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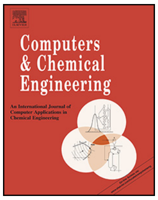

A comparative study of a direct discretization and an operator-splitting solver for population balance systems

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ABSTRACT

A direct discretization approach and an operator-splitting scheme are applied for the numerical simulation of a population balance system which models the synthesis of urea with a uni-variate population. The problem is formulated in axisymmetric form and the setup is chosen such that a steady state is reached. Both solvers are assessed with respect to the accuracy of the results, where experimental data are used for comparison, and the efficiency of the simulations. Depending on the goal of simulations, to track the evolution of the process accurately or to reach the steady state fast, recommendations for the choice of the solver are given.

1. Introduction

Population balance systems (PBSs) model particulate flows where not the behavior of the individual particles is of interest but the behavior of the particles in the mean. To this end, the particle population is described with a particle size distribution (PSD) and an equation for the PSD is derived whose terms model, e.g., transport, nucleation, growth, and aggregation of particles. Together with equations for the energy or mass balance and an equation which describes the flow field, the behavior of the particulate flow is modeled with a so-called PBS.

A major challenge for the numerical simulation of PBSs arises from the fact that the PSD does not only depend on time and space, like, e.g., the flow field and the temperature, but it depends also on properties of the particles, the so-called internal coordinates. After having applied a temporal discretization to the PBS, the equation for the PSD is given in a domain whose dimension is the sum of the spatial dimension and the number of internal coordinates.

One can find in the literature different proposals for dealing with the high dimensionality of the equation for the PSD. A direct discretization of the high-dimensional equation was studied, e.g., in Bordás et al. (2013), John et al. (2009), John and Roland (2010) and John and Suciu (2014). This approach is motivated by a potentially good accuracy of the computed solution, since no simplifications to the original problem were applied. However, the numerical solution of an equation in a higher-dimensional domain might be rather expensive. Motivated by performing more efficient simulations, other approaches were proposed. Moment-based methods, like the quadrature method of moments (QMOM) or the direct QMOM (DQMOM) (Marchisio and Fax, 2005; McGraw, 1997) replace the equation for the PSD by a system of equations for the first moments, with respect to the internal coordinates, of the PSD. These methods are quite popular in the engineering community. But the original PBS is modified quite strongly and the reconstruction of the PSD from the first moments is a severely ill-posed problem (John et al., 2007). Another approach motivated by efficiency, which does not change the original PBS, is the operator-splitting scheme proposed in Ganesan (2010). This scheme splits the computation of the solution into subproblems with respect to the spatial and to the internal coordinates (Ganesan, 2010; Ganesan and Tobiska, 2012). To the best of our knowledge, systematic numerical comparisons of these different schemes have not been performed in the literature so far.

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The goal of this paper consists in performing the first step in the systematic assessment of different solvers for PBSs. In this step, a direct discretization and an operator-splitting scheme are studied. This choice is motivated by our rich experience with these methods. By the way, it seems to be the first time that an operator-splitting method is applied for solving a PBS with aggregation.

For an assessment of numerical methods, one needs a problem where some reference values of the solution are known. To this end, a model of urea synthesis from Hackbusch et al. (2012), with a uni-variate population, will be used where some experimental data from Borchert and Sundmacher (2011) are available. This model will be considered in a comparable simple situation: the flow domain is a cylindrical pipe, the flow fields are stationary, the velocity field is given by a Hagen–Poiseuille profile, and the setup is such that the solution, in cylindrical coordinates, can be assumed to be independent of the angle. Since the velocity field is known, there is no need to solve the Navier–Stokes equations. Thus, the computing times of the different numerical methods for solving the equation for the PSD will constitute a large part of the overall computing times of the simulations. From the independence of the angle, it follows that the PBS can be written in axisymmetric form which reduces the spatial dimension from three to two.

The paper is organized as follows. Section 2 presents the population balance model of the urea synthesis. The solvers for the PBS are described in Section 3. Section 4 presents the numerical studies and an outlook will be given in Section 5.

2. The population balance model of the urea synthesis

This section presents the population balance system which models the urea synthesis. It is in principal the same model as considered in Hackbusch et al. (2012). Only, the flow domain has a different form, hence also the flow field, such that a 3D-axisymmetric form of this model can be used in the numerical simulations. It will be explained in Section 4 that the different flow field will also change the impact of growth and aggregation on the urea population compared with Hackbusch et al. (2012).

The model for the considered urea population consists of a system of equations describing the energy balance, the mass balance of the dissolved urea, and the behavior of the PSD.

For the flow field $\boldsymbol{u}$ [m/s] in the cylindrical domain $\Omega \subset \mathbb{R}^3$ a Hagen–Poiseuille profile is assumed. The boundary Γ of Ω is composed of the inlet Γ_{in}, the outlet Γ_{out}, and the wall Γ_{wall}.

