Numerical methods for the simulation of dispersed phase systems

Stefan Motz
motz@isr.uni-stuttgart.de
University of Stuttgart, Germany

S. Motz, A. Mitrović and E.D. Gilles
Institute for System Dynamics and Control Technology
Pfaffenwaldring 9, University of Stuttgart, 70550 Germany

Dispersed phase systems occur in chemical engineering in a large variety. They play an important role in industrial production processes, such like e.g. crystallization, granulation, polymerization or liquid-liquid extraction. A common characteristic of all those systems is that the dispersed phase consisting of e.g. particles, bubbles or drops is embedded in a continuous medium. A commonly accepted concept for the modeling of dispersed phase systems is the population balance approach [1,2,3].

The mathematical modeling of dispersed phase systems leads in general to partial integro-differential equations. For their solution different numerical methods will be discussed. The recently published 'Method of Space-Time Conservation Element and Solution Element' [4], which was originally designed for solving the Navier-Stokes and Euler Equations, was extended for the treatment of partial integro-differential equations. This rather new method will be compared to state of the art 'Method of Lines' based schemes, e.g. Finite Volume, Robust Upwind [5,6]. This comparison will be performed using a simple test model as well as a complex population balance model accounting for a continuously operated crystallizer. From the application of the discussed methods guidelines for a proper selection of numerical methods for the simulation of dispersed phase systems will be derived.

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