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Stabilized Finite Element Methods for the Simulation of Bulk Precipitations

*** Volker John[1], Michael Roland[2] and Ellen Schmeyer[3]**

[1] Universität des Saarlandes,
6.1 – Mathematik
Postfach 15 11 50, 66041 Saarbrücken, Germany
john@math.uni-sb.de
www.math.uni-sb.de/ag/john/

[2] Universität des Saarlandes,
6.1 – Mathematik
Postfach 15 11 50, 66041 Saarbrücken, Germany
roland@math.uni-sb.de
www.math.uni-sb.de/ag/john/MICHAEL_HOME/Homepage/home

[3] Universität des Saarlandes,
6.1 – Mathematik
Postfach 15 11 50, 66041 Saarbrücken, Germany
schmeyer@math.uni-sb.de
www.math.uni-sb.dw/ag/john/ELLEN_HOME/home

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ABSTRACT

Bulk precipitations are of great importance in chemical engineering applications. We will consider the barium sulphate precipitation which is particularly well understood from the chemical engineering point of view. The species $BaCl_2$ and Na_2SO_4 are reacting in a time–dependent flow field

$$BaCl_2 + Na_2SO_4 \rightarrow BaSO_4 + 2NaCl$$

leading initially to dissolved barium sulphate. After the local concentration of the dissolved barium sulphate exceeds a certain threshold, the precipitation starts and barium sulphate particles are produced. Currently, our model includes the nucleation and the growth of particles. While growing, the particles consume dissolved barium sulphate which balances the production of dissolved barium sulphate from the ongoing chemical reaction.

The mathematical model of this process, see [3], is a coupled system of

- the Navier–Stokes equations for describing the flow field,
- nonlinear convection–diffusion–reaction equations for the chemical reaction which are dominated by convection and reaction,
- a transport equation for the particle size distribution.

The particle size distribution depends not only on time and space but also on the size of the particles. That means, its domain of definition is one dimension higher than for the other equations.

This talk will present numerical approaches for solving the coupled population balance system which are mainly based on finite element methods. Numerical studies will be shown for the case that the flow field and the chemical reaction are given in a two–dimensional domain and the equation for the particle size distribution in a three–dimensional domain.

The talk will focus on the numerical solution of the convection–dominated reaction equation and the transport equation in the bulk precipitation model. Stabilization techniques for convection–dominated equations suffer often either from smearing of the layers, which leads to inaccurate solutions, or from spurious oscillations at the layers, which may result in instable simulations. The construction of non–smearing and non–oscillating discretizations is an active field of research. The talk will discuss several approaches to obtain such methods (residual based SOLD schemes [1,2], flux–corrected transport methods [4] and local projection schemes [5]) and study their performance in the simulation of bulk precipitation processes.

REFERENCES

[1] V. John and P. Knobloch. "A comparison of spurious oscillations at layers diminishing (SOLD) methods for convection–diffusion equations: Part I – a review". *Comput. Methods Appl. Mech. Engrg.*, Vol. **196**, 2197 – 2215, 2007

[2] V. John and P. Knobloch. "A comparison of spurious oscillations at layers diminishing (sold) methods for convection–diffusion equations: Part II – Analysis for P_1 and Q_1 finite elements". Technical report MATH–knm–2007/4, Charles University Prague, Faculty of Mathematics and Physics, Department of Numerical Mathematics, 2007

[3] V. John, M. Roland, T. Mitkova, K. Sundmacher, L. Tobiska and A. Voigt. "Simulations of population balance systems with one internal coordinate using finite element methods". Technical report, Universität des Saarlandes, FR. 6.1 – Mathematik, 2007

[4] D. Kuzmin and M. Möller. *Algebraic flux correction I. Scalar conservation laws*, in: R. L. D. Kuzmin, S. Turek (eds.), Flux–Corrected Transport: Principles, Algorithms and Applications, Springer, 155 – 206, 2005

[5] G. Matthies, P. Skrzypacz and L. Tobiska. "A unified convergence analysis for local projection stabilisations applied to the Oseen problem". *M2AN*, Vol. **41**, 713–742, 2007.