MODELING OF CHEMICAL REACTIONS USING FREE MATHEMATICAL PACKAGE SCILAB

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The study and modeling of chemical reactions is actual problem for modern chemistry. They allow to accelerate and optimize the procedure of creating of new preparations and prevent transformations of medicine compounds that lead to lose of consume or commercial characteristics. The investigation of the processes and application of the obtained results in medicine and agriculture allow to deal with the diseases and prevent the growing old of organism.

For analysis of obtained results one need the mathematical techniques and tools. Here the mathematical packages which are able to solve the systems of differential equations can be brought to the fore.

Modeling of chemical reactions is considered in this work. The problem of modeling is reduced to the system of differential equations relatively concentration of the reagents and reaction products. Different types of reactions are considered here: simple isothermal reversible reaction, complex parallel and consecutive isothermal reactions, isothermal reversible reactions of the second kind and non-isothermal reaction.

To solve the differential equations we use freeware mathematical package Scilab. The dependences of the substance concentration and its temperature (in the case of non-isothermal reaction) vs. time for every reaction are plotted.

Modeling of chemical reactions is conducted, solution of systems of differential equations to which these reactions are reduced is performed, the numerical results are presented and their comparison with results obtained in the commercial package Mathcad is made in this report. We can make a conclusion that the freeware package Scilab abilities to solve of systems of differential equations are not inferior to commercial package therefore it can be successfully used for modeling of chemical processes. The package also includes a great number of tools for editing of the displayed plots and it has considerable advantage, namely, it is freeware.