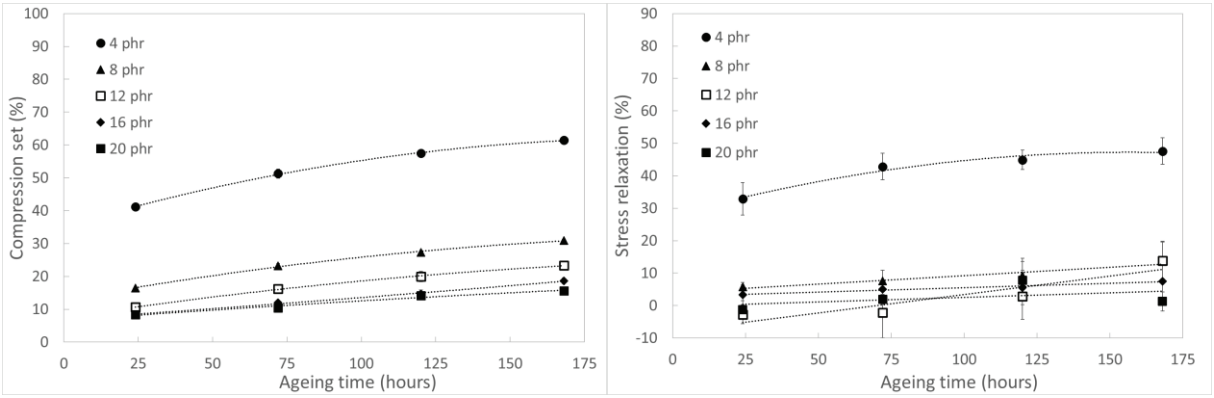

Figure 3. Compression set (a) and stress relaxation (b) dependence on ageing time at the temperature of 120 °C

Conclusion

This study confirmed that peroxide concentration significantly affects the thermal aging behaviour and mechanical performance of EPDM rubber. Higher peroxide levels increased crosslink density, resulting in improved hardness and enhanced resistance to compression set and stress relaxation. However, excessive crosslinking led to reduced elongation at break and, in some cases, a decline in tensile strength. Thermal exposure at 150 °C intensified these effects, particularly in samples with lower peroxide content, which exhibited pronounced degradation. The optimal balance between stiffness and elasticity was observed in formulations containing 12–16 phr of peroxide. Notably, stress relaxation was evaluated using a newly developed testing apparatus, which enabled discontinuous long-term measurements under controlled deformation and environmental conditions. This novel setup provided deeper insight into the viscoelastic behaviour of EPDM during thermal aging. Furthermore, reducing the aging temperature to 120 °C significantly improved material stability, highlighting the importance of temperature in long-term performance. These findings support the need for precise formulation design in thermally demanding applications.

Acknowledgement

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PROCESS ENGINEERING

SAMPLE FILLING IN ROTATIONAL RHEOMETRY AND CONDITIONS OF RHEOLOGICAL MEASUREMENT AND THEIR EFFECT ON THE FREE FALL OF A SPHERICAL PARTICLE IN A NON-NEWTONIAN FLUID

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Abstract

This study deals with the sample filling and conditions (air humidity content) of rheological measurement and their influence on the results of the numerical simulation of a free-falling spherical particle. A carboxymethyl cellulose *CMC* solution was chosen as a non-Newtonian, shear thinning fluid. For measuring the rheological properties of *CMC* solutions, a rotational rheometer HAAKE MARS I was employed. The measured data were fitted by power-law and Yasuda-Carreau models. Sample filling and conditions of rheological measurement can significantly influence the evaluation of the rheological properties (model parameters). The results show that the air humidity content during the rheological measurement has a more significant effect on evaluated model parameters than the overfilling of the sample. These changes in rheological model parameters can lead to numerical simulation results differences of tens of percents. The results of this study illustrate the importance of choosing the correct methodology and conditions of the rheological measurement corresponding to the expected conditions in hydrodynamic experiments.

Introduction

Understanding of the free fall of a spherical particle is a starting point for the characterization of the particle-fluid interaction and the prediction of the particle's terminal falling velocity. The terminal falling velocity is used in calculations of many hydrodynamic processes. Among others, these processes include sedimentation of suspensions, transport of suspensions in pipelines, or fluidization (e.g. literature[1]). Calculating the free-fall velocity in non-Newtonian fluids is complicated due to the complex rheological behaviour of non-Newtonian fluids. The prediction of the free-fall velocity can be influenced by the results of the rheological measurement, as well as by the rheological model used for the fitting of measured data. A very common problem in rheometry is finding proper conditions for measurement[2]. For example, sample overfilling or underfilling can influence the results of rheological measurement[3]. The evaporation of the solvent can also be a problem in rheometry[2]. Not only the rheological model but also a shear rate interval for the fitting of the measured data influences the prediction of the free-fall velocity. The importance of choosing the appropriate shear rate interval for determining the parameters of the power-law model is presented in the literature[4]. In that literature reference, the experimental terminal falling velocities and the terminal falling velocities calculated from the formula using the parameters of the power-law model are compared. The formula used for the calculation of the terminal falling velocities is based on the results of numerical simulations of different authors.
This study is focused on the influence of the sample filling in rotational rheometry and the influence of air humidity content on the results of the rheological measurements. The effect of these factors on the free fall of a spherical particle in a non-Newtonian fluid in the Stokes flow regime is numerically simulated. This study also compares the results of the numerical simulation performed with the parameters of the power-law and the Carreau-Yasuda rheological models.

Fundamentals

A rheology of purely viscous shear thinning non-Newtonian fluids is described by the viscosity curve, the dependence of the apparent viscosity η *[Pa·s]* on the shear rate $\dot{\gamma}$ *[s^{-1}]*. The viscosity curve can be described by rheological models. For shear thinning fluids, the simplest model is the power-law model

$$\eta = K \cdot \dot{\gamma}^{n-1} \tag{1}$$

where K *[Pa·s^n]* is the consistency coefficient and n *[-]* is the flow index. This model describe the dependence of viscosity on shear rate with sufficient accuracy only in a limited interval of the shear rate[4]. The rheology model that can describe shear thinning fluids in a wide interval of $\dot{\gamma}$ is the Carreau-Yasuda model

$$\eta = \eta_{inf} + (\eta_0 - \eta_{inf}) \cdot [1 + (\lambda \cdot \dot{\gamma})^a]^{(m-1)/a} \tag{2}$$

where η_{inf} *[Pa·s]* is the infinity shear rate viscosity, η_0 *[Pa·s]* is the zero shear rate viscosity, λ *[s]* is the Carreau-Yasuda model time parameter, a *[-]*, m *[-]* are the parameters of the Carreau-Yasuda model.

The free fall of a spherical particle in a non-Newtonian fluid is described by the drag coefficient and the particle Reynolds number. The drag coefficient C_D *[-]* is defined as

$$C_D = \frac{F_D}{0.5 \cdot \rho \cdot (\pi \cdot d^2/4) \cdot u_t^2} \tag{3}$$

where F_D *[N]* is the drag force, ρ *[kg·m^{-3}]* is the fluid density, d *[m]* is the particle diameter, u_t *[m·s^{-1}] is the* terminal falling velocity of the particle in the unbounded fluid. The particle Reynolds number Re_p *[-]* is expressed as

$$Re_p = \frac{u_t \cdot d \cdot \rho}{\eta_{eff}} \tag{4}$$

where η_{eff} *[Pa·s]* is the effective viscosity. For calculation of Re_p according to Eq. (4), η_{eff} is calculated according to Eq. (1) or (2) using the mean shear rate around the particle $\bar{\dot{\gamma}}$ *[s^{-1}].* The mean shear rate is expressed as

$$\bar{\dot{\gamma}} = u_t/d \tag{5}$$

Experiment and numerical simulation

A sodium salt of carboxymethyl cellulose *CMC* water solution in a concentration of 1.25% was used as a non-Newtonian, shear thinning fluid. The solution was prepared by dissolving a *CMC* powder in a mixture of tap water and formaldehyde and stirring for 8 *h*. Formaldehyde addition in concentration 1 *ml·l^{-1}* was used for stabilization of the *CMC* solution against biodegradation. The solution was stored in a beaker under foil to prevent evaporation. The density of the *CMC* solution was measured using a pycnometer. Rheological properties were measured on a rotational rheometer HAAKE MARS I with cone-plate geometry *CP* 35/2, truncation 0.105 *mm*, in the interval of $\dot{\gamma}$ = 0.01-1000 *s^{-1}*. The measurement temperature was set at 23 ± 0.1 *°C*. For selected measurement variants, the sample overflow was trimmed with a spatula in trimming position 0.115 *mm*. During the measurements, the relative humidity *RH* was measured using a humidity probe. Measurements were taken in three modes with respect to the *RH*: measurement at the laboratory *RH*, measurement with an additional hood, and measurement with the additional hood and humidification of air under the hood using a wet cloth. For each measurement variant, the viscosity curve was measured at least twice, and the mean viscosity curve was calculated. An overview of the measurement variants is listed in Table I.

The free fall of the particle was simulated, using the finite element method *FEM*, by steady-state flow over the fixed particle in the centre of the cylinder. The solution domain was chosen sufficiently larger than the diameter of the particle (d = 0.003 *m*) to avoid wall effects (height 0.6 *m*, diameter 0.5 *m*). The creeping flow package in COMSOL Multiphysics was used. The detail of the solution domain with mesh, schematically marked boundaries, and their description is in Figure 1.

