

Application of the regularization method to the analysis of the TPD spectra carried out under quasi-equilibrium conditions

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The paper deals with the problem of determination of the adsorption energy distribution function from the thermodesorption spectra recorded under the quasi-equilibrium conditions. It is shown that such quasi-equilibrium may be assumed for the majority of thermodesorption experiments carried out under the flow conditions. A mathematical model of the quasi-equilibrium thermodesorption is presented and discussed. Also, implementation of the regularization procedure based upon the quasi-equilibrium model is presented. The accuracy of this procedure is discussed by its application for the analysis of the quasi-equilibrium thermodesorption data obtained from simulations.

1. INTRODUCTION

The temperature programmed desorption (TPD) is one of the most popular experimental techniques used in surface science and catalysis to study the nature of gas-solid interactions. The principles of that method were first published in 1963 by Amenomiya and Cvetanovic, [1] and 9 years later the first theoretical paper on the application of that experiment to study energetic surface heterogeneity was published by Cvetanovic and Amenomiya. [2] The growing popularity of this method resulted in many publications concerning the technical side of this experiment as well as the theoretical analysis of the recorded TPD spectra. [3-7]

So far, that analysis of TPD spectra has usually been based on the Absolute Rate Theory (ART) [8] and the assumption of non-equilibrium nature of the

process, which led to the use of Polanyi-Winger equation or its modifications. [9-12] More recently the Statistical Rate Theory (SRT), developed by Ward et. al., [13] has also been applied for that analysis. First attempts to determine the adsorption/desorption energy distribution from the TPD spectra, using the SRT approach were made by Rudzinski et.al. [14-17]

The recent paper by Panczyk et. al. [18] shows that while applying the theoretical expression developed from the SRT approach for the quantitative analysis of the TPD spectra one may assume that the majority of thermodesorption processes carried out under flow conditions are quasi-equilibrium. It has been shown that the main reason for this quasi-equilibrium nature of thermodesorption is the readsorption occurring freely under the applied experimental conditions.

One of the advantages of the equilibrium thermodesorption is that it greatly simplifies its theoretical analysis because then the Langmuir isotherm can be used as the kernel in the integral equation. Moreover, differences between the ART and the SRT approach disappear since both approaches coincide at equilibrium. [19]

The regularization method [20] is frequently used to elucidate the adsorption energy distribution function from the experimental data based on the integral equation on equilibrium adsorption as well as from the thermodesorption data. [21] However, in the case of thermodesorption various kinetic expressions have been used as the kernel of the integral equation. Because the majority of the TPD experiments carried out under the flow conditions are the quasi-equilibrium ones, it seems reasonable to discuss the applicability of the regularization method to such a type of experimental data. This is the scope of this work.

2. THEORY

The SRT equation describing the adsorption/desorption rate has the following form, [13,22]

$$\frac{d\theta}{dt} = K'_{gs} \left[\exp\left(\frac{\mu_g - \mu_s}{kT}\right) - \exp\left(\frac{\mu_s - \mu_g}{kT}\right) \right] \quad (1)$$

where K'_{gs} is the so-called equilibrium exchange rate, θ is the fractional coverage of the surface, μ_s and μ_g are the chemical potentials of the adsorbed and gas phases, respectively. The meaning of kT is as usual, whereas t is the time.

Equation (1) is valid only for an isolated system but the generalization of the equation (1) proposed by Elliot and Ward [22] makes it also applicable for open systems and leads to a transformation of the equilibrium exchange rate K'_{gs} into

a certain function of the actual pressure p and coverage θ in the adsorption system under investigation.

In the case of an energetically heterogeneous surface the chemical potential in eq. (1) μ_s and the equilibrium exchange rate K'_{gs} become functions of the total coverage of the heterogeneous surface θ_t . [23,24]

$$K'_{gs} = K_{gs} p^{(e)} (1 - \theta_t) \quad K_{gs} = \frac{\xi S_A}{M \sqrt{2\pi m k T}} \quad (2)$$

