NOTE

SIMULATION OF NONLINEAR REACTION-DIFFUSION EQUATIONS

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Discrete particle simulation techniques developed for problems in plasma physics have been adapted to investigate one-dimensional dissipative structures. The results of the model are found to be consistent with bifurcation analysis of nonlinear reaction-diffusion equations. Two distinct types of behavior are observed corresponding to a localized steady-state solution and a time-dependent solution.

Introduction. In recent years there has been considerable interest in the phenomena which occur in open systems operating far from thermodynamic equilibrium. (Prigogine and Nicolis, 1971; Herschkowitz-Kaufman and Nicolis, 1972; Auchmuty and Nicolis, 1974; Herschkowitz-Kaufman, 1975). Such open systems which spontaneously evolve into spatially organized states are called dissipative structures (Prigogine, 1969). The discrete particle model presented here studies the effects of diffusion, initial and boundary conditions on the self-structuring processes. The results are compared with the computer simulation of bifurcation analysis presented by Herschkowitz-Kaufman (1975).

Method. The method of discrete particle simulation used by Ard, Hogan, and Stetson (1971), and as extended by Hogan and Stetson (1975), for solving

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coupled non-linear equations in plasma physics has been applied to this problem. The basic set of equations for this model is:

\[
\begin{align*}
A &\rightarrow X \\
B + X &\rightarrow Y + D \\
2X + Y &\rightarrow 3X \\
X &\rightarrow E
\end{align*}
\]

where the initial and final product concentrations \(B\), \(D\), and \(E\) are held independent of time and space throughout the system. The inverse reaction rates are neglected and the system is operating an infinite distance from thermodynamic equilibrium.

The time dependences of \(X\) and \(Y\) are

\[
\begin{align*}
\frac{dX}{dt} &= A(r) - (B + k)X + X^2 Y + DX_{rr}, \\
\frac{dY}{dt} &= BX - X^2 Y + DY_{rr},
\end{align*}
\]

where \(X_t = \frac{\partial X}{\partial t}, Y_t = \frac{\partial Y}{\partial t}, X_{rr} = \frac{\partial^2 X}{\partial r^2}, Y_{rr} = \frac{\partial^2 Y}{\partial r^2}, k\) is the forward kinetic rate coefficient, \(D_x\) and \(D_y\) are diffusion coefficients.

All other rate coefficients are set equal to unity and, for simplicity, diffusion is assumed to take place along the single spatial dimension \(r\). \(B\) is assumed to remain uniform in space and time. \(A\) is distributed non-uniformly and is completely determined by the closed equation

\[
\frac{dA}{dr} = -A(r) + DA_{rr}(r),
\]

where \(A\) is a given function of \(r\) only and \(DA\) is a diffusion coefficient.

Equations (5-7) are subject to the following boundary conditions where \(0 \leq r \leq 1\):

\[
\begin{align*}
A(0) &= A(1) = \bar{A}, \\
X(0) &= X(1) = \bar{X}, \\
Y(0) &= Y(1) = \bar{Y}.
\end{align*}
\]

There are only three independent variables \(A\), \(B\), and \(k\) so that for the steady non-uniform state

\[
\begin{align*}
X_0 &= A/k, \\
Y_0 &= kB/A.
\end{align*}
\]

Following the work of Herschkowitz–Kaufman and Nicolis (1972) we have set \(\bar{A} = 14\) and \(D_A = 1.97 \times 10^{-1}, D_x = 1.05 \times 10^{-3}, D_y = 5.25 \times 10^{-3}\). For the above conditions the steady-state solution for \(A\) is

\[
A(r) = c \cosh \left[D_A^{-1}(r - 1/2)\right],
\]

where \(c\) is a constant and \(0 \leq r \leq 1\).