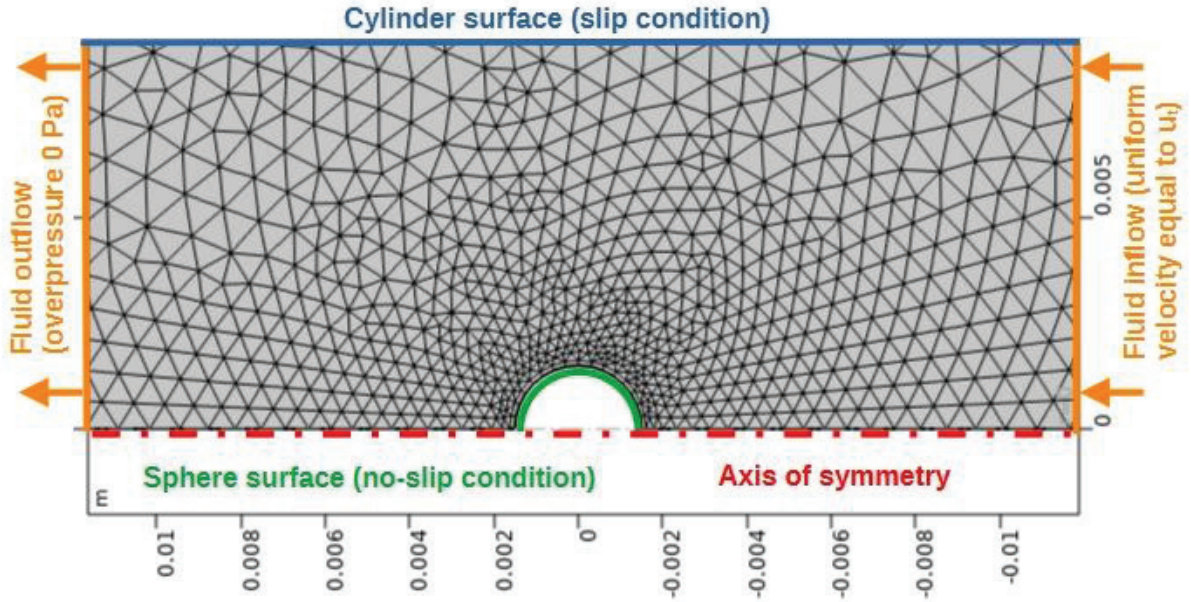

Figure 1: The detail of the solution domain

Results and discussion

The density of the *CMC* solution was 1003.1 $kg \cdot m^{-3}$ at 23 °C. The viscosity curve of each measurement variant was fitted by the Carreau-Yasuda model, Eq. (2), in the interval 0.01-1000 s^{-1}, see Figure 2 and Figure 3. The model parameters are listed in Table I. The numerical simulation was performed for all terminal falling velocities u_t listed in Table II with the parameters of the Carreau-Yasuda model for each measurement variant. The drag coefficients C_D were calculated according to Eq. (3) using the results of the drag force F_D from the numerical simulation. For variant 1, for all u_t, the numerical simulation was performed and values of C_D were calculated with the parameters of the power-law model, n = 0.643 and K = 2.100 $Pa \cdot s^n$ obtained in the interval from 0.01 s^{-1} to 1000 s^{-1}. The numerical simulation and the calculation of C_D was done also separately for each u_t with the model parameters obtained in the specific shear rate intervals corresponding to the mean shear rate around the particle $\bar{\dot{\gamma}}$, see Table II. Values of $\bar{\dot{\gamma}}$ were calculated from Eq. (5). The values of the particle Reynolds number Re_p, calculated according to Eq.(4), varied in the range of $6.2 \times 10^{-6} - 9.8 \times 10^{-2}$. The flow around the particle was in the Stokes flow regime.

Comparison of measurement variants

The viscosity curves measured under laboratory conditions (measurement variants 3 and 6) give the highest viscosity values, especially at low $\dot{\gamma}$. The variants 1 and 4 with the additional hood and humidification give the lowest viscosity values, see Figure 2 and Figure 3. It indicates that during the rheological measurement an evaporation occurred. Under the additional hood, the *RH* increased during approximately 20 *min* from laboratory *RH* to 40-60% and remained at this value until the end of the measurement (measurement time 40 *min*). The evaporation during the rheological measurement can also be observed in the relative weight loss of the *CMC* solution during the measurement. The range of the *RH* during the measurement and the relative weight loss are listed in Table I.

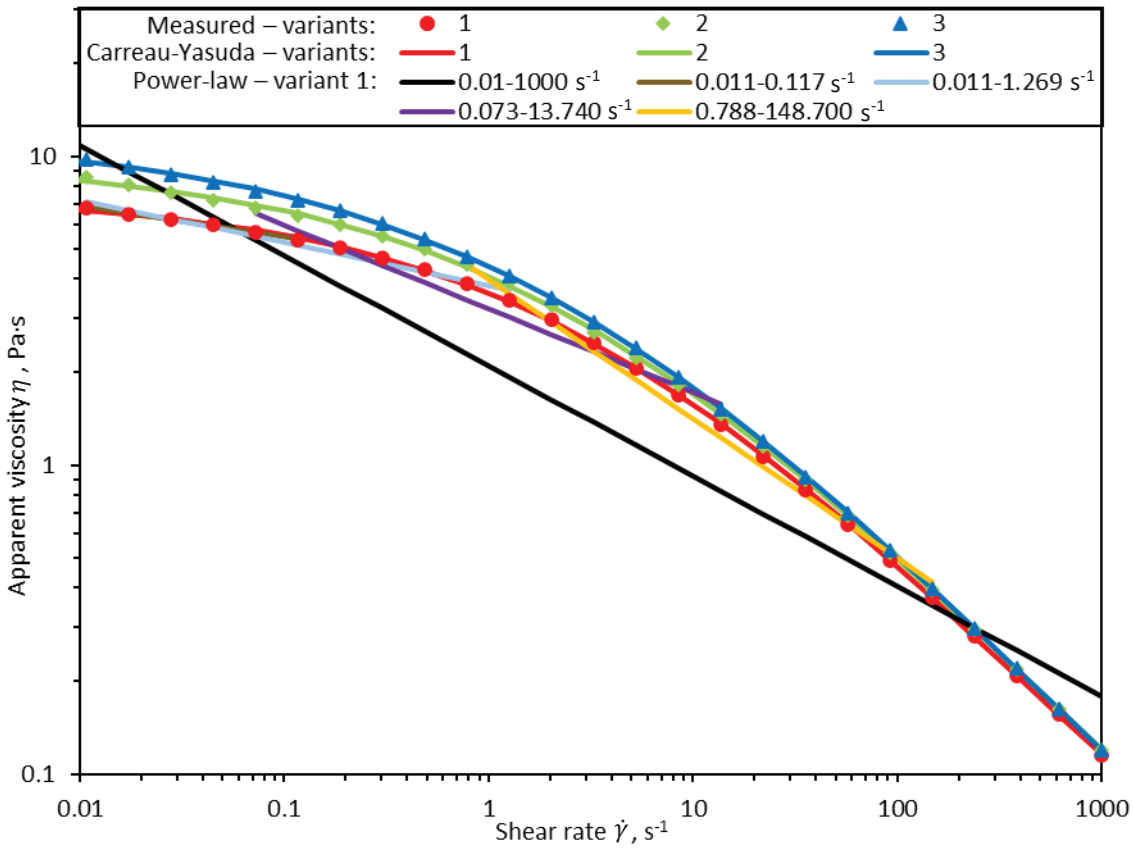

Figure 2. The viscosity curves and their fits by the rheological models for the measurement variants 1, 2, and 3

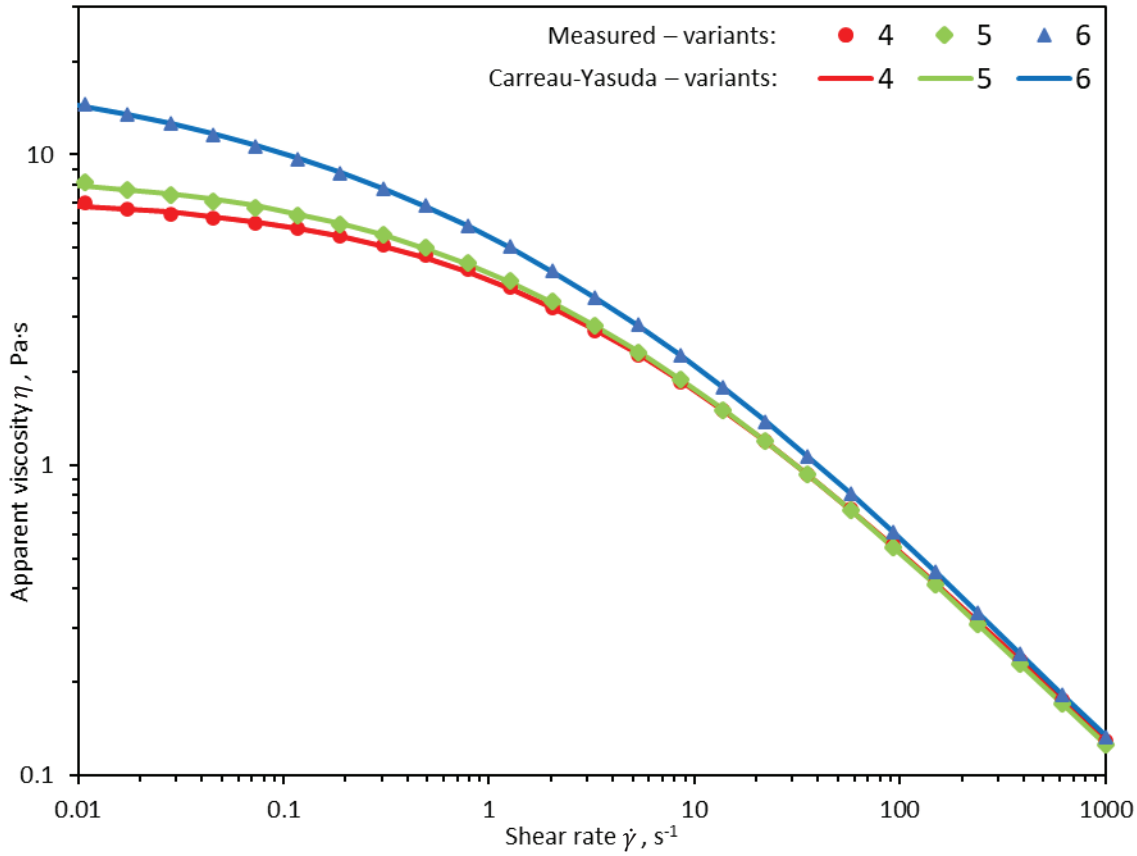

Figure 3. The viscosity curves and their fits by the rheological model for the measurement variants 4, 5, and 6

Table I
The overview of the measurement variants, weight loss and Carreau-Yasuda model parameters

Measurement variant	Overflow trimming	*RH* *[%]*	Measuring conditions	Relative weight loss *[%]*	Carreau-Yasuda model parameters				
					η_{inf} *[Pa·s]*	η_0 *[Pa·s]*	λ *[s]*	a *[-]*	m *[-]*
1	yes	80-100	humidification	6	0.012	7.404	0.311	0.461	0.275
2	yes	40-60	hood	10	0.006	9.533	0.472	0.446	0.298
3	yes	20-30	laboratory	19	0.014	11.636	0.349	0.400	0.227
4	no	80-100	humidification	9	0.000	7.299	0.458	0.536	0.350
5	no	40-60	hood	27	0.001	8.814	0.511	0.487	0.329
6	no	20-30	laboratory	86	0.020	21.218	0.251	0.316	0.134

The drag coefficients of the different measurement variants and the drag coefficients obtained using the different rheological models were compared as the relative difference of the drag coefficients ΔC_D *[-]*. The relative difference of the drag coefficients ΔC_D is expressed as

$$\Delta C_D = \frac{C_D - C_{D,variant\ 1,Carreau-Yasuda}}{C_{D,variant\ 1,Carreau-Yasuda}} \cdot 100 \quad (6)$$

where $C_{D,variant\ 1,Carreau-Yasuda}$ *[-]* is the drag coefficient of the measurement variant 1 obtained using the Carreau-Yasuda model for curve fitting in the interval 0.01-1000 s^{-1}. The drag coefficient C_D *[-]* was obtained with the parameters of the Carreau-Yasuda model (fitting interval 0.01-1000 s^{-1}) of the measurement variants 2, 3, 4, 5, or 6, or the drag coefficient obtained using the power-law model parameters of the measurement variant 1 (fitting interval 0.01-1000 s^{-1}) or the specific fitting intervals from Table II.