Let $m_{\text{mol}} = 60.06 \times 10^{-3}$ [kg/mol] be the molar mass of urea, then the saturation concentration of the dissolved urea is given by

$$c_{\text{sat}}(T) = \frac{35.364 + 1.305(T - 273.15)}{m_{\text{mol}}} [\text{mol/m}^3], \tag{1}$$

where T is the temperature in the system. Further, the growth rate of the urea particles is modeled by

$$G(c, T) = \begin{cases} k_g \left(\dfrac{c - c_{\text{sat}}(T)}{c_{\text{sat}}(T)} \right)^g, & \text{if } c > c_{\text{sat}}(T), \\ 0, & \text{else}, \end{cases} \quad [\text{m/s}], \tag{2}$$

with the growth rate constant $k_g = 10^{-7}$ [m/s] and the growth rate power $g = 0.5$ [·]. Here, c[mol/m^3] is the molar concentration of the solute, and its evolution is described by

$$\frac{\partial c}{\partial t} - D\Delta c + \boldsymbol{u} \cdot \nabla c + \frac{H_\ell}{m_{\text{mol}}} = \frac{f_\ell}{m_{\text{mol}}} \quad \text{in } (0, t_e) \times \Omega, \tag{3}$$

where

$$H_\ell = 3\rho^d k_V G(c, T) \int_{\ell_{\min}}^{\ell_{\max}} \ell^2 f \; d\ell, \quad \text{and} \quad f_\ell = -\rho^d k_V \ell_{\min}^3 B_{\text{nuc}}.$$

In this equation, $D = 1.35 \times 10^{-9}$[m^2/s] is the diffusion coefficient of urea in ethanol, $\rho^d = 1323$ [kg/m^3] is the density of urea (dispersed phase), $k_V = \pi/6$ [·] is the scaling factor from diameters to volume (where it is assumed that all particles are of spherical shape) and t_e [s] is the final time for the simulations. The nucleation rate B_{nuc} is defined by

$$B_{\text{nuc}} = \begin{cases} \alpha_{\text{nuc}} \exp \left(\dfrac{-\beta_{\text{nuc}}}{\ln^2(c/c_{\text{sat}}(T))} \right), & \text{if } c > c_{\text{sat}}(T), \\ 0, & \text{else}, \end{cases}$$

where $\alpha_{\text{nuc}} = 1 \times 10^8$ is the nucleation constant and $\beta_{\text{nuc}} = 1.66667 \times 10^{-4}$ is a model constant. The PSD is denoted by f [1/m^4] and the diameter of the particles is ℓ [m], where $\ell_{\min}$ is the smallest diameter (nuclei size) and $\ell_{\max}$ is an upper bound for the largest diameter. The last term on the left-hand side of (3) describes the decrease of dissolved urea due to the growth of particles and the term on the right-hand side models the consumption of dissolved urea due to the nucleation of particles. Eq. (3) has to be equipped with initial and boundary conditions. The boundary condition is given by

$$\begin{cases} c(t, \boldsymbol{x}) = c_{\text{sat}}(T_{\text{in}}), \boldsymbol{x} \in \Gamma_{\text{in}}, \\ D \dfrac{\partial c}{\partial \boldsymbol{n}_\Gamma} = 0, \boldsymbol{x} \in \Gamma_{\text{out}} \cup \Gamma_{\text{wall}}, \end{cases} \tag{4}$$

where $\boldsymbol{n}_\Gamma$ is the outward pointing unit normal on Γ and T_{in} is the temperature at the inlet, see (6). In addition, an initial condition is needed for closing equation (3). Since such a condition is not known from the experiments, the inlet concentration value is used as the initial value, that is

$$c(0, \boldsymbol{x}) = c_{\text{sat}}(T_{\text{in}}) \quad \boldsymbol{x} \in \Omega.$$

The model for the energy balance is of the same type as the model of the mass balance

$$\rho c_p \left(\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T \right) - \lambda \Delta T + \delta h_{\text{cryst}} H_\ell = \delta h_{\text{cryst}} f_\ell \quad \text{in } (0, t_e) \times \Omega. \tag{5}$$

In this energy equation, $\rho = 789$ [kg/m^3] is the density of ethanol at 298 K, $c_p = 2441.3$ [J/(kg K)] is the specific heat capacity of ethanol, $\lambda = 0.167$ [J/(K m s)] is its thermal conductivity, and $\delta h_{\text{cryst}} = 2.1645 \times 10^5$[J/kg] is the heat of solution (enthalpy change of solution). The term on the right-hand side of (5) describes the decrease of temperature resulting from the nucleation of particles and the last term on the left-hand side the decrease of the temperature due to the consumption of energy by the growth of the particles. The known boundary conditions from the experiments are

$$\begin{cases} T(t, \boldsymbol{x}) = T_{\text{in}}, & \boldsymbol{x} \in \Gamma_{\text{in}}, \\ \lambda \dfrac{\partial T}{\partial \boldsymbol{n}_\Gamma} = 0, & \boldsymbol{x} \in \Gamma_{\text{out}}, \\ T(t, \boldsymbol{x}) = T_{\text{wall}}, & \boldsymbol{x} \in \Gamma_{\text{wall}}, \end{cases} \tag{6}$$

with $T_{\text{in}} = 301.15$ [K] and $T_{\text{wall}} = 291.15$ [K]. Hence, the suspension is cooled at the wall. The initial condition was used in the same way as for the mass balance, that is,

$$T(0, \boldsymbol{x}) = T_{\text{in}} \quad \boldsymbol{x} \in \Omega.$$

Finally, the model for the behavior of the PSD is presented. Since it is assumed that the particles are of spherical shape, they can