In eq. (2) S_A [m²/g] is the area of adsorbing/desorbing solid surface, M [g⁻¹] is the density of the adsorption centers, m is the mass of molecule and ξ is some Boltzmann factor related to the activation energy of adsorption. The quantity $p^{(e)}$ is the equilibrium pressure (in the isolated system) corresponding to a given value of coverage of energetically heterogeneous surface θ_t . If we assume the ideal gas behavior of the molecules in the bulk gas phase then the following relation between the equilibrium pressure and chemical potential exists,

$$p^{(e)} = \exp\left(\frac{\mu_s(\theta_t) - \mu_g^0}{kT}\right) \quad (3)$$

Thus, the more particular form of eq. (1) reads

$$\frac{d\theta_t}{dt} = K_{gs} \exp\left(\frac{\mu_s(\theta_t) - \mu_g^0}{kT}\right) (1 - \theta_t) \left[\exp\left(\frac{\mu_g(p) - \mu_s(\theta_t)}{kT}\right) - \exp\left(\frac{\mu_s(\theta_t) - \mu_g(p)}{kT}\right) \right] \quad (4)$$

where μ_g^0 is the standard chemical potential of the ideal gas.

Expressing chemical potentials as functions of the actual coverage and pressure p means physically that there is quasi-equilibrium throughout each phase, but non-equilibrium exists between these phases. Also, the equilibrium pressure in the auxiliary isolated system is expressed as the function of $\mu_s(\theta_t)$ since the *solid dominated* limit implies that $\theta_t^{(e)} \approx \theta_t$. [23,24]

Let us introduce the following function:

$$\varepsilon_c(\theta_t) = -\mu_s(\theta_t) - kT \ln q \quad (5)$$

where q is the partition function of the adsorbed molecules related to the internal degrees of freedom. Then, eq. (4) can be modified to the following form:

$$\frac{d\theta_t}{dt} = \frac{K_{gs}}{K} e^{-\frac{\varepsilon_c(\theta_t)}{kT}} (1-\theta_t) \left[Kp e^{-\frac{\varepsilon_c(\theta_t)}{kT}} - \frac{1}{Kp} e^{-\frac{\varepsilon_c(\theta_t)}{kT}} \right] \quad (6)$$

where

$$K = q e^{\frac{\mu_g^0}{kT}} \quad (7)$$

Let us notice, that in the case of energetically homogeneous surface the relation (5) leads to:

$$\varepsilon_c = -kT \ln \frac{\theta}{1-\theta} + \varepsilon \quad (8)$$

Rearranging equation (8) gives the Langmuir isotherm equation:

$$\theta(\varepsilon, \varepsilon_c) = \frac{\exp\left(\frac{\varepsilon - \varepsilon_c}{kT}\right)}{1 + \exp\left(\frac{\varepsilon - \varepsilon_c}{kT}\right)} \quad (9)$$

where ε is the energy (heat) of adsorption on the energetically homogeneous surface and ε_c is the adsorption potential. This equation becomes the kernel of the integral equation,

$$\theta_t = \int \theta(\varepsilon, \varepsilon_c) \chi(\varepsilon) d\varepsilon \quad (10)$$

for the energetically heterogeneous surface where χ is the distribution function of adsorption energy on this surface.

Looking at equation (6) one can notice that at equilibrium ($d\theta_t/dt = 0$), the adsorption potential becomes the explicit function of pressure.

$$\varepsilon_c = -kT \ln Kp \quad (11)$$

and the pressure p in eq. (11) becomes equal to the pressure in the auxiliary isolated system.

Equation (6) links the three important parameters in the thermodesorption process i.e. ε_c , T and θ_t . Solving eq. (6) with respect to ε_c gives,

$$\varepsilon_c(\theta_t, T) = \frac{1}{2} kT \ln \frac{K_{gs}(1-\theta_t)}{K^2 p \left(K_{gs} p (1-\theta_t) - \beta \frac{d\theta_t}{dT} \right)} \quad (12)$$

where the heating rate $\beta = dT/dt$ and $d\theta_t/dt = \beta (d\theta_t/dT)$. The pressure p is related to the desorption rate, (F – the flow rate of carrier gas, m_s – the mass of the sample), i.e.:

$$p = -\frac{m_s M k T \beta}{F} \frac{d\theta_t}{dT} \quad (13)$$

It can be noted that equation (12) reduces to eq. (11) when

$$\left| K_{gs} p (1-\theta_t) \right| \gg \left| \beta \frac{d\theta_t}{dT} \right| \quad (14)$$

It is obvious that for equilibrium ($d\theta_t/dt = 0$) the same transformation takes place. Thus, when $d\theta_t/dt$ is negligibly small compared to $K_{gs} p (1-\theta_t)$ the quasi-equilibrium occurs. For typical values of the parameters of the thermodesorption process carried out under the flow conditions relation (14) is usually fulfilled [19]. There might be some exceptions when the readsorption is hindered by strong activation barriers.

