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A COMPUTER PROGRAM FOR THE EVALUATION OF NON-ISOTHERMAL KINETIC PARAMETERS

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Abstract

A program for the evaluation of non-isothermal kinetic parameters is presented. The program allows evaluation of the kinetic parameters under constant heating rate or constant reaction rate conditions. The simulation of temperature *vs.* conversion curves is also possible. A regression method is included, which allows a discrimination between various conversion functions and also evaluation of the activation paramaters.

The program was tested with various simulated decomposition curves and the non-isothermal decomposition curves of calcium oxalate. The program is written in Visual BASIC 4.0 and can be run under Windows 95 ©.

Keywords: computer program, non-isothermal kinetics

Introduction

The recent development of non-isothermal kinetics requires the elaboration of computer programs for evaluation of the kinetic parameters [1–3].

We earlier developed the computer programs Versatile for the evaluation of non-isothermal kinetic parameters. The programs allow the computation of non-isothermal kinetic parameters by means of several integral and differential procedures.

The present work reports an improved variant of the program. Besides the thermogravimetric procedures to evaluate non-isothermal kinetic parameters, the new variant includes a DTA method [4], a CRTA method [5] and also a procedure to discriminate between various forms of the differential conversion function [6].

This program can simulate non-isothermal kinetic decomposition curves and draw graphical representations of simulated, calculated and experimental curves.

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The program

The use of this program leads to a number of advantages:

– the integral and differential methods can be applied to the same experimental data points (if necessary, the data are integrated or differentiated),

– a discrimination between various conversion functions is possible,

– constant decomposition rate data can be analysed,

– a simulation of temperatures *vs.* conversion curves is possible for both constant heating rate and constant decomposition rate procedures.

This program utilizes a Windows environment with sensitive on-line help capabilities (there are other functions, such as editing the data file by importing ASCII files, writing in data at the keyboard or reading the data from a picture).

Table 1 Values of non-isothermal kinetic parameters calculated by four methods (the data were simulated with the parameters n=1.0, A=10^{12} s^{-1} and E=120 kJ mol^{-1} for a heating rate of 5 K min^{-1})

	CR	*FW*	*A*	*US*
E/kJ mol^{-1}	119.8±0.2	120.4±0.1	120.0±0.03	116.5±0.05
$10^{-12}A/s^{-1}$	0.89±0.10	1.12±0.04	1.02±0.03	0.35±0.04
n	1.0	1.0	1.0	0.9
r	0.999999	0.999998	0.999999	0.99992

CR, *FW*, *A* and *US* stand for Coats-Redfern [7], Flynn-Wall [8], Achar [9] and Urbanovici-Segal [10]

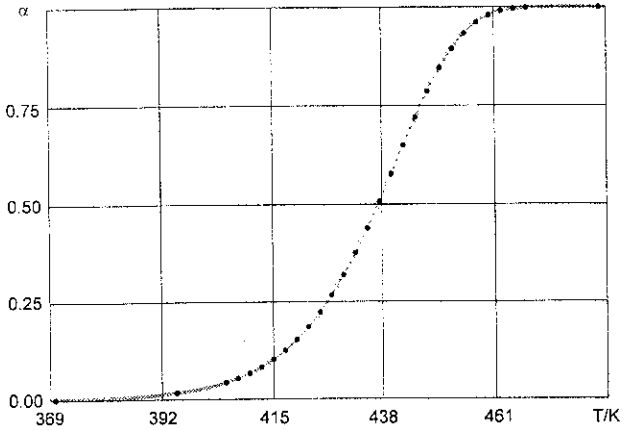

Fig. 1 (α, T) curves for data simulated with the parameters A=10^{12} s^{-1}, E=120 kJ mol^{-1} and heating rate=5 K min^{-1} (circles) and for parameters obtained by the Coats-Redfern method (crosses)

Program testing

In order to check this program, kinetic parameters were evaluated for simulated data curves with either constant heating rate or constant decomposition rate, and also for the dehydration of calcium oxalate.

Table 1 lists the results obtained by using the integral and differential methods for a simulated curve. The parameters taken in the simulation were $A=10^{12}$ s^{-1}, $E=120$ kJ mol^{-1} and heating rate=5 K min^{-1}. It may be seen that the parameters obtained are in good agreement with the simulated ones. The temperature *vs.* conversion curves obtained by means of the same program for these parameters are plotted in Fig. 1.

The possibility of direct graphical evaluation of the kinetic parameters by manual variation of the parameters is also included in this program, both for constant heating rates and for constant decomposition rates.

Conclusions

A computer program for the evaluation of non-isothermal kinetic parameters is presented. This program allows

– a discrimination between various conversion functions,
– an evaluation of constant reaction rate data,
– simulation of temperature *vs.* conversion curves for constant heating rate as well as constant decomposition rate data.

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