

Letter to the editor

*Kinetics analysis project*

A Kinetics Workshop was held during the 11th International Congress on Thermal Analysis and Calorimetry (ICTAC) in Philadelphia, USA, in August 1996. One of the suggestions which arose was that sets of kinetic data should be prepared and distributed to volunteer participants for their analysis using any, or several, methods as desired. These sets are now available and will be distributed to those who volunteered (and provided usable addresses) at the Workshop. Anyone else wishing to participate should contact:

Prof. Michael Brown, Chemistry Dept., Rhodes University, Grahamstown, 6140 South Africa. Fax: +461-25109; E-mail: chmb@wartho-g.ru.ac.za

Any comments, suggestions, or queries concerning the project should be directed to Prof. Brown, or to:

Dr. Marek Maciejewski, Laboratorium für Technische Chemie, ETH-Zentrum, Universitätsstrasse 6, CH-8092 Zürich, Switzerland. Fax: +41-1-632-1163; E-mail: maciejewski@tech.chem.ethz.ch

or else

Dr. Sergey Vyazovkin, Department of Chemistry, University of Utah, Salt Lake City, UT 84112, USA; fax: +1-801-585-3207; E-mail: Svyazov@atlas.chem.utah.edu

*The data sets*

*SET 1*

Fig. 1 illustrates six experimental alpha-temperature curves for the decomposition of calcium (CC) *in vacuum*, obtained at different heating rates (1.8, 2.5, 3.5, 5.0, 6.2 and 10 K min<sup>-1</sup> as shown) by Dr. Maciejewski.

File: *CCVKPM.TXT*

*SET 2*

Fig. 2 illustrates six experimental alpha-temperature curves for the decomposition of calcium carbonate (CC) *in nitrogen*, obtained at different heating rates (1.0, 3.0, 5.0, 7.5, 10, 15 and 25 K min<sup>-1</sup> as shown) by Dr. Maciejewski.

File: *CCNKPM.TXT*

*SET 3*

Fig. 3 illustrates six experimental alpha-time curves for the decomposition of calcium carbonate (CC) *in vacuum*, obtained at different temperatures (550, 540, 535, 530, 520 and 515°C as shown) by Dr. Maciejewski.

File: *CCVISO.TXT*

*SET 4*

Fig. 4 illustrates seven experimental alpha-time curves for the decomposition of calcium carbonate (CC) *in nitrogen*, obtained at different temperatures (773, 750, 740, 732, 719, 710 and 700°C as shown) by Dr. Maciejewski.

File: *CCNISO.TXT*

*SET 5*

Fig. 5 illustrates six experimental alpha-temperature curves for the decomposition of ammonium perchlorate (AP) *in nitrogen*, obtained at different heating

rates ( $a=2.52$ ,  $b=5.16$ ,  $c=7.58$ ,  $d=10.49$ ,  $e=12.79$  and  $f=15.45 \text{ K min}^{-1}$ ) by Dr. Vyazovkin.

File: *APKPM.TXT*

### STEP 6

Fig. 6 illustrates five isothermal alpha–time curves for the decomposition of ammonium perchlorate (AP) in flowing nitrogen, obtained at different temperatures ( $a=558$ ,  $b=553$ ,  $c=548$ ,  $d=543$  and  $e=548 \text{ K}$ ) by Dr. Vyazovkin.

File: *APISO.TXT*

### SET 7

Fig. 7 illustrates five simulated alpha–temperature curves calculated at heating rates of 0.5, 1.0, 2.0, 4.0 and  $8.0 \text{ K min}^{-1}$  by Dr. Vyazovkin.

File: *SIMKPM.TXT*

### SET 8

Fig. 8 illustrates five simulated isothermal alpha–time curves calculated at temperatures of  $a=380$ ,  $b=375$ ,  $c=370$ ,  $d=365$  and  $e=360 \text{ K}$  by Dr. Vyazovkin.

File: *SIMISO.TXT*

These data sets (about 100 points each) are available on diskette (MS-DOS) from Michael Brown (address above) in ASCII text format. Other formats can be provided on request.

