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Simulation of Kinetics of Chemical Reactions.

by

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The relationship between velocity of the chemical reactions with activities or concentrations of their reactants, temperature and pressure is established through application of the experimental data into the integral or the differential rate models conjugated with the isolation method. Since the traditional way of doing these calculations is often time - consuming and tedious, a computer software called CRS has been developed to assist investigators. The less expert and the infrequent users would benefit from the software too.

A menu-style data entry and readily accessible database make the program easy to learn and to utilize. The present version allows the input of up to 24 concentration - time points on each curve, the fixing of the set limits for each calculation, the pre-specification of the acceptable error plus the output of the kinetic information in both tabular and graphical forms. The first version called 1.00 was written in Quick Basic but because of considerable need to the database, it has been rewritten in Clipper. The present version called 2.01 can be used to simulate various problems of metallurgical interest with enhanced levels of accuracy and speed.

The procedure is to calculate the rate constant k for all values of the reaction order n being iterationally raised within the limits specified by the user. The integrated rate equation is used for calculation of the order with respect to each isolated reactant at each stage. If the fit does not prove satisfactory, the procedure can be repeated with another equation. The mathematical algorithm used is based on obtaining the minimum in standard deviations of k. A window is eventually opened to demonstrate the best fit of the data for the least standard deviation.

The differential method is used for determination of both apparent and true orders, n_t and n_c, along with the appropriate rate constants of the reaction. The method of Regression Analysis is used to find the best fitted line with the most appropriate slope and intercept. The work is underway to add a chemical mechanism data base for comparison of the predicted and the experimental rate equations and/or curves. The present version is able to calculate the frequency factor and the activation energy of the reaction.

Availability -
Information about CRS may be obtained by writing to Dr. K. Sadrnezhaad, Department of Metallurgical Engineering, Sharif University of Technology, P.O. Box 11365-9466, Tehran, Iran. Phone: 3011-9821-918620. Fax: 3011-9821-662254.