MODELING AND SIMULATION OF DISPERSED TWO-PHASE FLOW TRANSPORT PHENOMENA IN ELECTROCHEMICAL PROCESSES

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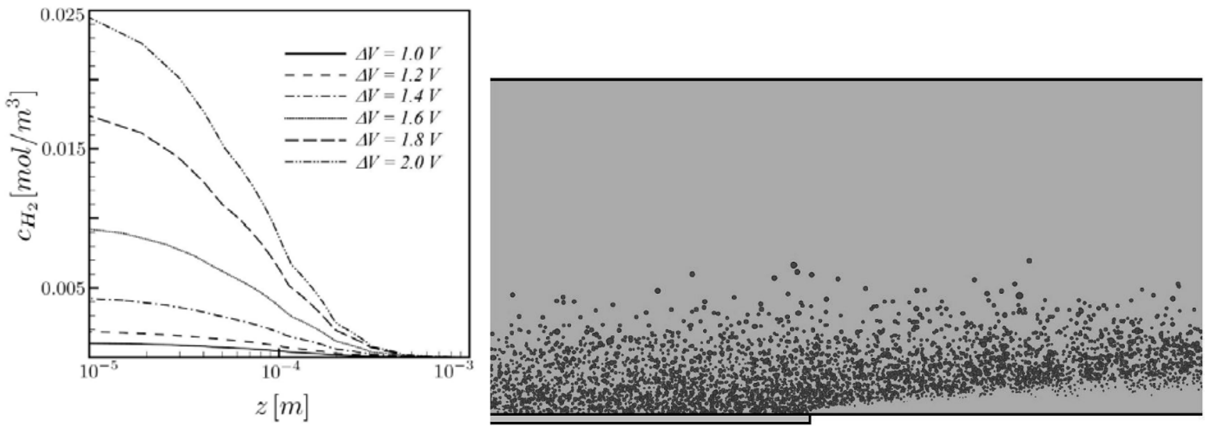
Numerical simulation of dispersed multiphase flows is a main challenge in modern CFD. Dispersed flows include particle-laden, droplet-laden and bubbly flows. We use an Eulerian-Lagrangian model for the numerical treatment of such type of flows. In this approach we treat the carrier fluid in a continuous manner, while the dispersed entities are tracked individually, approximated by mass-points and regarded as spherical in terms of computing their drag coefficient. The dispersed entities exchange momentum with the carrier phase, modeled by a two-way coupling approach. Since collisions play a significant role in particle and bubble dispersion, a stochastic four-way coupling approach to model these interactions has recently been implemented. In addition, energy coupling and droplet vaporization models have been implemented lately.

The parallel Lagrangian solver PLaS has been developed and implemented during the present Ph.D. work. Its purpose is to track a set of dispersed entities, which interact with the carrier phase computed by the flow solver. PLaS has been successfully coupled to the flow solvers Morpheus, SFELES and COOLFluiD. Several test cases have been set-up and computed for particle-laden, droplet-laden and bubbly flows.

A further challenge in nowadays CFD is the integration of combined simulation approaches, e.g. the combination of dispersed two-phase flow and electrochemical phenomena. An approach for the modeling of bubbly two-phase flow combined with ion transport, reaction kinetics and gas-producing electrodes has been carried out. In this approach, ion transport has been taken into account by the MITReM model, the electrode reaction kinetics has been modeled by the Butler-Volmer kinetics and a stochastic approach for bubble generation on electrode surfaces has been used.

Two-phase flow and electrochemical effects in a parallel flow channel reactor have been simulated. The obtained results show that for an increasing electrode potential difference, the supersaturation of the gaseous species increases and the amount of bubbles evolving from the gas-producing electrode rises. The novel simulation approach pointed out in the present Ph.D. work proved to work well. Promising initial results for a parallel channel flow reactor test case have been obtained and were compared to experimental results in the scope of the IWT-SBO project MuTEch. Figure 1 shows the molecular hydrogen concentration profiles normal to a gas-producing electrode in the parallel flow reactor and the according gas bubbles, which are transported away from the electrode by means of buoyancy and fluid flow motion.



(a) (b)

Figure 1: Simulation results for electrochemical bubble generation: (a) Molecular H2-concentration profiles normal to a gas-producing electrode, (b) Gas bubbles at an electrode potential difference of 1.0V