Modeling Fast Reactions and Particle Flow

Applications of OpenFOAM in the Pharmaceutical Industry

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Abstract

To model complex multiphase systems involving a high hold-up, mass transfer and fast reactions is a major challenge. In the pharmaceutical industry, the current modeling efforts are driven by both regulatory aspects as well as the need of the industry to constantly improve their production technology to manufacture increasingly complex products. The flexible programming platform "OpenFOAM" is an excellent tool to meet the expectations of researchers to face these challenges and provide complex and still maintainable software applications.

The basis of our Euler-Lagrange (EL) Large Eddy Simulations (LES) is a solver that can handle dense particle swarms as well as solves for the filtered concentration field for reactive species. The effects of liquid displacement, particle-particle and particle-wall collisions, as well as the influence of sub-grid-scale turbulent motion on the particle flow are taken into account. By solving the transport equation for the filtered mixture fraction as well as its variance, the probability density function (PDF) of each species can be reconstructing assuming its shape. This methodology has found interest only recently [1], and has shown that there is a big need in developing LES as a tool to predict the outcome of reaction-networks. Within the last two years we have implemented and tested above features in OpenFOAM and can now provide a sophisticated solver that has been validated for dilute bubbly flow [2, 3] as well as fast chemical reactions [4].

In the presentation we will reflect on our previous work involving the flow in bubble columns (see Fig. 2). Here, we were able to predict the low-frequency motion of the bubbly plume as well as mixing in the liquid phase. Also, we will provide details on our latest development involving a sophisticated film model that has been implemented via a look-up table [4]. This enables the prediction of the outcome of fast reactions near the gas-liquid interface without their explicit resolution. Finally, we show our implementation of a PDF-based approach for predicting mixing in a micro-reactor for the production of nanoparticles. An outlook for the implementation of a population-balance-equation-based methodology in the solver, as well as general perspectives for the use of OpenFOAM in the pharmaceutical industry is provided.

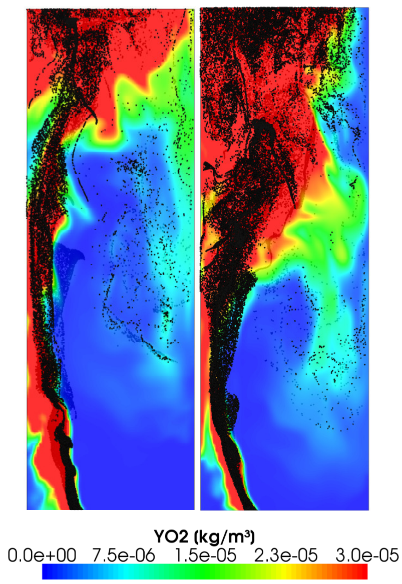

Fig. 1: Oxygen distribution in a gassed bioreactor [2].

Key words: large eddy simulation, reactive mixing, mass transfer, bubble columns, micro reactors

References

[1] D.L. Marchisio: *Large Eddy Simulation of Mixing and Reaction in a Confined Impinging Jets Reacto*r, Computers & Chemical Engineering 33, 2009.

[2] S. Radl, J.G. Khinast: *Multiphase Flow and Mixing in Dilute Bubble Swarms*, AIChE J (accepted for publication), 2010.

[3] S. Radl, R. Sungkorn, D. Suzzi, J. Derksen, J.G. Khinast: *High Performance Simulation of Bubbly Flows: Pushing the Limit by Using Conventional CFD and LBGK*, Multi-Scale Modelling Symposium, Melbourne (Australia), 2009.

[4] S. Radl, D. Suzzi, J.G. Khinast: *Fast Reactions in Bubbly Flows: Film Model and Micro-Mixing Effects*, submitted to Industrial & Engineering Chemistry Research, 2010.