### Kinetic analyses

Please send a brief summary of the Methods and Results of your kinetic analyses of calcium carbonate, ammonium perchlorate, or simulated data (you may choose to try one or more?) including any rate equation(s) identified as applicable, and estimates (with uncertainties) of the Arrhenius parameters, to Michael Brown, *WITHIN SIX MONTHS OF THE DATE OF*

*APPEARANCE OF THIS NOTE.* The contributions will be combined and compared and a report on the Project, acknowledging all participants (with their permission of course!) will be submitted to *Thermochimica Acta* for publication.

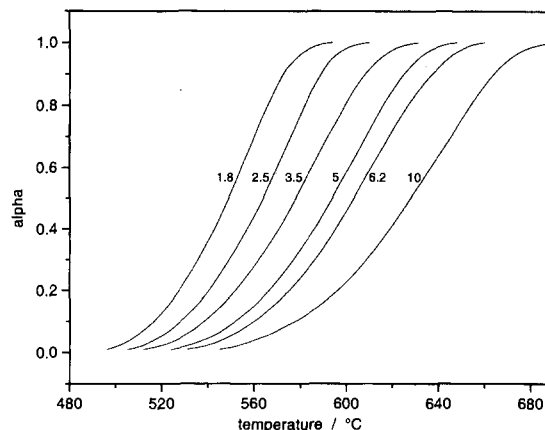


Fig. 1. Experimental alpha–temperature curves for the decomposition of calcium carbonate (CC) *in vacuum*, obtained at different heating rates (1.8, 2.5, 3.5, 5.0, 6.2 and  $10 \text{ K min}^{-1}$  as shown).

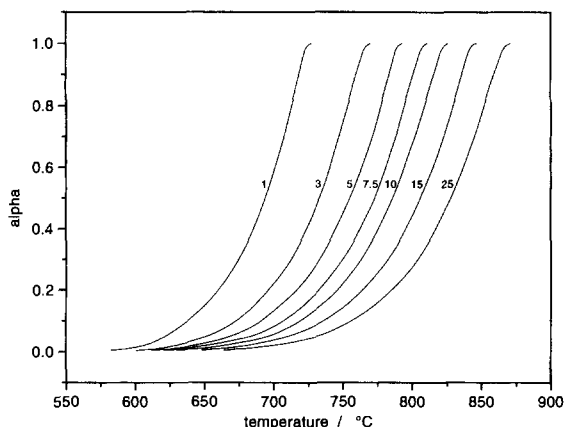


Fig. 2. Experimental alpha–temperature curves for the decomposition of calcium carbonate (CC) *in nitrogen*, obtained at different heating rates (1.0, 3.0, 5.0, 7.5, 10, 15 and  $25 \text{ K min}^{-1}$  as shown).

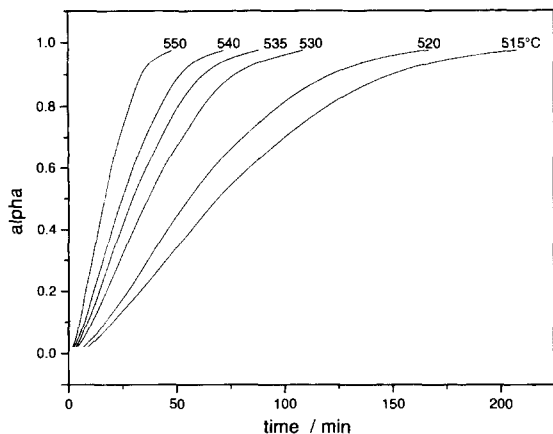


Fig. 3. Experimental alpha–time curves for the decomposition of calcium carbonate (CC) *in vacuum*, obtained at different temperatures (550, 540, 535, 530, 520 and 515°C as shown).

