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Note

NON-ISOTHERMAL KINETICS IN THERMAL DESORPTION. DESORPTION CURVE SIMULATION

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In a previous note [1] the Coats–Redfern method was used [2] to evaluate the kinetic parameters of thermal desorption. If the kinetic order of desorption equals two, the linearised form of the Coats–Redfern equation takes the following form

$$\ln\left[\frac{\alpha}{(1-\alpha)T^2}\right] = \ln\left[\frac{AR}{\beta E_d}(1-2RT/E_d)\right] - E_d/RT \tag{1}$$

where α is the conversion degree at temperature T (K), E_d the activation energy of the desorption, A the pre-exponential factor, and β the heating rate. From the slope and intercept of the plot $\ln[\alpha/(1-\alpha)T^2]$ vs. $1/T$, the activation energy of thermal desorption and the pre-exponential factor can be determined.

This note aims to recheck the applicability of the method for TPD studies through simulation of the TPD curves and their subsequent comparison with the experimental ones. In order to do this, four TPD curves (thermal programmed desorption curves), $p(T)$, concerning the H_2/Fe-catalyst system, have been chosen to be worked by help of the Coats–Redfern method using the technique of linear regression.

Actually, a simplified version of eqn. (1) was applied in which $2RT/E_d \ll 1$, a condition which holds for all the desorption temperatures. The sample was heated with $\beta = 0.16$ K s^{-1}. Using the experimental values of E_d and A, a value of α_{calc} can be evaluated from eqn. (1). On the other hand

$$p(T) \propto d\alpha/dT = (A/\beta)\exp(-E_d/RT)(1-\alpha)^2 \tag{2}$$

By introducing the known values of E_d, A and α_{calc} into eqn. (2), the desorption rates can be evaluated for all desorption temperatures, and thus the TPD curve can be simulated.

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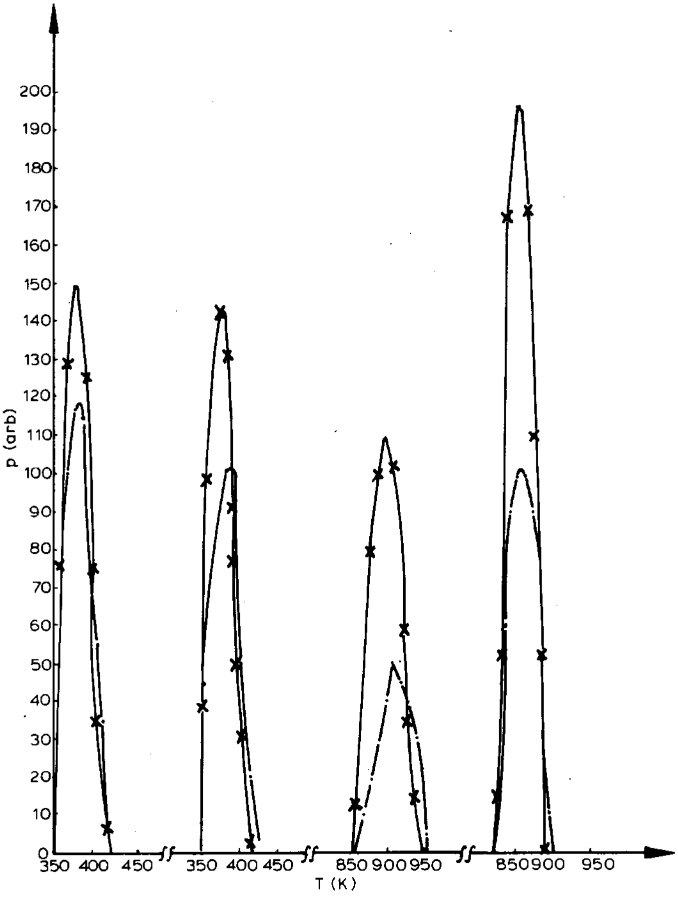

Fig. 1. Experimental (– • –) and simulated (– × –) TPD curves.

The experimental and simulated TPD curves are given in Fig. 1. One can notice a quite satisfactory location of the simulated curves, the difference between the peak temperatures, T_p, of the simulated and original curves being lower than 10 K. This again shows the usefulness of non-isothermal kinetics in investigations concerning thermal desorption.

REFERENCES

1 E. Segal, Thermochim. Acta, 53 (1982) 379.
2 A.W. Coats and J.P. Redfern, Nature (London), 201 (1964) 68.