The relative differences ΔC_D between C_D of variant 1 and C_D of variants 2, 3, 4 ,5 and 6 are more significant for the low values of $\dot{\gamma}$. They can be in the order of tens of percents, see Figure 4. The influence of sample overfilling

is the most significant for measuring at the laboratory *RH*. Compare the results for variants 3 and 6 with the results for variants 2 and 5 in Figure 4. The relative difference of C_D for variant 4 indicates that for higher *RH* values, the differences between measurements with trimming and with the sample overflow are not significant.

Table II
The terminal falling velocities, mean shear rates, specific shear rate intervals and power-law model parameters

u_t [m·s^{-1}]	$\bar{\dot{\gamma}}$ [s^{-1}]	$\dot{\gamma}$ specific intervals [s^{-1}]	Power-law model parameters measurement variant 1	
			K [Pa·s^n]	n [-]
0.00003	0.01	0.011-0.117	4.364	0.901
0.0003	0.1	0.011-1.269	3.810	0.861
0.003	1	0.073-13.740	3.209	0.729
0.03	10	0.788-148.700	4.000	0.549

Comparison of the power-law and the Carreau-Yaasuda model for measurement variant 1

Using the power-law model in the wide shear rate interval can lead to serious relative differences ΔC_D between C_D calculated for this case and C_D calculated with the parameters of the Carreau-Yasuda model. The smaller differences can be obtained by fitting the viscosity curve in the specific interval for each $\bar{\dot{\gamma}}$, see Figure 4.

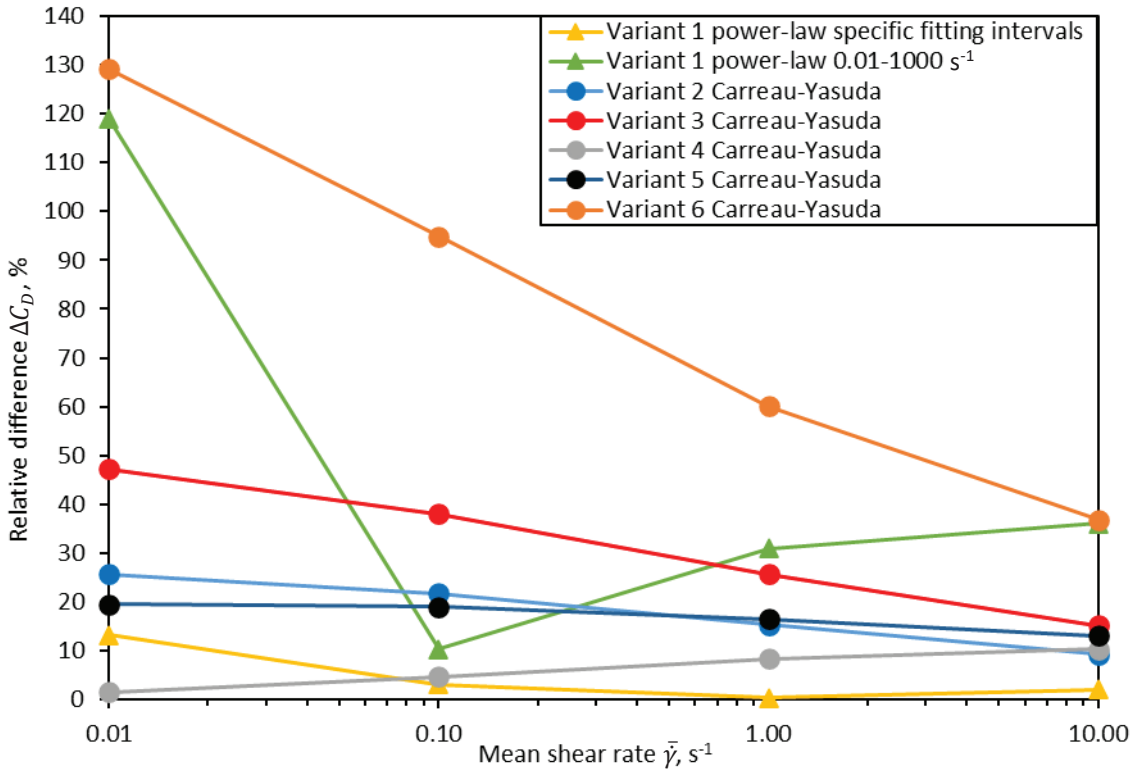

Figure 4. The relative differences of the drag coefficients calculated from Eq. (6)

Conclusions

The water evaporation during the rheological measurement of the *CMC* solution can lead to significant errors in the evaluation of the free fall of a spherical particle in a non-Newtonian fluid. Relative differences in the drag coefficients ΔC_D, due to evaporation during rheological measurement, can be in the order of tens of percent. Air humidification can significantly reduce evaporation. The influence of the sample amount was less significant than the influence of the relative humidity.

These results indicate the importance of choosing the correct methodology and conditions of the rheological measurement that correspond to the conditions in the hydrodynamic experiments.

For the evaluation of the free fall of a particle in a non-Newtonian fluid, the power-law model should be used only in a specific interval of the shear rate $\dot{\gamma}$. The results obtained using the power-law model in the wide interval of the shear rate $\dot{\gamma}$ can significantly differ from those obtained using the Carreau-Yasuda model.

Acknowledgement

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Nomenclature

a *[-]*	Carreau-Yasuda model parameter	*RH [%]*	relative humidity
C_D *[-]*	drag coefficient	u_t *[m·s^{-1}]*	particle terminal falling velocity
CMC	carboxymethyl cellulose	$\dot{\gamma}$ *[s^{-1}]*	shear rate
CP	Cone-plate geometry	$\bar{\dot{\gamma}}$ *[s^{-1}]*	mean shear rate around the particle
d *[m]*	particle diameter	ΔC_D *[-]*	drag coefficients relative difference
F_D *[N]*	drag force	η *[Pa·s]*	apparent viscosity
FEM	finite element method	η_{eff} *[Pa·s]*	effective viscosity
K *[Pa·s^n]*	consistency coefficient	η_{inf} *[Pa·s]*	infinity shear rate viscosity
m *[-]*	Carreau-Yasuda model parameter	η_0 *[Pa·s]*	zero shear rate viscosity
n *[-]*	flow index	λ *[s]*	Carreau-Yasuda model time parameter
Re_p *[-]*	particle Reynolds number	ρ *[kg·m^{-3}]*	fluid density

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THE REALISTIC OPTIONS FOR THE DECARBONISATION OF ORLEN UNIPETROL'S STEAM CRACKER

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Abstract

The decarbonisation of the industry is the chemical industry is a very challenging task especially from the point of view the chemical industry itself belongs together with the power generation and transport among the largest sources of carbon dioxide. Thus the ethylene production represents the biggest producer of carbon dioxide among the (petro)chemical processes it is obvious the overall decarbonisation of any petrochemical complex should start with the decarbonisation of the steam cracker.
The decarbonisation of the steam cracker is a very complex process which have to be focused on every aspect of the plant operation. The frequently spoken transition to electric pyrolysis furnaces as well as compressors and pumps driven by electro motors instead of steam turbines is unrealistic being very far from the feasible reality. The feasible decarbonisation have to be based on the complex analysis of the operated plant, its specific process arrangement, availability of the renewable energy, transition to different (more environment friendly) feed stocks and detailed internal process parameters optimization. The finally proposed path to the decrease of the carbon footprint of particular plant has to take into the account also the age of the operated plant thus the most European plants are very old being limited by the technical solutions (e.g. cracked gas compressor, pyrolysis section, etc.)
The paper describes a realistic options for the decarbonisation of the ORLEN Unipetrol's steam cracker – a plant which is in operation since 1980. The decarbonisation of naturally mixed/liquid cracker is quite a challenge especially from the point of the limited availability of the renewable energy. The paper analyses the position of the unit among others as well as brings a brief introduction of the first European low emission cracker (Ineos Project ONE)

Introduction

The decarbonisation is defined as the process of reducing or eliminating emissions of carbon dioxide (CO2) and other greenhouse gases in order to prevent further global warming. The goal of decarbonisation is to reduce dependence on fossil fuels in order to establish a low-emission or carbon-neutral economy. The decarbonisation comprises of different measures such as switch to renewable energy, improvement of energy efficiency and developing carbon capture and storage technologies. Based on the origin of produced emissions the direct emissions (linked to productions), indirect emissions (power generation) and other indirect emissions (mainly logistics) are defined.
The decarbonisation is inevitable not only due to the wide implementation of European legislation but especially from the competitiveness point of you. Despite the fact it brings lot of challenges such as financing, timing and limited readiness of commercially available solutions it is clear it will bring the significant savings of energy due to the improvement of energy efficiency. It can also improve the overall status of the plant simply from the point of view the old and worn equipment can be replaced by new one thus the return of investment is ensured now. Therefore, from the above definition, it is necessary to ensure that the decarbonisation of any steam cracker minimises production of emissions during operation, maximises the use of renewable energies and implements solutions that reduce or at least do not increase logistics requirements. The minimization of the emissions during the plant operation is a very complex task which depends on the multiple factors either design or process based. The important design based factors are plant age (i.e. technology constraints related to particular solutions used in the past), design of pyrolysis heaters, plant configuration and plant location (e.g. the plant located in the Middle East have got different design of cooling systems than plant located in the Scandinavia). The process based factor can be type and composition of used feeds, cracking severity, temperature and pressure of the main products, charge gas compressor suction pressure, etc.
How important the mentioned parameters are can be easily illustrated in the following three figures 1-3. The figure 1 shows the development of the specific charge gas compressor power consumption ($kW.t^{-1}$ ethylene) during the period of last fifty years. It is clearly visible big burden the older plant has in the comparison to the more efficient recent designs – in case of ORLEN Unipetrol's cracker the charge gas compressor has specific power consumption worse approximately by one third (135 per cent of contemporary machines). Such a difference represents not only the huge challenge for the decarbonisation but it also significantly increases its costs. Moreover, the competitiveness of the plant on the market it is remarkably negatively influenced too.

