

Fast Numerical Methods for Simulation of Chemically Reacting Flows in Catalytic Monoliths

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Abstract: Chemically reacting flows in catalytic monoliths are investigated. The fluid dynamics are modelled by the boundary layer equations (BLEs), which are a large system of parabolic partial differential equations (PDEs) with highly nonlinear boundary conditions arising from the coupling of surface processes with the flow field inside the channel. The BLEs are obtained by simplifying the comprehensive model described by the Navier-Stokes equations and applying the boundary approximation theory. The surface and gas-phase chemical reactions are described by detailed models.

The PDEs are semi-discretized using the method of lines leading to a structured system of differential-algebraic equations (DAEs). The DAEs are solved by an implicit method, based on the backward differentiation formulas (BDF). Solution of DAEs by BDF methods requires the partial derivatives of the DAE model functions with respect to the state variables. By exploiting the structure of the DAEs, we develop efficient methods for computation of the partial derivatives in the framework of automatic differentiation and of finite differences. Applying these methods, we obtain a significant improvement in computing time. Moreover, the results also show that for solution of our DAE systems computation of the derivatives by automatic differentiation always outperforms computation of derivatives by finite differences. Numerical results for a practical application of catalytic oxidation of methane with a complex reaction mechanism are presented.

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