Quasi-equilibrium nature of thermodesorption process allows to use the Langmuir isotherm (9) for the theoretical/mathematical description of the process. This isotherm can be written in the following form:

$$\theta(p, T) = \frac{K p e^{\frac{\varepsilon}{kT}}}{1 + K p e^{\frac{\varepsilon}{kT}}} \quad (15)$$

While expressing the pressure p in eq. (15) by the rhs of eq. (13) and next solving the so-obtained equation with respect to $d\theta/dT$ we arrive at the following expression,

$$\frac{d\theta}{dT} = -\frac{F e^{\frac{\varepsilon}{kT}}}{m_s M K \beta k T} \frac{\theta}{1-\theta} \quad (16)$$

Eq. (16) is the differential equation which allows predicting the equilibrium TPD spectra not only for the Langmuir model of adsorption (energetically uniform surface) but also for an energetically heterogeneous surface. This is because equation (16) can be used as the kernel of integral equation (10). After solving eq. (16) with the boundary condition $\theta(T_0)=1$ (where T_0 is the value of temperature corresponding to the initial coverage assumed to be equal to 1), the explicit form of $\theta(T, \varepsilon)$ function is obtained.

$$\theta(T, \varepsilon) = -\text{PLog}\left[-\exp\left[\frac{F * \text{EEi}[-\varepsilon/kT]}{\kappa} - \frac{\kappa + F * \text{EEi}[-\varepsilon/kT_0]}{\kappa}\right]\right] \quad (17)$$

where $\kappa = \beta k K M m_s$.

Expression (17) requires using a few special functions implemented in the *Mathematica* program. Particularly, $\text{EEi}[x]$ function which is equivalent to the *Mathematica* internal function $\text{ExpIntegralEi}[x]$ defined as follows:

$$\text{EEi}[x] = \int_{-x}^{\infty} \frac{\exp[-t]}{t} dt \quad (18)$$

$\text{PLog}[z]$ function is equivalent to the *Mathematica* function $\text{ProductLog}[z]$ that gives the principal solution for w in $z = we^w$. After differentiation of eq. (16) with respect to T , we obtain

$$\frac{d\theta}{dT} = \frac{\exp(-\varepsilon/kT)F - \text{PLog}\left[-\exp\left(\frac{F}{\kappa} \text{EEi}[-\varepsilon/kT]\right) - \frac{\kappa + F \text{EEi}[-\varepsilon/kT_0]}{\kappa}\right]}{\kappa \left(1 + -\text{PLog}\left[-\exp\left(\frac{F}{\kappa} \text{EEi}[-\varepsilon/kT]\right) - \frac{\kappa + F \text{EEi}[-\varepsilon/kT_0]}{\kappa}\right]\right)} \quad (19)$$

Equation (19) will be used by us as the kernel in the differentiated integral equation (10) to calculate the TPD spectrum for the energetically heterogeneous surface. It can also be used for the reverse procedure, *i.e.* determination of the distribution function from the simulated TPD spectra by means of the regularization method.

3. RESULTS AND DISCUSSION

In order to demonstrate the applicability of the regularization method for the determination of the adsorption energy distribution from the quasi-equilibrium

TPD spectra, we first simulate such data using some predetermined distribution function. So, let us assume that the adsorption energy distribution has the following quite complicated shape.

$$\chi(\varepsilon) = 0.25e^{-\frac{1}{\sqrt{8\pi}}\frac{(\varepsilon-140)^2}{8}} + 0.4e^{-\frac{1}{\sqrt{16\pi}}\frac{(\varepsilon-115)^2}{16}} + 0.25e^{-\frac{1}{\sqrt{4\pi}}\frac{(\varepsilon-95)^2}{4}} + 0.1e^{-\frac{1}{\sqrt{3\pi}}\frac{(\varepsilon-86)^2}{3}} \quad (20)$$

Next, the ‘experimental’ TPD spectra were calculated using integral equation (10) with eq.(19) as the kernel and assuming different heating rates together with the distribution function (20).

Figure 1 shows the plot of function (20) whereas Figure 2 shows the simulated TPD spectra corresponding to distribution (20) and a few heating rates β . These spectra (Figure 2) will be used as experimental ones while recovering the adsorption energy distribution function, $\chi(\varepsilon)$.

