

Fast Simulation of 2-D Convection-Diffusion, Reacting Flows

H.-D. Minh

*Institute for Chemical Technology and Polymer Chemistry, University of Karlsruhe (TH),
hdminh@gmail.com*

2-D convection-diffusion, reacting flows in a single channel of catalytic monoliths are investigated. The fluid dynamics are modelled by a steady state, boundary-layer equations, which is a large system of parabolic partial differential equations (PDEs) with nonlinear boundary conditions arising from the coupling between the gas-phase and surface processes. The chemical processes are modelled using detailed chemistry. The PDEs are semi-discretized by a method of lines leading to a large-scale, structured differential algebraic equations (DAEs). The DAEs are solved using a tailored BDF code. We exploit the structure of the Jacobian and freeze the diffusion coefficients during approximation of Jacobian by the finite difference. By applying our approach, the computation times have been reduced by a factor of ten and more depending on the particular problem. The larger the problem is, the bigger the speed up is.