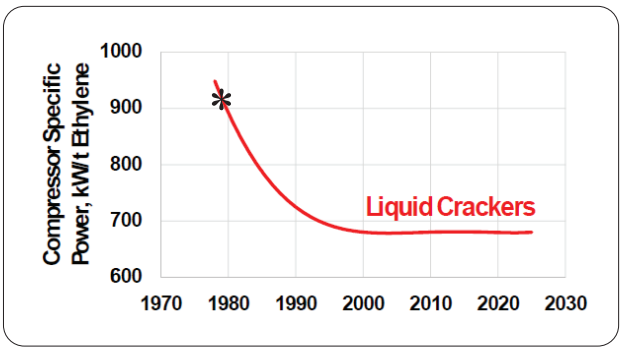

Figure 1. The specific power consumption of charge gas compressor [1] (Position of ORLEN Unipetrol cracker indicates asterisk)

The other decisive and determinative parameter is a feedstock slate, i.e. type and amount of feedstock the plant is processing. The feedstock slate determines the energy consumption in two ways – via plant configuration and via the operation of the pyrolysis section. The significant deviations between the ethane and liquid (feeds) crackers shows figure 2 where the comparison of plant energy indexes ($GJ.t^{-1}$ ethylene) is made.

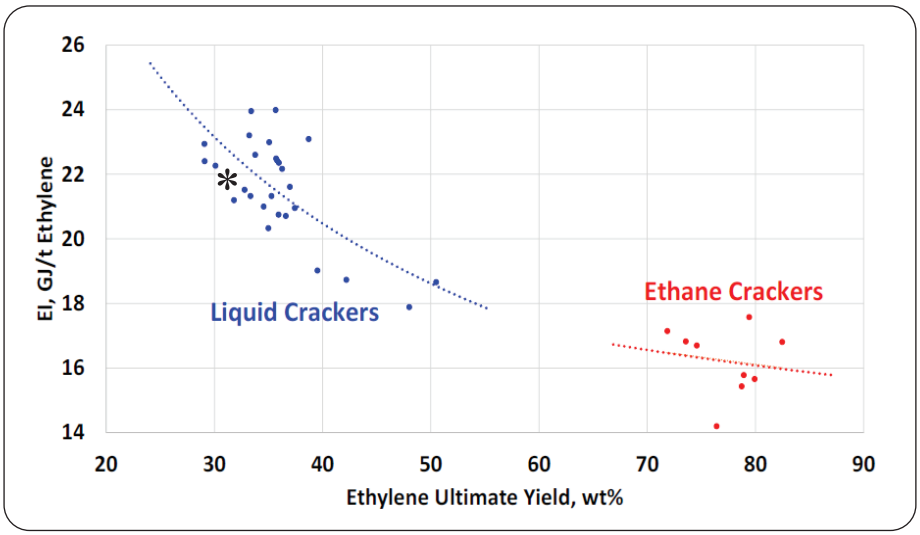

Figure 2. The energy index of ethane and liquid crackers [1] (Position of ORLEN Unipetrol cracker indicates asterisk)

The following figure 3 shows confirms the worse position of the liquid crackers in case of the carbon dioxide specific production – despite the fact the ethane crackers need more energy (higher energy index values) their specific production of carbon dioxide is lower.

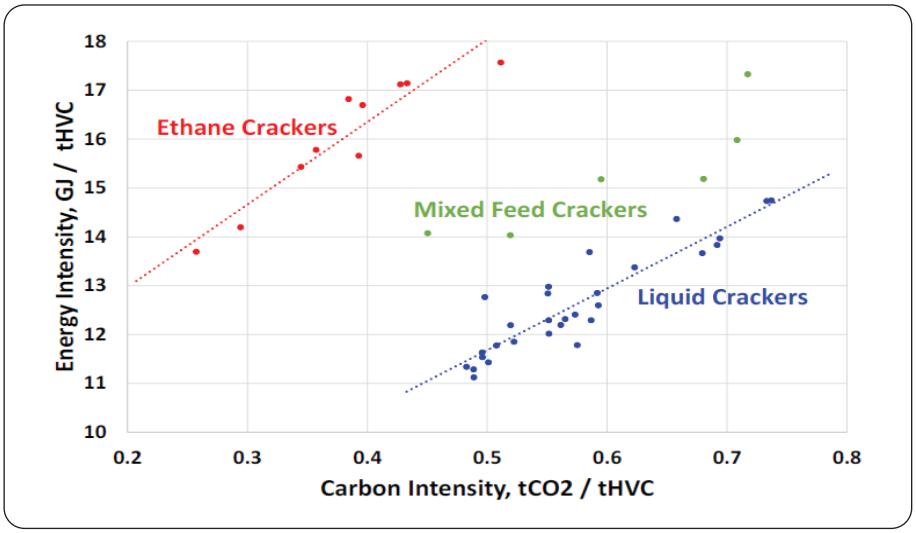

Figure 3. The comparison of specific energy intensity based on specific CO_2 production [1] (different cracker

type)

(Position of ORLEN Unipetrol cracker indicates asterisk)

Taking into the account the constraints presented in previous figures it is clear the decarbonisation of the steam cracker has to be a complex and multi directional task. It is clear the way how to decarbonize the cracker has to be chosen based on feedstock slate, age of the plant, process layout and process parameters optimization. The specific carbon dioxide production of existing European crackers varies between 0,7 and 2,0 t $CO_2.t^{-1}$ ethylene. The carbon dioxide is produced mainly at pyrolysis section (90 – 95 per cent) and the pyrolysis section itself consumes 60 – 65 per cent of energy. The other important contributor to the total production of the carbon dioxide at the cracker site is the boiler house used for the production of the of high-pressure steam (majority of this steam is produced at TLEs of pyrolysis heaters). Such an arrangement means this two process nodes are the primary candidate for the decarbonisation – the only problem is the decreasing of the carbon footprint is strongly conditioned either by the availability of electricity from renewable sources or availability of the hydrogen as the alternative fuel. Anyway, the huge surplus of the methane will be an issue in this case so that its utilization is a key condition.

More probable way than electrification a complex optimization of the plant represents a feasible way. The first step has to be focused on the combination of energy savings, enhancement of thermal integration and optimization of process parameters. This first step can be further boosted by the second one - full or partial utilization of the hydrogen as the fuel and increase of the lighter feed stocks where it makes sense (e.g. replacement of heavy feeds by LPG). The third step can be partial replacement of turbines and reasonable revamp of identified pieces of equipment due to the higher CAPEX requirements. The massive electrification of the plant as well as implementation of CCR (carbon capture storage) and FGR (flare gas recovery systems) are with the highest probability the last option thus these measures needs really massive investment.

Decarbonization of an already operating plant

The decarbonisation of an already operating plant, i.e. plant designed without the requirements related to the reduction of carbon footprint is always a compromise – simply from the point of view of total available CAPEX and possibilities and conditions at particular location. In general, two possible options of minimization energy consumption (reduction of carbon dioxide emissions) are always present – the optimization of the process parameters and revamp/retrofitting of existing equipment.

The most effective ways of plant energy consumption decrease include

- optimization of the pyrolysis heaters operation in order to reduce the energy requirements. The side effect of such a optimization is the worse economy of the pyrolysis process – increased coking rate and the negative impact on yields. The measures should comprise the COP optimization (increase of the suction pressure of charge gas compressor), increase of the cracking severity in order to mitigate the negative yield impact and the reduction of S/O ratio (decrease of process steam consumption). The revamp of existing equipment have to be focused on the implementation of the combustion air preheat.
- minimization of cracked gas compressor power. The measures have to be focused on the plant traffic reduction (minimization of any recycles) and the decrease of the pressure drop and temperatures. The minimization of inter-stage coolers outlet temperature is recommended as well as the reduction of the turbine condenser back pressure. The increase of the suction pressure was mentioned above. The revamp of existing equipment has to be focused on additional cooling of streams and decrease of pressure drop (e.g. replacement of demisters in knocking drums)
- minimization of refrigeration power. The operational measures in this area have to include the minimization of the cryogenic product rundown to storage area and a minimization of the condensing pressure of propylene refrigerant. The revamp activities can be focused especially on the optimization of the number of propylene refrigerant levels (increase of the number of stages and the reduction of delta T). The replacement of the ethylene refrigerant compressor steam turbine by an electro motor can be also good solution in case the electricity from renewable sources is available.
- optimization of cracker flow sheet. The measures related to the optimization of cracker flowsheet always include the revamp activities. These activities are conditioned by the deep analysis of the existing process thus they represents the significant intervention into the equipment. The revamp activities have to be focused on the heat integration activities, optimization of the steam balance, mitigation of cooling water temperature increase, optimization/minimization of utility requirements, etc. The examples of activities can include the heating of process streams with low-level heat sources (quench oil, quench water, low pressure steam) where possible, improvement of process heat integration, replacement of

trays in distillation towers (reduction of reflux flow), replacement of steam turbines by electro motors or implementation of enhanced surface heat exchangers.

The scope of decarbonisation activities is expected to be tailor-made for a particular plant being determined by local conditions, plant layout and constraints as well as the CAPEX possibilities.