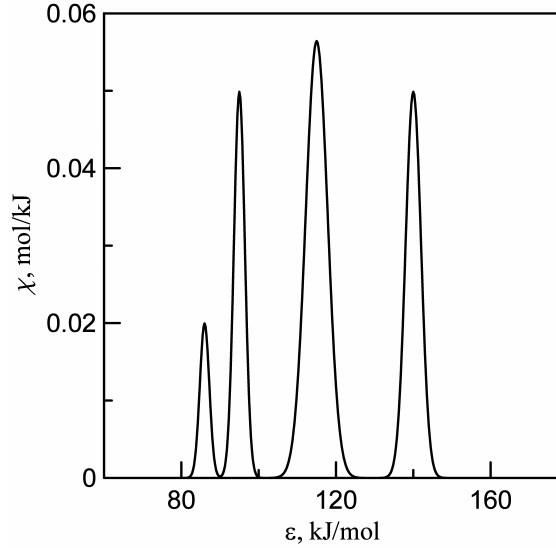


Fig. 1. Plot of the distribution function χ defined in eq. (20) which will be used for simulation of the TPD spectra.

Implementation of the regularization algorithm in the *Mathematica* program is very simple. Main part of the code can be condensed in only a few lines, that is:

```

result=Solve[Table[Sum[(dtht[[j,2]]- Sum[ $\alpha$ [i] *
dtt[Enx[[i]],dtht[[j,1]]],{i,1,n} ])*
*(-dtt[Enx[[i]],dtht[[j,1]]]),{j,1,m}]+ $\gamma$  $\alpha$ [i]==0,
{i,1,n}],Table[ $\alpha$ [i],{i,1,n}]]

```

The object `dtht` is the two-dimensional table containing m experimental data points in the form $\{-d\theta/dT, T\}$, `Enx` is the one-dimensional table containing the sampled energy points, `dtt` is the kernel (19) implemented as a function of energy and temperature. The table `α` contains n values of the distribution function corresponding to n values of the energy from the table `Enx`. γ is the regularization parameter. The object `result` contains the results of calculations which are to be used in further operations.

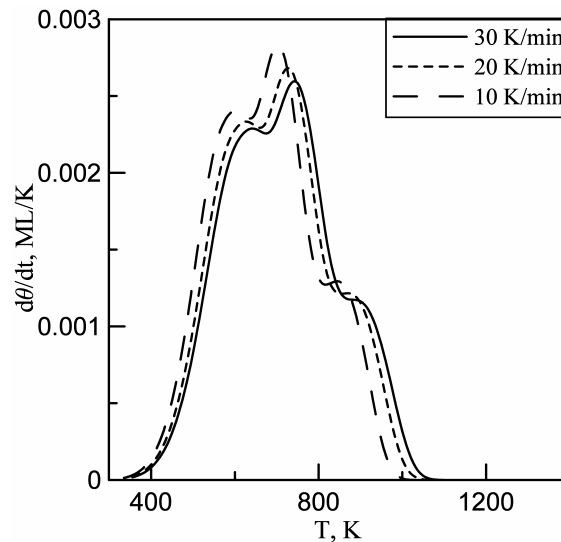


Fig. 2. TPD spectra calculated from eq. (10) with eq. (19) as the kernel and the function (20) as the adsorption energy distribution function χ . Calculations were carried out using the following set of parameters: $K = 10^{-10} \text{ Pa}^{-1}$; $\epsilon = 100 \text{ kJ/mol}$; $m_s = 0.1 \text{ g}$; $M = 10^{-4} \text{ mol/g}$; $F = 30 \text{ cm}^3/\text{min}$; $\theta_0 = 1$, $T_0 = 300\text{K}$. The values of the assumed heating rates are shown in the legend.

The results of calculations based upon the above simple algorithm are shown in the next two figures. Figure 3 shows the results for various values of the regularization parameter γ . Its correct choice is usually the weakest point of the regularization method. [21] Thus, the calculations have been carried out for various values of the regularization parameter γ to show its influence on the results of calculations. The values of other parameters were identical to those

used for simulation of the spectra. Left panel of Figure 3 shows the comparison between the ‘experimental’ TPD spectrum drawn as the solid lines, whereas the symbols ‘•’ shows the ‘theoretical’ spectrum calculated using the determined distribution function (shown in the right panel and denoted by the symbol ‘•’). The solid line in the right panel is the pre-determined function from Figure 1. Every row in Figure 3 shows the results of calculations for a fixed value of the regularization parameter γ shown in the legends.