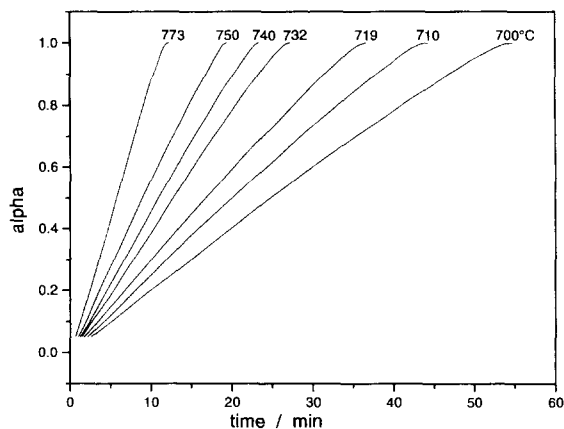


Fig. 4. Experimental alpha–time curves for the decomposition of calcium carbonate (CC) *in nitrogen*, obtained at different temperatures (773, 750, 740, 732, 719, 710 and 700°C as shown).

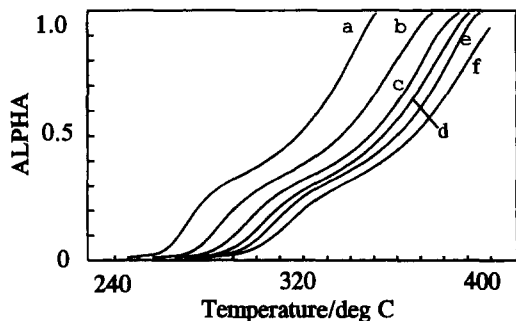


Fig. 5. Experimental alpha–temperature curves for the decomposition of ammonium perchlorate (AP) *in nitrogen*, obtained at different heating rates ( $a=2.52$ ,  $b=5.16$ ,  $c=7.58$ ,  $d=10.49$ ,  $e=12.79$  and  $f=15.45$  K min<sup>-1</sup>).

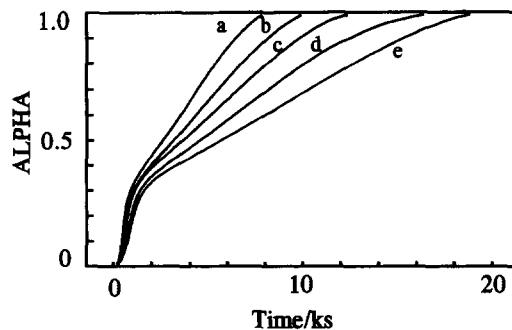


Fig. 6. Isothermal alpha–time curves for the decomposition of ammonium perchlorate (AP) in flowing nitrogen, obtained at different temperatures ( $a=558$ ,  $b=553$ ,  $c=548$ ,  $d=543$  and  $e=548$  K).

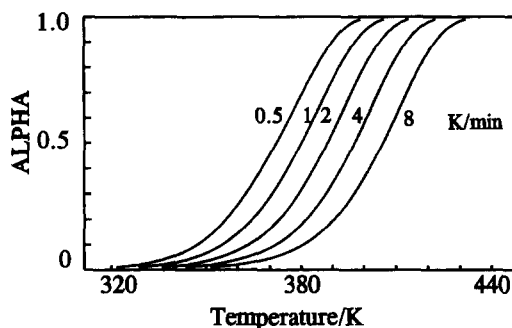


Fig. 7. Simulated alpha–temperature curves calculated at heating rates of 0.5, 1.0, 2.0, 4.0 and 8.0 K min<sup>-1</sup>.

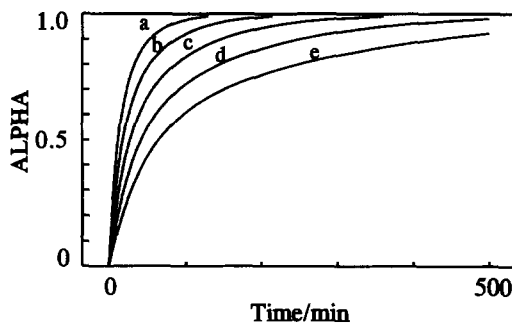


Fig. 8. Simulated isothermal alpha–time curves calculated at temperatures of  $a=380$ ,  $b=375$ ,  $c=370$ ,  $d=365$  and  $e=360$  K.