Decarbonization of a new plant

The example of the implementation of decarbonisation approach into the design of a new steam cracker represents the current INEOS Project One [2]. The new cracker is built in Antwerp since 2021 for INEOS company. The cracker was designed by T.EN (Technip Energies) as a low emission modular steam cracker with nameplate capacity of 1450 tons of ethylene. The plant is designed to process imported ethane only. The cracker flowsheet (Figure 4) is optimized in order to achieve the following goals

- maximum specific carbon dioxide emission threshold 0,7 t $CO_2.t^{-1}$ ethylene (be better than the best 10 crackers in Europe)
- maximum specific energy consumption threshold 17 $GJ.t^{-1}$ ethylene (be the best in Europe)

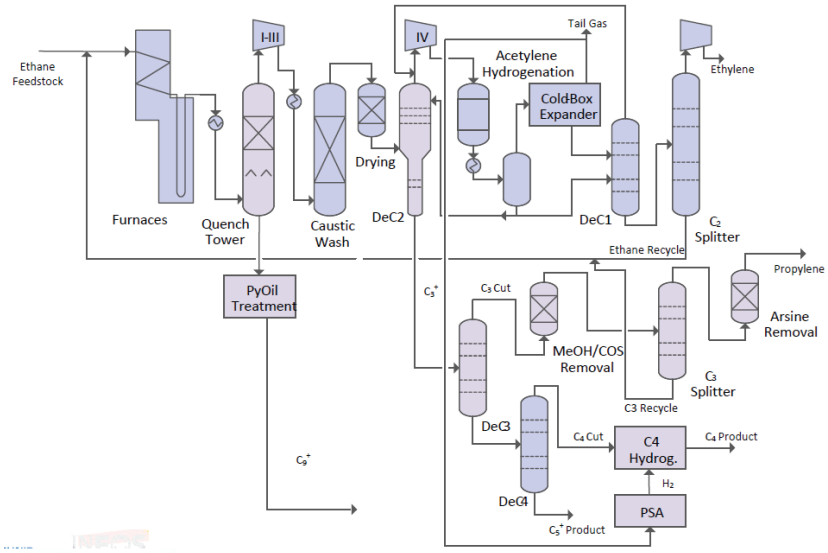

Figure 4. INEOS Project ONE steam cracker flowsheet[2]

In order to fulfil these goals the following measures were applied:

- ethane was chosen as the only feedstock – the cracking of ethane at high conversion (72 per cent) provides high ethylene yields
- the fuel gas has at standard operational conditions very high content of hydrogen (85 per cent)
- the radiant box of pyrolysis heaters was designed in a way to achieve high efficiency – (firing pattern, air preheat system)
- the design of pyrolysis heater was optimized in a way to maximize the production of HP-steam as well as to achieve high coil inlet temperatures
- all pumps are driven by electro motors (including quench oil circulation pumps and BFW pumps)
- deep thermal integration techniques and design applied

The recent calculation show the design goals will be not only met but significantly exceeded – the maximum specific carbon dioxide emission threshold is expected to reach 0,3 t $CO_2.t^{-1}$ ethylene and the maximum specific energy consumption is expected to be within the range 14,3 - 15 $GJ.t^{-1}$ ethylene. This success is conditioned by the availability of the electric energy from renewable sources (contracted by INEOS on long time basis).
The estimated values of both parameters can be even improved – this step is expected after the successful commissioning and start-up of the plant. The pyrolysis section was designed for the implementation of CCS (no carbon dioxide will be emitted into the atmosphere). The hydrogen content in fuel gas will be further optimized (100 per cent possible). Last but not least the flare gas recovery system is ready to be implemented too.

The realistic options for the decarbonisation of ORLEN Unipetrol's cracker

The ORLEN Unipetrol steam cracker is forty five years old plant designed and commissioned in the late seventies of the last century. The plant is a mixed/liquid cracker with nameplate capacity of 544 kta of ethylene processing wide range of feedstock (LPG, mixed naphtha, hydrocracker residue and recycled ethane/propane stream). The plant is fully integrated with the downstream units (DPG, thermal hydrodealkylation of BTX fraction and benzene extraction). The plant also operated its own boiler house where approximately 40 per cent of high pressure steam is produced. Plant was revamped twice (2000, 2007) nevertheless no modification/improvement of utilities (especially boosting of cooling water system) was made. The cracker suffered a major accident in 2015 when four pyrolysis heaters were burnt down as the consequence of the quench oil pool fire. The five new units supplied by T.EN (Technip Energies – four heaters in 2016, the fifth one was commissioned in 2023) are BAT units fully comparable with heaters used for INEOS Project One. The original boiler house was replaced by new unit in 2021 which is capable to burn methane and pyrolysis oils meeting all valid environmental limits. Plant has very limited possibility for an extensive change of feedstock slate and no electricity from renewable sources is available. The carbon footprint of the cracker site is alarming (2,25 t $CO_2.t^{-1}$ ethylene) nevertheless there is a real opportunity to utilize the potential of new equipment.

The decarbonisation strategy of the ORLEN Unipetrol cracker has to be based on the combination of activities in four areas

1. optimization of feedstock slate (partial replacement of hydrocracker residue by LPG)
2. optimization of operation parameters
3. equipment modification/revamp
4. implementation of new equipment

The decarbonisation strategy is based on the availability of LPG. The abandonment of the Russian crude oil processing brings a nice opportunity for the steam cracker decarbonisation – the possibility to operate in parallel two pyrolysis heaters cracking LPG seems to become feasible for the first time in the plant history. If this arrangement becomes reality it would be possible to make two important steps towards the decarbonisation of the plant

a) put higher amount of hydrogen into the fuel gas (decrease CO_2 production, save methane) [3]
b) utilize saved methane in order to stop the burning of heavy pyrolysis oil (PFO) at boiler house (decrease CO_2 production)

Such a joint optimization can paw the way for the utilization of the potential of the new equipment installed between the years 2016 and 2022 (new pyrolysis heaters and boiler house). The principle of proposed cyclic swap of fuels proposed for the standard plant operation shows Figure 5.

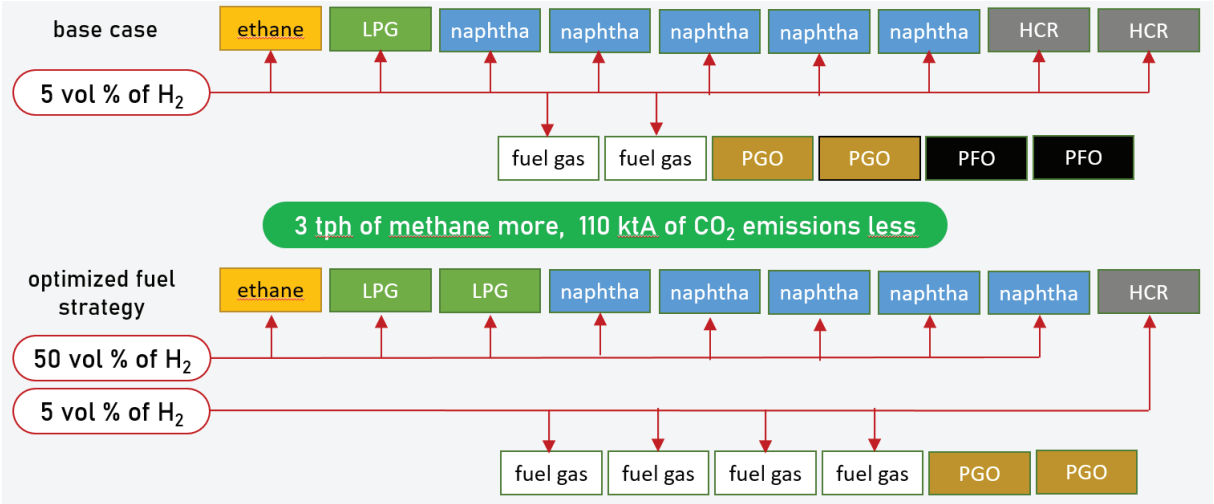

Figure 5. Arrangement of the optimized fuel strategy in case of standard plant operation

The proposed solution is based on the two separate fuel systems – new one designed for the higher content of hydrogen (minimum 50 vol. per cent) and existing one capable to handle the lower content of hydrogen (up to 5 vol. per cent). In total eight pyrolysis heaters (five existing plus three revamped) is expected to burn hydrogen rich fuel gas while remaining one will be fired with standard methane with low content of hydrogen. The excess of methane (approximately 3 tons per hour) is expected to be used at boiler house where it substitutes the heavy pyrolysis oil. The new fuel strategy can be implemented relatively soon and with moderate CAPEX requirements

– at least five pyrolysis heaters is fitted with burners capable to burn even pure hydrogen and the LPG evaporators and feed lines are ready – only the new fuel system pipelines and LPG supply line have to be provided. The change of process operational parameters can be executed without extra costs. The minor modification of equipment or its revamp related CAPEX requirements are varying in a broad range – the most important project is definitely the revamp of three pyrolysis heaters and provision of combustion air preheat. Finally, the implementation of a new equipment is optional due to the significant CAPEX requirements.
All proposed projects of this realistic plant decarbonisation strategy are listed in the table 1.

Table I. Identified potential of particular decarbonisation project

No.	Particular project title	Category	CO_2 reduction potential		reduction of specific CO_2 emission
			tph	tpA	per cent
1	HP-steam minimization	optimization of parameters	1,2	10512	0,93
2	LPG instead HCR	feedstock slate modification	1,1	9636	0,86
3	cyclic swap of fuels at boiler house	feedstock slate modification	6,4	56064	4,99
4	pyrolysis heaters process parameters optimization	optimization of parameters	2,8	24528	2,18
5	CGC suction pressure increase	optimization of parameters	1,4	12264	1,09
6	PRC suction pressure decrease	optimization of parameters	0,3	2628	0,23
7	PRC condensers - remote control of cooling water supply	modification/revamp	0,9	7884	0,70
8	increase of the hydrogen content in fuel gas	feedstock slate modification	5,3	46428	4,13
9	replacement of quench oil circulation pumps	modification/revamp	1,1	9636	0,86
10	replacement of quench water coolers	modification/revamp	0,9	7884	0,70
11	replacement of LPG evaporators	modification/revamp	1,0	8760	0,78
12	electromotors for HCR pumps	modification/revamp	0,9	7884	0,70
13	combustion air preheat - humidifier implementation	new equipment	1,4	12264	1,09
14	implementation of turboexpander GT/GB-302	new equipment	2,6	22776	2,03
15	revamp of pyrolysis heater BA-101	modification/revamp	1,6	14016	1,25
16	revamp of pyrolysis heater BA-103	modification/revamp	1,6	14016	1,25
17	revamp of pyrolysis heater BA-105	modification/revamp	1,6	14016	1,25
18	reconstruction of old boiler BF-1201B (start up booster)	modification/revamp		550	0,05
19	revamp of CGC and PRC turbine condensers	modification/revamp	4,8	42048	3,74
20	revamp of ERC turbine	modification/revamp	2,4	21024	1,87
21	revamp of CGC compressor	modification/revamp	3,0	26280	2,34
22	operation of electric driven BFW pumps only	optimization of parameters	4,4	38544	3,43

Results and discussion

The proposed ORLEN Unipetrol decarbonisation strategy is based on execution of the feedstock and fuel portfolio change. Thus there are no available sources of the renewable energy the only way how to decrease the carbon footprint of the plant is (besides the recycling which is not included in this paper) the introduction of lighter feed and replacement of heavy fuels. The proposed changes in this area can deliver the reduction of the carbon dioxide production by 10 per cent.
Nearly eight per cent of carbon dioxide production can be in addition achieved relatively simply by the optimization of process parameters or plant procedures. In this area is clear that the optimization of process parameters towards the reduction of carbon footprint has negative impact on the plant economy, especially in case of reduction of pyrolysis yields and higher coking rate.
The modification or revamp of existing equipment can secure additional reduction of 15 per cent of total carbon dioxide production. The feasibility of execution of these projects strongly depends on the CAPEX requirements which varies in the broad range between units to hundreds of millions CZK. Last 4 per cent of carbon dioxide

production can be secured by implementation of a new equipment nevertheless the CAPEX requirements are very high.