Analysis of Figure 3 leads to the conclusion that the value of the parameter $\gamma = 10^{-2}$ is too high. There is no agreement between the experimental and calculated spectra based upon this value of the regularization parameter. Of course, there is also very weak agreement between the assumed and the determined distribution function. The decreasing value of γ leads to better and better agreement between the spectra and the distributions functions. Here, the second row in Figure 3 shows the results for $\gamma = 10^{-13}$. The observed perfect accuracy of the regularization method is kept over quite a wide range of the γ values (from 10^{-4} to 10^{-30}). Only for extremely low values of γ , *i.e.* 10^{-50} one can observe the typical noise generated by the regularization method for too small values of the regularization parameter.

The results presented in Figure 3 would suggest that the choice of a correct value of the regularization parameter is rather a simple task. Moreover one would expect a perfect accuracy in the determination of the adsorption energy distribution function when applying this method. However, the experimental TPD spectrum applied in these calculations is free of experimental errors. The true experimental data are always more or less noisy. Therefore, we repeated all calculations using as the input the TPD spectrum with the random noise added to the signal. The applied noise is uniform ($\pm 2\%$) and proportional to the signal. The results of calculations based upon this ‘rationalized’ spectrum are shown in Figure 4.

Now, it can be seen that the overall accuracy of the regularization method decreases. This, however, is to be a fully expected result since some part of the ‘experimental’ information has been lost after introduction of errors. The function χ obtained for the most correct value of $\gamma = 10^{-5}$ (determined using the trial and error procedure) is quite far from the true distribution. However, some of its important features are correctly recovered despite the errors introduced. One can easily notice that the distribution function consists of four peaks having various mutual intensities (correctly recovered), also positions of the successive maxima of these peaks are correctly determined.

