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Direct discretizations of bi-variate population balance systems with finite difference schemes of different order

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HIGHLIGHTS

- Direct discretizations are used to simulate a bi-variate population balance system.
- A hybrid finite difference – finite volume discretization is presented.
- A monotone first order upwind and an ENO method of order three are applied.
- Important outputs of interest are predicted very differently.
- The impact on numerical errors on the computational results is shown.

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ABSTRACT

The accurate and efficient simulation of bi-variate population balance systems is nowadays a great challenge since the domain spanned by the external and internal coordinates is five-dimensional. This report considers direct discretizations of this equation in tensor-product domains. In this situation, finite difference methods can be applied. The studied model includes the transport of dissolved potassium dihydrogen phosphate (KDP) and of energy (temperature) in a laminar flow field as well as the nucleation and growth of KDP particles. Two discretizations of the coupled model will be considered which differ only in the discretization of the population balance equation: a first order monotone upwind scheme and a third order essentially non-oscillatory (ENO) scheme. The Dirac term on the right-hand side of this equation is discretized with a finite volume method. The numerical results show that much different results are obtained even in the class of direct discretizations.

1. Introduction

Population balance modeling has gained a lot of attention in the last few years, since many particulate processes can be described with its help, e.g., crystallization, comminution, precipitation, polymerization, aerosol, and emulsion processes. In particular, population balance systems for crystallization processes model the interaction of the surrounding medium and particles, which are described by a particle size distribution (PSD). Moreover, this interaction leads to different phenomena, e.g., nucleation, growth, aggregation, breakage, and transport of particles (Hulburt and Katz, 1964; Gerstlauer, 1999). Physical quantities in those systems, like temperature and concentrations, depend on time and so-called external coordinates, i.e., the spatial or geometrical coordinates, whereas the PSD depends on time, external coordinates, and so-called internal coordinates, which describe additional properties of the individual particles, e.g., diameter, volume, or main axes in the case of anisotropic particles. Population balance systems take into account a flow field transporting the particles. This approach results in a system of partial differential equations where the Navier–Stokes equations for the fluid velocity and pressure are coupled to convection–diffusion equations for the concentration of the species and the temperature of the system and a transport equation for the PSD. The flow field, temperature field, and concentration field are defined in a three-dimensional domain while the PSD is defined in a higher-dimensional domain, spanned by the external and internal coordinates.

There are different goals of numerical simulations. One goal consists in gaining a deeper insight into physical processes (models) by such simulations. In this case, one should use accurate (high order) numerical methods. Of course, such methods are generally computational expensive. Another goal might be to utilize numerical simulations for a real time control of processes.

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In this situation, very efficient methods have to be applied. However, such methods are usually of low order, i.e., one has to expect only a low accuracy of the numerical results. Altogether, different goals of numerical simulations require the use of numerical methods with different properties and one should choose the method according to the goal. This report focuses on the accuracy of numerical methods. Main goals of this report consist, on the one hand, in increasing the sensitivity of the population balance community on the possible size of numerical errors and on the other hand, in motivating careful and systematic studies of the properties of numerical methods for solving multi-variate population balance systems in order to obtain guidelines on which method is appropriate for which goal.

To this end, the crystallization process of potassium dihydrogen phosphate (KDP) is considered as a bi-variate model, i.e., with two internal coordinates. These coordinates are the characteristic length scales of the crystals. Particle transport as well as temperature-dependent nucleation and growth are taken into account. The coupling is modeled as one-way coupling, which means that the flow field is used for the computation of concentration, temperature, and the PSD. The back coupling can be neglected in the used model because of a sufficiently small amount of particles, suspended in a dilute dispersion medium, and of the presence of sufficiently small temperature gradients.