In total, the proposed decarbonisation strategy has a potential to reduce the CO_2 emissions by 36,5 per cent.

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SYNTHESIS AND PRODUCTION OF DRUGS

APPLICATION OF DFT CALCULATIONS FOR CRYSTAL STRUCTURE VERIFICATION OF PHASES FROM SALT-COCRYSTAL CONTINUUM AREA

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Abstract

Pharmaceutical solid forms, such as salts and cocrystals, are essential in drug formulation. Despite differing primarily in the position of a single hydrogen atom, salts and cocrystals are subject to markedly different regulatory requirements set by the US Food and Drug Administration (FDA)[1,2]. We previously developed a computational method based on Density Functional Theory (DFT) to distinguish salts from cocrystals by optimizing artificially constructed incorrect structures[3].
In the present work, we expanded the studied dataset to 404 cocrystal models and used the rSCAN functional instead of the previously used PBE functional. The analysis confirmed that 301 of the evaluated structures were indeed cocrystals, while 87 represented salt–cocrystal continuum forms. Additionally, 16 cocrystals were classified as potential salts. These problematic structures were further investigated. We reproduced the crystallization process and performed data collection using single-crystal X-ray diffraction (SCXRD) for 7 of them. Complete experimental data were available for 2 problematic structures from the original authors and, data reinterpretation was possible. To obtain the best possible hydrogen positions, we used the Hirshfeld atom refinement (HAR) method for refinement as implemented in Olex2 software and NoSpherA2.
The findings revealed that rSCAN occasionally provided unreliable results for strong hydrogen bonds; however, the discrepancies were often corrected by using better-renormalized or hybrid functionals, such as r2SCAN, PBE0, and PBE50. Among the structures exhibiting salt-like behavior, five structures were confirmed as salts. Our results suggest that the r2SCAN functional offers a reliable balance between accuracy and computational efficiency, particularly for O–H···N bonds longer than 2.554 Å[4].

Introduction

Pharmaceutical molecules can exist in various solid forms. Cocrystals are stoichiometric multicomponent solids formed from two or more neutral components, while pharmaceutical salts involve an ionizable drug and a counter-ion[1,5,6]. The key distinction between the two is given by the position of a single hydrogen atom, making accurate identification essential for regulatory and quality control purposes[2]. Numerous well-established techniques exist for distinguishing salts from cocrystals, including single-crystal X-ray diffraction, solid-state NMR or neutron diffraction—the latter being the most precise but limited by high cost, low intensity, and the requirement for large single crystals. Each method has limitations and may not be universally applicable[7-9]. We are developing a Density Functional Theory (DFT) based method for distinguishing salts from cocrystals. Our DFT method optimizes an artificially constructed wrong structure (hydrogen atom placed in salt position near the potential acceptor for cocrystals and vice versa cocrystal position with hydrogen atom placed near the potential donor of the salts). The verification of the method was done based on a comparison of the results with an experimentally confirmed hydrogen position. 16 cocrystals from the studied set were identified as salt, in disagreement with experimental data. These cases were investigated further: 7 were recrystallized and analyzed using single-crystal X-ray diffraction, and for 2, the original data were reinterpreted. Hydrogen positions were refined using the Hirshfeld atom refinement (HAR) in Olex2/NoSpherA2. We also tested whether more advanced functionals (r2SCAN, PBE0, PBE50) could better match experimental results in these problematic cases.

Methodology

The DFT calculations were performed using CASTEP code. Since the cell parameters were assumed to be accurately obtained experimentally, we solely performed only optimization of atomic positions. We used the rSCAN functional with MBD dispersion correction and automatic fine basis precision[10,11]. The data were prepared in checkCIF-DFT software[12]. The optimization was always performed from both artificial salt and cocrystal starting models. Computation was performed on Karolina supercomputer at TU Ostrava, Czech Republic.
For cases where we crystallized the structure or reinterpreted the data of the original authors, we used HAR method as implemented in Olex2 software and NoSpherA2 module [13-16]. For the wavefunction calculation we

had used def2-TZVP localized base, r2SCAN functional and Orca 5.0 software[17]. The refinement was performed using two methods in all cases. The first method was based on refinement of the problematic hydrogen in single position. The second method was based on refinement of this hydrogen in two positions as disordered one. The donor and acceptor distances to the hydrogen were in the second case restrained to the value 0.95 Å with weight corresponding to 0.01 Å esd.

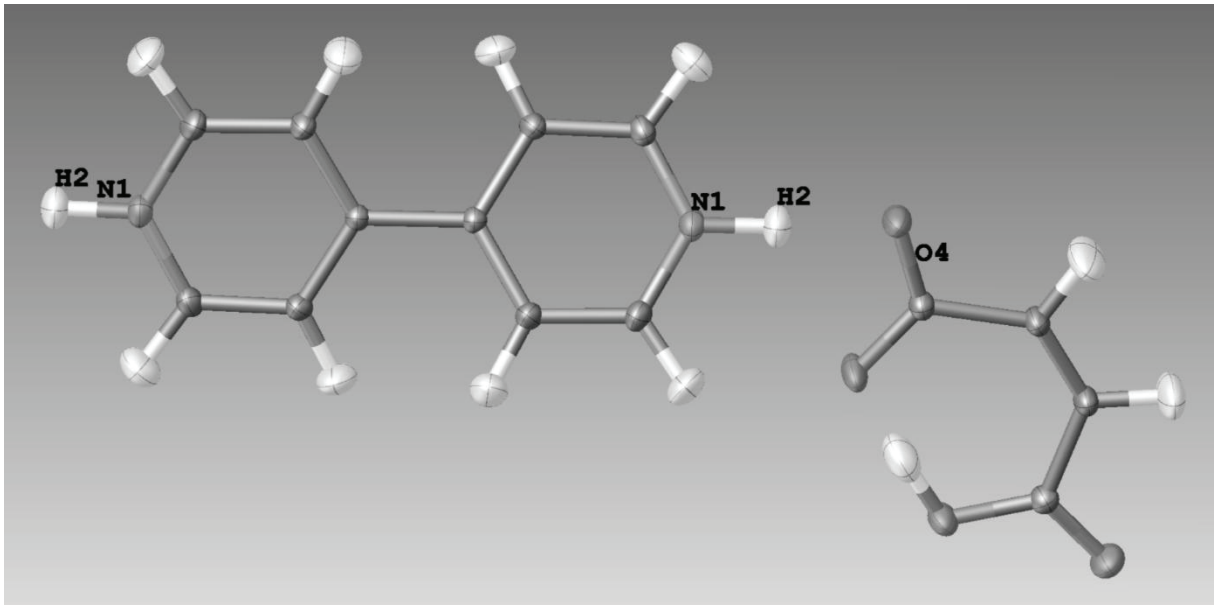
Conclusions

We confirmed the correct cocrystal structure determination in 301 cases. For 87 structures we had identified that the phase determination is suspicious, and the structures probably create a salt-cocrystal continuous phase.

Table I
Results of calculation on 404 structures from the zone with -1 ≤ *ΔpKa* ≤ 4 (rSCAN fine + MBD)

Pure cocrystal	Salt-cocrystal continuum phase	Pure salt
301	16	87

Figure 1 Structure of 4,4'bipyridine and maleic acid (GIPQAX) in Olex2 refined by HAR method with hydrogen atoms treated as anisotropic. The structure was originally solved incorrectly as cocrystal.



From the 16 phases exhibiting consistent salt behaviour by our methodology, we experimentally proved that 2 are true salts. We believe that 3 others were incorrectly solved by the original authors, and our DFT method using rSCAN functional correctly identified these as salts. In some cases we confirmed that the DFT method based only on rSCAN functional is not reliable and unsuitable for cocrystal/salt distinguishing with strong H-bond. However, advanced functionals (r2SCAN, PBE0, PBE50) were able to correct these discrepancies in some cases. For future prediction we suggest using the r2SCAN functional for salt–cocrystal differentiation, which provides correct results for O–H···N bonds longer than 2.554 Å, compared to our previous 2.613 Å limit. The computational cost of r2SCAN is comparable to rSCAN, making it suitable for large-scale screening[18].

Acknowledgements

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TECHNOLOGY FOR ENVIRONMENTAL PROTECTION

TESTING THE ECOTOXICITY OF CIGARETTE BUTTS AND THEIR IMPACT ON THE ENVIRONMENT

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Abstract

The work deals with experimental testing of the ecotoxicity of cigarette butts applying their extract on three types of living systems: freshwater crustacean *Daphnia m*agna, freshwater algae *Desmodesmus subspicatus* and sewage sludge. The tests were carried out using procedures corresponding to the relevant OECD methodologies for ecotoxicological testing.

Introduction

Cigarette butts (CB) are one of the few wastes that have been systematically addressed. The scientific community has been studying their issue for several years, mainly due to their potential toxicity[1] and high annual production volume[2]. The impact of chemicals on the environment is assessed by ecotoxicological tests. They are classified into many different groups according to their nature. The most common classification parameters are the duration of the test (acute, subchronic and chronic)[3], the environment in which it is carried out (terrestrial or aquatic)[4], and the organism tested.

Experiments

In this work, three toxicity tests were performed in collaboration with VÚOS a.s., Rybitví according to OECD methodologies: (i) acute immobilization test corresponding to OECD Guideline No. 202[5] on the freshwater crustacean *Daphnia m*agna, (ii) growth inhibition test No. 201[6] on the freshwater alga *Desmodesmus subspicatus* and (iii) activated sludge respiration inhibition test No. 209[7].

(i) Acute Immobilization Test No. 202
Daphnia magna (Figure 1 a) is a primary consumer in freshwater and it is sensitive to water purity. Therefore, it is used as a standard organism for ecotoxicological tests. The EC50 lethal concentration values achieved in acute toxicity tests on this organism are used for the evaluation of substances in the REACH system[8].
An extract of cigarette butts (Marlboro) from the outdoor environment was prepared for the test. 4 Cigarette butts (1.296 g) were extracted in 2 L of dilution water (demineralized water containing salts: $CaCl_2$, $MgSO_4$, $NaHCO_3$, KCl) for 24 h at room temperature and the solution was filtered[9,10,11].
6 Concentrations were prepared and 20 daphnia were placed in each. Extinction was recorded after 24 and 48 h.