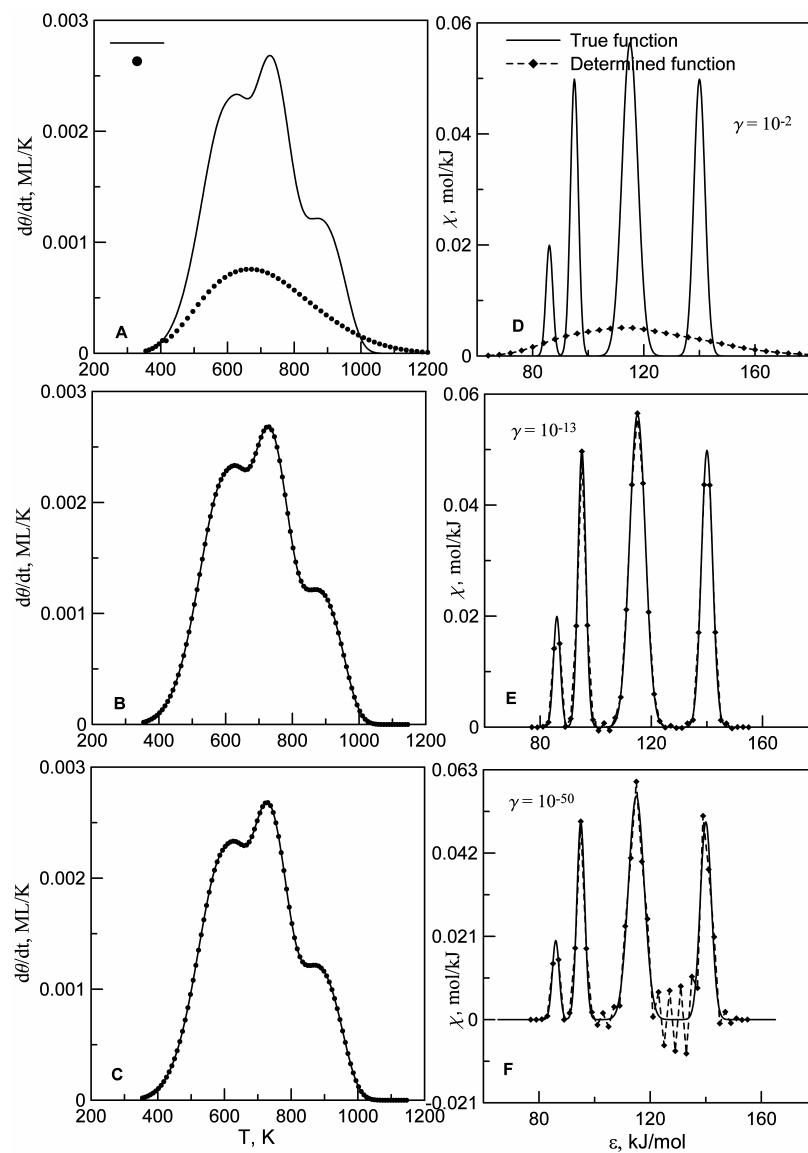


Fig. 3. Results of application of the regularization method to the TPD spectrum shown in Figure 2 for the heating rate $\beta=20\text{K/min}$. Left panel shows the comparison between the 'experimental' TPD spectrum drawn as the solid lines, whereas the symbols ' \bullet ' show the 'theoretical' spectra calculated using the determined distribution functions (shown in the right panel and denoted by the symbol ' \bullet '). The solid line in the right panel is the pre-determined function from Figure 1. Every row in Figure 3 shows the results of calculations for a fixed value of the regularization parameter γ marked in the legends.

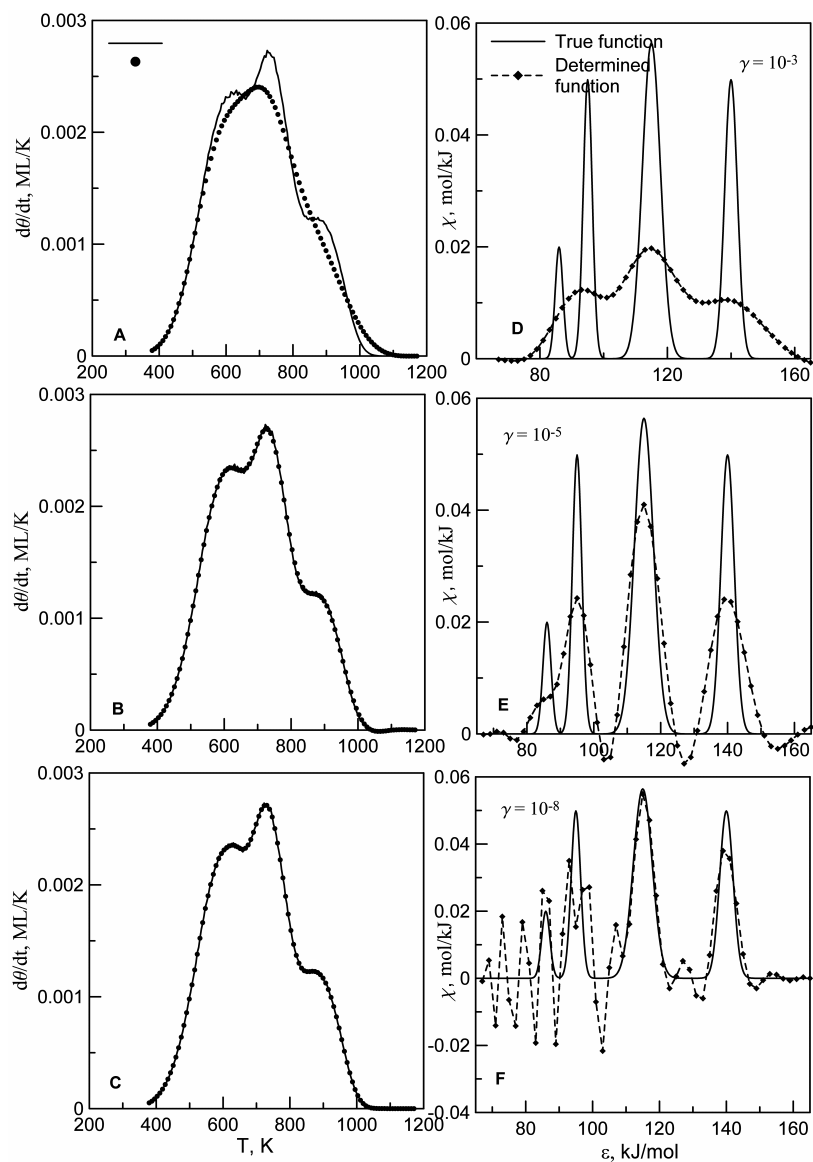


Fig. 4. The same results as in Figure 3 but here the random errors ($\pm 2\%$) are added to the input TPD signal.

