On some mathematical models arising in chemical kinetics

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When constructing mathematical models for some chemical reaction processes, systems of ordinary differential equations (called reaction-systems) or systems of partial differential equations (called reaction-diffusion systems) are arisen. The aim of this research paper is establishing mathematical models and investigating their numerical solutions, corresponding chemical reaction processes like:

$$A \xrightarrow{k_1} B$$

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$$

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} AB \equiv C$$

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} AB \equiv D \qquad 2A + C \underset{k_4}{\overset{k_3}{\rightleftharpoons}} A_2C \equiv E.$$

Here A, B, C, D and E denotes chemical components and $k_1, \ldots, k_4$ denote reaction rates.

A brief introduction on how to construct mathematical models for chemical reaction processes and chemical reaction-diffusion processes is given. Finite difference schemes, C-programming language and the mathematical package MATHEMATICA are used to find numerical solutions for the mathematical models corresponding to above reactions. Also in numerical simulations of these models, no-flux boundary conditions and some hypothetical initial data are used. Two dimensional spatial dispersion behaviors and time evolution of the relevant chemicals in above reactions are observed by numerical simulation of the corresponding mathematical models.

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