(ii) Growth Inhibition Test No. 201
Desmodesmus subspicatus (Figure 1 b) is found in the plankton of habitats such as ponds and lakes, especially in eutrophic waters. It is one of the most common species of freshwater plankton. It can also be found in soils and biological soil layers.

a)  b) 

Figure 1. a) *Daphnia magna*, b) *Desmodesmus subspicatus*

A seed culture with a concentration of 5000 cells/mL was prepared so that exponential growth could prevail. Cells were counted using the standard method in a Büchner chamber (Figure 2 a). For a statistically correct evaluation, 40 squares in four rows were counted as indicated in Figure 2 b. The seed culture was added to 100 mL of nutrient solution[6] and allowed to grow for 4 days.

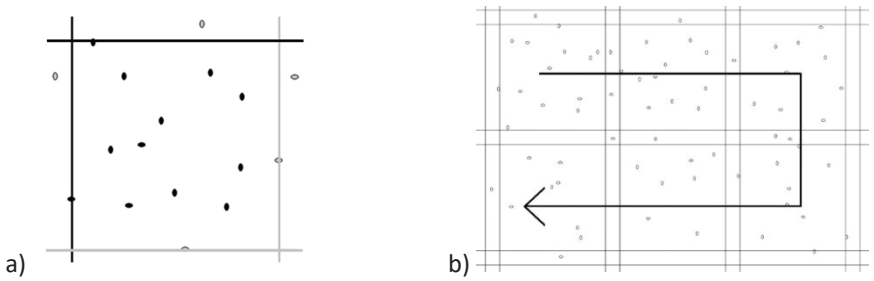

Figure 2. a) Illustration of cell counting in one square of a Büchner chamber[12], b) Illustration of cell counting in a grid of a Büchner chamber[12]

For the test, an extract of cigarette butts from the outdoor environment was prepared. 20 Cigarette butts were extracted in 2 L of water for 24 h at room temperature and the solution was filtered[9,10,11]. 6 Concentrations were prepared. The required amount of the resulting inoculum culture was added to each concentration, the samples were irradiated with constant stirring for 72 h[6] and evaluated.

(iii) Activated Sludge Respiration Inhibition Test No. 209

First, synthetic wastewater was prepared by mixing distilled water, meat extract, peptone, urea and salts (NaCl, $CaCl_2$, $MgSO_4$, K_2HPO_4)[7]. And 2 L of extract from 40 cigarette butts was prepared. Synthetic wastewater was added to sedimented activated sludge (3 g dry matter/L) from a wastewater treatment plant and the solution was aerated for 24 h. 5 Concentrations of extracts from cigarette butts in the mixture with the sludge solution was aerated for 180 min and the decrease in dissolved oxygen concentration was monitored.

Results/discussion

In all tests, the mortality of organisms was evaluated using the ToxRatPro Version 3.3.0 program and the values of lethal concentrations EC50 and ErC50 were obtained (Table I).

In the acute toxicity test on daphnia, it was noted that immobilized organisms (unlike individuals from low concentrations) had antennae stuck together by droplet deposits of a yellow precipitate, which was also contained in their digestive tract. At higher concentrations, this substance formed fibres that connected different individuals to each other. Precipitation of fibres mentioned could initiated by the movement of daphnia, because these fibres were not observed in the sample containing algae, although higher concentrations of the extract were used in it. The precipitate also prevented daphnia from moving and breathing. Chemical analysis was not performed, but it is probably one of the components of tar.

Table I
Results of ecotoxicological tests

Test No.	Time [h]	EC50 [1/L]	ErC50 [1/L]
202	24	0.81	
	48	0.39	
201	72	-	23.03
209	3	-	could not be determined

Conclusion

Based on the tests performed, cigarette butts cannot be included in the list of acutely ecotoxic substances according to current legislation.

Acknowledgements

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COMPARISON OF CATALYTIC PERFORMANCES OF PT/$TI_XCE_YO_N$ CATALYSTS AND TRANSITION METAL (TI, CU, FE) AND LANTHANIDE (CE) - BASED OXIDE CATALYSTS FOR DICHLOROMETHANE OXIDATION

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Abstract

The aim of this work is to compare the catalytic performance of two sets of granulated catalysts prepared by co-precipitation in dichloromethane oxidation. The first set of catalysts contains impregnated Pt on various TiO_2-CeO_2, the second set of catalysts is composed of a mixture of TiO_2, CeO_2, CuO and Fe_2O_3. The prepared catalysts were tested in dichloromethane oxidation using light-off tests in temperature range of 100-500°C in a flow reactor connected to online FTIR.

Introduction

Dichloromethane is classified as a Class 2A compounds, a probable human carcinogen. Dichloromethane (DCM) is one of many substances classified as a chlorinated volatile organic compound (CVOC) that definitively pose a risks to a human health and the environment[1,2]. Catalytic oxidation is one of the most technologically and economically acceptable technologies for the CVOCs reduction due to its simplicity and high efficiency. In recent years, efforts have been made to develop a highly active, selective and durable catalyst for CVOCs oxidation and to reduce the carbon footprint[3,4]. The catalysts may be formed from metals and transition metals[5], lanthanides[6] and noble metals[7] to maximize activity and selectivity. The methods of preparation of catalysts can be different, the most common preparation methods are coprecipitation[8], sol-gel technique[9], hydrothermal[10] preparation and impregnation[8]. The catalytic oxidation of dichloromethane includes the adsorption and disproportion of C-Cl and C-H bonds on acidic centers of the catalyst and subsequent oxidation of unwanted by-products (CH_2O and CO) to the deisred CO_2[11,12,15]. The acidity of the catalyst itself can be influenced by the use of an acidic precursor in the preparation of the catalyst[13], or alternatively by the final acid treatment of the prepared catalyst[14]. The reducibility of the catalyst can be influenced by the addition of a component which is well self-reducing and thus leads to the oxidation of by-products ($CH_2O \rightarrow CO \rightarrow CO_2$)[15]. For this reason, titanyl sulfate was used as an abundantly acidic precursor for TiO_2 and other added oxides due to its good reducibility.

Experimental part

Catalysts preparation

The prepared catalyst sets were prepared by co-precipitation method using titanyl sulphate as a precursor for TiO_2. As additional precursors for the other oxides present were: $Fe(NO_3)\cdot 9H_2O$, $Ce(NO_3)_3\cdot 6H_2O$ and $Cu(NO_3)_3\cdot 3H_2O$. The calcination conditions were the same for both prepared sets, namely 550 °C for 4 h. The calcination was followed by sieving to the desired grain size (0.315 - 0.160 mm). For the first prepared set, Pt was impregnated using as a precursor for platinum chloroplatinic acid. The impregnation was again followed by calcination and sieving to the desired grain size (Figure 1.). For catalytic testing 500 ppm of DCM, 1.5 vol.% of water, and 0.89 g of catalyst were used. The air flow rate was established at 1.05 dm^3/min. These conditions correspond to the space velocity (SV) of 71 $m^3/kg_{cat}\cdot h$.

Figure 1. Photos of fresh powder catalysts.

Catalysts testing

Catalytic testing of the prepared powder catalysts was carried out in a quartz tube reactor in the temperature range of 100 - 500 °C with a heating rate of 5 °C/min[9]. Output gas emissions were analysed using an online FTIR analyser calibrated for a wide range of hydrocarbons, chlorinated hydrocarbons and oxyderivatives. Before start of each catalytic test, the catalyst was first heated in a stream of air from 25 °C to 500 °C and then cooled to the reaction start temperature. Prepared powder catalysts were characterized by selected techniques (XRF, XRD, SEM-EDS, N_2 physisorption at 77K, H_2-TPR and NH_3-TPD) to determination their physico-chemical properties.

Results

Catalysts characterization

From the XRF results, in the first set of platinum impregnated catalysts, the amount of impregnated platinum is ~ 1 wt.%, which was required during preparation. Further, it is evident from the XRF results that both the prepared sets of catalysts exhibit the presence of sulphur in the form of SO_4^{2-} ranging from 8 to 17 wt. %. The first prepared set of catalysts indicates from the XRD results the presence of the crystalline phases $Ce_2(SO_4)_3$ and $Ce_2(SO_4)_3 \cdot 4\ H_2O$. For the second prepared set of catalysts, the presence of amorphous $CuSO_4$ is confirmed from XPS analysis in the $Ti_9Ce_1Cu_{0.3}S_zO_n$ catalyst. For the remaining two prepared catalysts, the presence of neither crystalline nor amorphous phase was confirmed, but the formation of $Fe_2(SO_4)_3$ is probably due to the overlap of the individual components that can be observed in the SEM-EDS images.

The textural parameters including specific surface area, volume and pore distribution (Table I) of all the prepared catalysts were evaluated based on adsorption-desorption isotherms from the N_2 physisorption method at 77 K. The first prepared set of platinum-impregnated catalysts exhibit a combination of type I and IV isotherms, which denote mesoporous-macroporous catalysts with pore sizes of ~ 5 - 50 nm for both fresh and spent catalysts. For the $Pt/Ti_3Ce_7S_zO_n$, $Pt/Ti_5Ce_5S_zO_n$ and $Pt/Ti_7Ce_3S_zO_n$ catalysts, crystallization occurs during catalytic testing and is manifested by an increase in specific surface area and pore volumes. The second set of catalysts prepared is based on adsorption-desorption isotherms of the IV isotherm, which denotes mesoporous catalysts with pore sizes of ~ 3-25 nm. For all the prepared catalysts in the second prepared set, crystallization also occurs during catalytic testing, thereby increasing the specific surface area and pore volume.

Table I
Textural properties for both prepared sets of catalysts.

