Mathematics in the XXI Century
Novosibirsk, June 25–28, 2003
(Abstracts of Talks)

A Parallel Implementation of 3-D Unsteady Reaction-Diffusion Model

L. P. Kamenshchikov and V. I. Bykov

The processes of sorptions, diffusions and chemical reactions on a surface of a solid-state catalyst may be written as:

$$(1)\quad \frac{\partial Y_i}{\partial t} = D\left[Z\left(\frac{\partial^2 Y_i}{\partial x^2} + \frac{\partial^2 Y_i}{\partial y^2}\right) - Y_i\left(\frac{\partial^2 Z}{\partial x^2} + \frac{\partial^2 Z}{\partial y^2}\right)\right] + f_i(Y_1, \ldots, Y_N), \quad i = 1, \ldots, N,$$

where $Y_i(t, x, y)$ is the concentration of i-th substance on the catalyst surface, D is the surface diffusion coefficient, f_i is the nonlinear function presenting kinetics of the process, N is the number of substances, $Z = 1 - \sum_i Y_i$.

Generally, it is necessary to take into account a diffusion of reagents not only on the surface but also in the bulk of the catalyst. The example with the bulk diffusion only for one substance (marked as i_0) is considered in the given report:

$$(2)\qquad \frac{\partial Y_{i_0}}{\partial t} = D_v\left(\frac{\partial^2 Y_{i_0}}{\partial x^2} + \frac{\partial^2 Y_{i_0}}{\partial y^2} + \frac{\partial^2 Y_{i_0}}{\partial z^2}\right),$$

where $Y_{i_0}(t, x, y, z)$ is the concentration i_0-th substances in the bulk, D_v is the bulk diffusion coefficient, x, y, z are the Cartesian coordinates, t is time. All mentioned values are dimesionless. The equation (2) are solved in an unit cube, such that the equations (1) are valid on an upper face of the cube. Dirichlet condition is set for the equation (2) on the upper bound of the cube, and zero Neumann conditions are set on the rest faces.

The problem of a loss stability of a stationary state and occurrence in the system of self-oscillations is researched. Conditions of bifurcations of homogeneous stationary solutions of (1) are obtained. Influence of exchange process of the catalyst surface with the bulk is analyzed. Conditions at which oscillations on a surface induce time-dependent mass transfer in the bulk of the catalyst are defined. The numerical solutions indicating presence of self-oscillations as on the surface and in the bulk of the catalyst are resulted. As physics-chemical model the mechanism of adsorption of hydrogen on the metal catalyst and bulk diffusion of hydrogen from the surface was considered.

The equations (1)–(2) were solved numerically by the method of lines on the clusters MBC-1000/16 and MBC-1000/M which allow to apply the large computational grids. The parallelization of calculations consists in splitting the cube by some horizontal planes; calculations in each layer were fulfilled on the individual

©2003 L. P. Kamenshchikov and V. I. Bykov

processor. Before execution of the next time step each processor receives a number of 2-D arrays with necessary values of function Y_{i_0} from the adjacent processors. The code was written in Fortran-DVM language (developed in the Keldysh Institute of Applied Mathematics, Russian Academy of Science) which allows to automize the process of parallelization to a certain extent. Fortran-DVM gives programmers the ability to write a code at a high level. And though (1)–(2) may be quite solved on a serial computer, the offered technique for parallelization can be used for more complex systems when, for example, there are a lot of equations of type (2) and/or with the more complex right part.

Institute of Computational Modelling SB RAS, Krasnoyarsk, 660036, Russia