Fractional Model of Danckwerts Tubular Catalytic Reactor

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Abstract

Modeling of anomalous diffusion in closed domain $\mathcal{D} \subset \mathbb{R}^d$ is a complex problem with many chemical, physical, and mathematical aspects. When the isotropic anomalous diffusion is unlimited, the fundamental solution of corresponding fractional PDE has to be radially symmetric. Previous condition motivates us to use only Riesz derivative as a model of fractional Laplacian and Feller derivative as a model of fractional gradient also in one-dimensional case of the anomalous tubular catalyst reactor. Danckwerts in 1950's supposed catalytic bed which is fixed inside the tube of chemical reactor. The fluid (gas or liquid) pass thorough the catalyst bed of fixed length with constant flow rate and therefore the advection occurs in front of, inside, and behind the catalyst bed. But there are two significant suppositions: both chemical reaction and the traditional diffusion occurs only inside the bed. The classical model is represented by parabolic PDE with well defined boundary conditions.

We suppose one-dimensional anomalous diffusion of single substance inside the catalyst bed with the first order chemical reaction and study various formulations of Fractional Advective Diffusion Equation (FADE). First, using Feller fractional gradient instead the traditional one and mass balance, we obtain fractional PDE with Riesz fractional Laplacian and fractional boundary conditions which is not useful for analytic or numeric solution. The second case is pure stochastic model of particle movement with spatially constrained anomalous diffusion part and unlimited particle translation via advection. The third model combines the exact solution of motionless anomalous diffusion with Neumann boundaries with spatial shift $h \to 0_+$. Resulting integro-differential equation enables to study the properties of fractional diffusive, advection, and reaction terms. The fourth model is based on the Finite Volume Method (FVM) and is suitable for direct numerical simulation including nonlinear chemical kinetics. The catalyst bed is decomposed into N identic segments to obtain resulting system of ODE using only the mass balance and Feller derivative as model of fractional gradient. First numerical results will be presented at the end of presentation.