Catalysts Fresh	S_{BET} ($m^2 \cdot g^{-1}$)
Pt/CeO_2	44
Pt/TiS_zO_n	42
$Pt/Ti_3Ce_7S_zO_n$	14
$Pt/Ti_5Ce_5S_zO_n$	14
$Pt/Ti_7Ce_3S_zO_n$	7
$Pt/Ti_9Ce_1S_zO_n$	4
$Ti_9Ce_1Cu_{0.3}S_zO_n$	24
$Ti_{8.2}Ce_{0.5}Fe_{1.3}S_zO_n$	38
$Ti_{8.2}Fe_{1.8}S_zO_n$	94

To determine the reducibility of both prepared catalyst sets, the catalysts were subjected to a temperature - programmed reduction by hydrogen (H_2-TPR) in the temperature range of 0-500 °C (Table II). The first prepared set of platinum impregnated catalysts exhibits the following order of reducibility $Pt/Ti_9Ce_1S_zO_n$ > $Pt/Ti_7Ce_3S_zO_n$ > $Pt/Ti_5Ce_5S_zO_n$ > $Pt/Ti_3Ce_7S_zO_n$ > Pt/TiS_zO_n > Pt/CeO_2. For the Pt/CeO_2 catalyst, the presence of one shoulder (100 °C) and two peaks (180 °C, 380 °C) is evident in the TPR profiles. The presence of a shoulder at 100 °C indicates the reducibility of platinum oxides (Pt_xO_y). The peak at 180 °C marks the reducibility of surface oxygen in CeO_2 and the peak at 380 °C marks the interaction between the metal and the support, causing increased lattice oxygen mobility in the CeO_2 crystal lattice. For the $Pt/Ti_5Ce_5S_zO_n$ catalyst, one peak with a maximum at 330 °C was recorded indicating the reduction of Ce^{4+} ions to Ce^{3+} ions. For the Pt/TiS_zO_n and $Pt/Ti_3Ce_7S_zO_n$ catalysts, peaks at 332 °C and 350 °C indicating reduction of Ti^{4+} ions are evident. The second prepared set of catalysts had reducibility in the following order: $Ti_{8.2}Fe_{1.8}S_zO_n$ > $Ti_{8.2}Ce_{0.5}Fe_{1.3}S_zO_n$ > $Ti_9Ce_1Cu_{0.3}S_zO_n$. Only two peaks were recorded in the temperature range 0-500 °C with maxima at 421 °C and 481 °C. In the $Ti_9Ce_1Cu_{0.3}S_zO_n$ catalyst, the reduction of Ce^{4+} ions to Ce^{3+} ions occurs at 421 °C. In the $Ti_{8.2}Fe_{1.8}S_zO_n$ catalyst, Fe^{3+} ions are reduced to Fe^{2+} ions at 481 °C. At temperatures above 500 °C, the reduction of surface Ce^{4+} ions to Ce^{3+} ions (501 °C) and the reduction of Ce^{2+} ions to Cu^0 (580 °C) occurs. Compared to the first set of catalysts prepared with impregnated platinum, the second set of catalysts prepared shows reducibility at higher temperatures due to suppression of oxide formation by the presence of sulphur.

A temperature-programmed desorption of ammonia (NH_3-TPD) was used to determine the acidity of the prepared catalyst sets (Table II). In the first prepared set of platinum impregnated catalysts the acidity was as follows: Pt/TiS_zO_n > $Pt/Ti_5Ce_5S_zO_n$ > Pt/CeO_2 > $Pt/Ti_3Ce_7S_zO_n$ ~ $Pt/Ti_7Ce_3S_zO_n$ > $Pt/Ti_9Ce_1S_zO_n$. For the second prepared set of catalysts, the acidity is as follows: $Ti_{8.2}Fe_{1.8}S_zO_n$ > $Ti_{8.2}Ce_{0.5}Fe_{1.3}S_zO_n$ > $Ti_9Ce_1Cu_{0.3}S_zO_n$. For both prepared sets of catalysts, there is the presence of weak (0 - 200 °C) and strong (400 - 500 °C) acidic centres that affect the oxidation of dichloromethane

Table II
Reducibility and acidity for both sets prepared catalysts by H_2-TPR and NH_3-TPD.

Catalysts	Reducibility* H_2-TPR ($mmol \cdot g^{-1}$)	Peak maximum H_2-TPR (°C)	Acidity* NH_3-TPD ($mmol \cdot g^{-1}$)	Peak maximum NH_3-TPD (°C)
Pt/CeO_2	0.7	100; 180; 380	0.2	61
Pt/TiS_zO_n	1.9	332	0.4	62; 464
$Pt/Ti_3Ce_7S_zO_n$	2.6	350	0.2	100
$Pt/Ti_5Ce_5S_zO_n$	2.3	330	0.2	105
$Pt/Ti_7Ce_3S_zO_n$	2.2	480	0.2	104
$Pt/Ti_9Ce_1S_zO_n$	3.7	< 500	0.1	62
$Ti_9Ce_1Cu_{0.3}S_zO_n$	2.1	421	0.6	66; 430
$Ti_{8.2}Ce_{0.5}Fe_{1.3}S_zO_n$	4.4	501	1.0	66; 423
$Ti_{8.2}Fe_{1.8}S_zO_n$	5.4	481	1.6	66; 416

* For temperature range 0-500 °C

Catalytic activity and selectivity

The catalytic activity and selectivity results for both prepared sets of catalysts are summarized in Figure 2 a and b, where T_{50}, T_{90} and the yields of main reaction products (HCl and CO_2) are presented. Achieved DCM conversion for both prepared catalyst sets moved in the range of 98-100 %, which correspond to complete oxidation of DCM within tested temperature range. For the first prepared set of catalysts, the best catalyst is Pt/TiS_zO_n, which shows the highest activity and has the second best selectivity to desired reaction products HCl and CO_2. The Pt/CeO_2 catalyst exhibits the lowest present concentration of unwanted by-products CH_2O and CO, but formation of unwanted chlorinated by-product chloroform ($CHCl_3$) was detected. The yield of HCl in the catalytic oxidation of DCM is in the range of 82-97 % for both prepared sets of catalysts, which is good up to excellent. The good activity and high HCl selectivity of TiO_2-based catalysts may be associated with increased acidity of the catalysts, which causes dichloromethane adsorption and subsequent disproportionation of C-Cl and C-H bonds on the acidic sites of the catalysts. The yield of CO_2 is in the range of 91-99 % for the first prepared set of platinum impregnated catalysts. The second prepared set of catalysts shows comparable activity to the first prepared set with impregnated platinum but shows worse CO_2 selectivity and formation of unwanted reaction by-products, which is due to the reducibility of the catalysts at higher temperatures compared to the first set of catalysts.

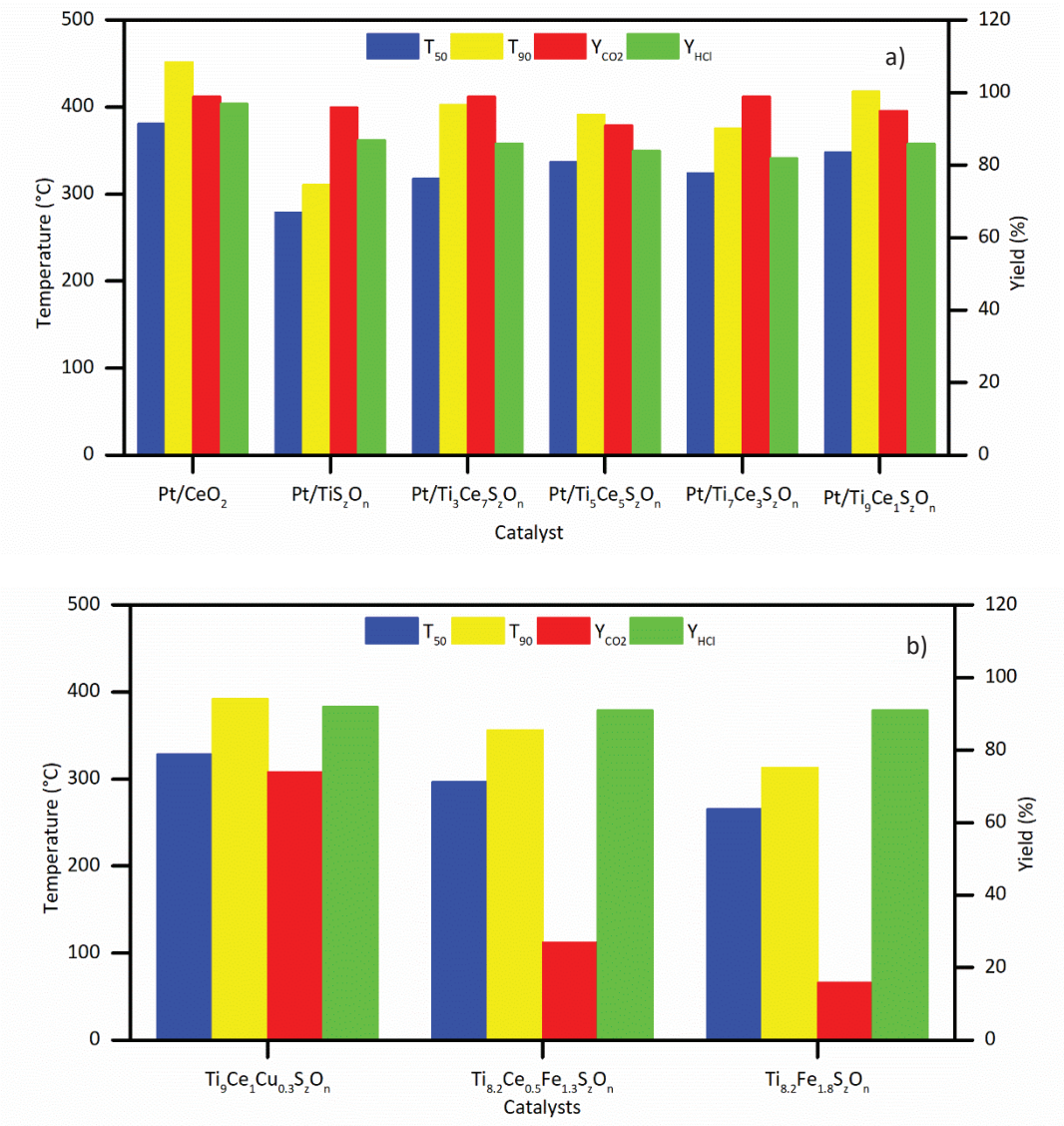

Figure 2. Catalytic efficiency of powder catalysts in DCM oxidation for both prepared set of catalysts; (a) platinum impregnated TiO_2-based catalysts, (b) mixed TiO_2, CeO_2, CuO and Fe_2O_3-based catalysts.

Conclusion

The prepared powder catalyst sets were tested in the catalytic oxidation of dichloromethane, as one of the widely used harmful solvents in the pharmaceutical industry and chemical synthesis. Titanyl sulphate was used as an acidic precursor in the additions, which was found to have a positive effect on the catalytic activity for both prepared sets, as it possessed the presence of weak and strong acidic centres in the catalyst, which affect the adsorption and disproportionation of C-Cl and C-H bonds. The 98-100% conversion of dichloromethane was reached over all tested catalysts at set experimental conditions. The CO_2 selectivity of the prepared catalyst sets varied due to different reducibility. It was better for Pt impregnated powder catalysts at lower temperatures (bellow 400 °C), which resulted in their enhanced CO_2 selectivity of 91-99% and the detected concentrations of unwanted by-products (such as CH_2O, CO) were lower compared to the second prepared set where the CO_2 yields ranged only from 16-74% and the concentrations of unwanted by-products were high. The HCl selectivity of all tested catalysts moved in the range of 82-97 %, which is generally very high.

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