The numerical solution of bi-variate population balance systems is computationally challenging since the equation for the PSD is given in a five-dimensional domain in each discrete time. In order to overcome the increase in dimension, techniques based on model simplification are widely employed. One approach consists in replacing the higher-dimensional equation for the PSD by a system of equations for the first moments of the PSD, which is a system in three dimensions (Hulburt and Katz, 1964). The most popular approaches in this direction are the quadrature method of moments (QMOM) (McGraw, 1997) and nowadays the direct quadrature method of moments (DQMOM) (Marchisio and Fox, 2005). The DQMOM has been used for the simulation of multi-variate population balance systems, e.g., in Buffo et al. (2013). However, it is well known that the reconstruction of a PSD from a finite number of its moments is a severely ill-posed problem (John et al., 2007; de Souza et al., 2010). Other approaches consider directly the equation for the PSD, for instance, numerical methods based on operator-splitting techniques or direct discretizations (the so-called discrete methods). The basic idea of operator-splitting techniques is to split the high-dimensional equation into two low-dimensional equations, one with respect to the external coordinates and one with respect to the internal coordinates, and solve them sequentially, e.g., see Ganesan and Tobiska (2012) for the use of such methods for the simulation of a crystallization process. However, this approach introduces splitting errors whose magnitude is known only in model situations (Ganesan, 2012). With the increase of computational power, direct discretizations of the population balance equation become an interesting option. In these methods, the external and internal coordinates are discretized together, thus additional errors from simplifying the equation are not introduced. In this report, it will be shown that this approach is nowadays possible. To our best knowledge, the presented simulations are the first ones with direct discretizations for bi-variate population balance systems. Altogether, we think that among the numerical approaches mentioned here, potentially the most accurate simulations can be performed by using direct discretizations. For this reason, two methods from the class of direct discretizations will be studied.

This report focuses on the accuracy of the considered two methods from the class of direct discretizations. In both methods, the flow field is simulated with a higher order finite element method, the convection-dominated equations for temperature and concentration with a linear flux-corrected transport (FCT) finite element method, and the transport equation for the PSD with methods based on finite difference schemes. Both studied methods differ only in the concrete finite difference approximation: a first order monotone upwind scheme and a third order essentially non-oscillatory (ENO) scheme. In the considered setup, the five-dimensional domain spanned by the external and internal coordinates can be decomposed by a tensor-product mesh, which enables the utilization of finite difference methods for the differential operator of the population balance equation, which describes the convection with respect to internal and external coordinates. However, the model for the nucleation used in this equation contains a Dirac distribution such that a finite difference approach cannot be applied for this term. In this report, a finite volume method will be used for the the nucleation term and it is explained in detail how the correct scaling has to be chosen to obtain finally a hybrid finite difference – finite volume discretization for the population balance equation.

The report is organized as follows. The studied process is described in Section 2. In Section 3, the system of equations modeling the bi-variate population balance system is introduced. A brief description of the numerical methods and the couplings

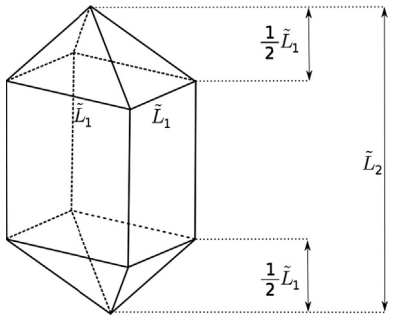

Fig. 1. Characteristic lengths of KDP crystals.

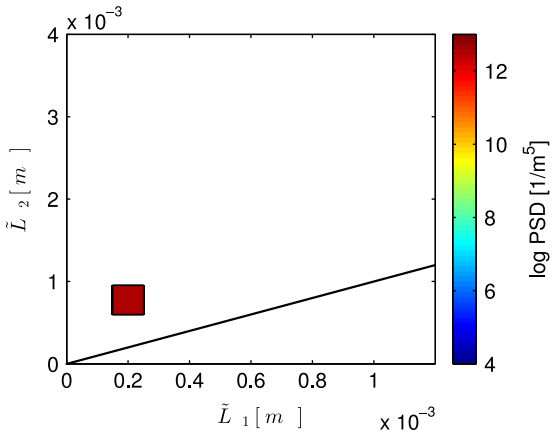

Fig. 2. Equally distributed seed PSD at the inlet of the channel for $\tilde{t} \in [0, \tilde{t}_{inj}]$ s.

Table 1
Degrees of freedom for simulating the population balance system.

Simulation quantity	Number of d.o.f.
Velocity	496 875
Pressure	76 032
Temperature	22 477
Concentration	22 477
PSD	45 515 925