Nowak, U.; **Grah, A.**; **Schreier, M.**

Parameter estimation and accuracy matching strategies for 2-D reactor models. (English)

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The paper deals with a description of a numerical scheme applied to the solution of the PDE used in mathematical modeling of chemical reactions. The authors consider a 2-d time-dependent model in a cylindrical reactor module. The governing eqs. result from the balance equations for mass and energy, but the development is not described. The model also includes some uncertain parameters, which are determined in the numerical procedure combined with measurements. After spatial discretization a very large system of differential-algebraic equations is integrated by a one-step method using the linearly implicit extrapolation code LIMEX. The parameter identification procedure requires supplementing the governing equations with the sensitivity analysis equations. Then, the parameters can be obtained minimizing the nonlinear least-squares functional created from the simulation solutions and their measurement counterparts. For this purpose, the damped Gauss-Newton algorithm is employed. To increase the computational efficiency, the master/slave mode is used to control the Gauss-Newton iterations. Finally, some numerical experiments are presented.

Reviewer: Vladimir Sládek (Bratislava)

MSC:

80A32	Chemically reacting flows
65N40	Method of lines for boundary value problems involving PDEs
65L06	Multistep, Runge-Kutta and extrapolation methods for ordinary differential equations
65H10	Numerical computation of solutions to systems of equations
92E20	Classical flows, reactions, etc. in chemistry

Keywords:

chemical reactions; parameter estimation; sensitivity analysis; least-squares method; Gauss-Newton algorithm

Software:

NewtonLib; pchip; Schittkowski

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