The negative parts of the distribution function are typical for the simple Tikhonov regularization. [20,21] Such effect might be avoided by applying a more sophisticated non-negative regularization. [21] This method, however, would be much more complicated and the calculations are then much slower.

The method presented can be applied to experimental spectra and one can expect reliable results. When applying this method to analyze experimental data one has to choose correct values of parameters. Most of them are usually known, but K must be determined from other experiments or by using one of the methods described by Pańczyk et. al. [18] The choice of the regularization parameter is the main difficulty when applying this method to experimental data. If the experimental spectrum is not sufficiently smooth, determination of true shape of the distribution function might not be possible.

4. SUMMARY AND CONCLUSIONS

We have presented the method for determination of the adsorption energy distribution function from the quasi-equilibrium TPD spectra. In such a type of experiment the mathematical model of thermodesorption process takes a specific form consistent with the Langmuir equilibrium isotherm. While using the SRT formalism one may assume that the majority of the thermodesorption experiments carried out under flow conditions are quasi-equilibrium.

Determination of the adsorption energy distribution function from the quasi-equilibrium TPD data can be done by using the classical regularization method. In turn, application of the *Mathematica* software makes the implementation of the regularization procedure extremely simple and the calculations are very fast.

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CURRICULA VITAE



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Tomasz Pańczyk was born in Zamość, Poland in 1972. Studies of chemistry in the Faculty of Chemistry, Maria Curie-Skłodowska University in Lublin in 1992–1997. Individual course of studies supervised by professor Władysław Rudziński. Received Ph.D. degree in physical and theoretical chemistry from the Maria Curie-Skłodowska University in Lublin in 2001. At present he is employed as an assistant professor in the Institute of Catalysis and Surface Chemistry, Polish Academy of Science in Kraków. The main field of interest is the theoretical study of various dynamic processes related to the gas adsorption on solids. The investigations resulted in over 30 original papers.



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the Institute of Catalysis and Surface Chemistry of the Polish Academy of Sciences in Cracow. He was also the Chairman of the Committee for Interface Chemistry of the Polish Chemical Society, and served also one year as the President of the Society. Professor Rudziński was a member of the Board of Directors of the International Adsorption Society, and served as a member of the Scientific Committees of such international conferences as the largest world conference on adsorption FOA (Fundamentals of Adsorption), or the Pacific Adsorption Conference. He is also a corresponding member of the European Academy of Arts Sciences and Humanities.

He published over 250 papers, and the monograph co-authored by Professor D.H. Everett "Adsorption of Gases on Heterogeneous Surfaces" (Academic Press, 1992). Together with Professors W. A. Steele and G. Zgrablich, he edited the monograph "Equilibria and Dynamics of Gas Adsorption on Heterogeneous Solid Surfaces" (Elsevier, 1997). He was the Member of Editorial Boards of "Langmuir" journal, and is now member of the Editorial Boards of "Adsorption" journal, and of the journal "Adsorption Science & Technology".

He organised the four international symposia: "Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids"-ISSHAC (Poland, 1992, 1995, 1998, 2001, 2004), and the Polish-Israeli Symposium "Current Trends in Interface Chemistry", in 2000.

For his outstanding scientific achievements, he was awarded five times by the Polish Ministry of Education and once by the Rector of Maria Curie-Skłodowska University. He was also awarded by the Polish Chemical Society.

Besides many short visits to many Universities of the world, he also paid long-term visits to Queens University (Canada), University of Vienna (Austria), University of Leipzig (Germany), Tohoku University (Japan), CNRS Laboratory at the University of Montpellier (France), Ruhr University in Bochum (Germany), Seoul National University (Korea), Chonnam National University (Korea), CNRS Laboratory in Nancy (France), University of San Luis (Argentina), and National Chung Cheng University (Taiwan).

Main scientific interests: Theoretical description of adsorption of simple ions and of surfactants at oxide/electrolyte interfaces (Special attention focused on enthalpies of adsorption and on effects of surface heterogeneity), equilibria and kinetics of gas adsorption on energetically heterogeneous solid surfaces, (also thermodesorption), and mixed-gas adsorption.