

## Theoretical studies of the heat effects accompanying mixed-gas adsorption by using Vacancy Solution and Regular Adsorbed solution theories

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The theoretical studies of the enthalpic effects accompanying mixed-gas adsorption equilibria by using Vacancy Solution Theory are presented. Besides heterogeneity the interaction effects by using the Regular Adsorbed Solution theory are taken into account. The theoretical predictions of adsorption phase diagrams and accompanying them calorimetric effects requires only the knowledge of single-gas adsorption and calorimetric data. It is shown that, in general, the VST approach gives the results that are in good agreement with experimental data.

### 1. INTRODUCTION

The theoretical predictions of mixed-gas adsorption based on pure-component isotherms can be applied in industrial separation of gases by adsorption processes. Application of this modern technology is also imposed also by less energy consumption. Such processes are controlled by computer programs in which a subroutine calculating gas adsorption equilibria play a substantial role. The accuracy and speed of calculations result in higher degree of purity of separated gases. As adsorption of gases is accompanied by enthalpic effects possibility of taking it into account may have unquestionable influence on the process productivity.

In our recent studies we have investigated the theoretical methods of predicting heat effects accompanying mixed-gas adsorption by using the Integral Equation (IE) approach [12], the Ideal Adsorbed Solution (IAS) theory [11,13] and the Potential Theory (PT) [14]. A basic principle in theoretical investigations proposed by us is the possibility to calculate the mixed-gas

adsorption equilibria and enthalpic effects accompanying them by using only information which can be determined from theoretical analysis of single-gas systems. In the present paper we show some results of the theoretical studies concerning the application of the Vacancy Solution Theory (VST) to describe the isosteric heats accompanying mixed-gas adsorption [15].

## 2. THEORY

The vacancy formalism was proposed by Dubinin [1] in 1977. He treated the single-component adsorption as equilibrium between two 'vacancy solutions' having different compositions. Lucassen-Reynders [2-4] used a similar idea to describe the surfactant adsorption and his considerations can be extended to predict the adsorption equilibrium of mixed surfactant system. On the basis of the achievements by Dubinin and Lucassen-Reynders, Suwanayuen and Danner [5] the approach known as the Vacancy Solution Theory is proposed. The adsorption equilibrium is defined in the following way:

- Both gas and adsorbed phases are considered to be solutions of adsorbates in a hypothetical solvent called "vacancy". A vacancy (vacuum entity) can be filled by adsorbate molecules;
- The properties of the adsorbed phase are defined as excess properties in relation to a dividing surface;
- The entire system including the solid is in the thermal equilibrium, but only the gas and the adsorbed solutions are in the osmotic or phase equilibrium with each other;
- The equilibrium of the system is maintained by a pressure usually called surface, osmotic or spreading pressure which arises from a potential force field at the surface.

For the model presented above, the gas adsorption equilibrium can be considered as an equilibrium between a bulk adsorbent solution and its surface phase. So, a pure gas adsorption equilibrium thus becomes an equilibrium between binary vacancy solutions. Briefly speaking, the model of adsorption equilibrium assumes that the gas and adsorbed phases are the solutions of adsorbates in a hypothetical solvent called 'vacancy'. A vacancy (i.e. empty site) can be filled by adsorbate molecules.

Rudziński et al. [6] applied VST for the case of mixed-gas adsorption equilibria on heterogeneous solid surfaces. By using the Regular Adsorbed Solution (RAS) theory as the model of non-ideality the following expression for the case of single-gas adsorption can be obtained:

$$\theta_{ii} = \frac{\left[ K_i p_i \exp\left\{\frac{\varepsilon_i^0}{kT}\right\} \right]^{kT/c_i} \exp\left\{\frac{\omega_{ii} \theta_{ii}}{c_i}\right\}}{1 + \left[ K_i p_i \exp\left\{\frac{\varepsilon_i^0}{kT}\right\} \right]^{kT/c_i} \exp\left\{\frac{\omega_{ii} \theta_{ii}}{c_i}\right\}} \quad (1)$$

where  $\theta_{ii}$  is the surface coverage,  $c_i/kT$  - the heterogeneity parameter,  $K_i \exp\{\varepsilon_i^0/kT\}$  - the Langmuir constant ( $\varepsilon_i^0$  - the most probable value of adsorption energy) and  $\omega_{ii}$  is the interaction parameter of the molecules adsorbed on the neighbouring adsorption sites.

On the basis of single-gas isotherm equation (1) we can calculate the heat effects accompanying adsorption processes by using the well-known expression:

$$q_i^{st} = -k \left[ \frac{\partial \ln p_i}{\partial (1/T)} \right]_{\theta_{ii}} \quad (2)$$

where  $q_i^{st}$  is the isosteric heat accompanying the single-gas adsorption. So, the combination of eqs (1) and (2) leads to the following result:

$$q_i^{st} = q_i^{st0} - c_i \ln \frac{\theta_{ii}}{1 - \theta_{ii}} + \omega_{ii} \theta_{ii} \quad (3)$$

where  $q_i^{st0} = k \frac{d \ln K_i'}{d(1/T)}$  is frequently called the 'non-configurational' isosteric heat of adsorption and  $K_i' = K_i^0 \exp\{\varepsilon_i^0/kT\}$ .  $\omega_{ii}$  is the same interaction parameter as in eq. (1) so the simultaneous analysis of the isotherms and isosteric heats of single-gas adsorption gives the possibility to increase the accuracy of  $\omega_{ii}$  determination. The value of the parameter  $q_i^{st0}$  only shifts the heat curve on y-axis.

The use of the single-gas adsorption isotherm (1) gives all information necessary to calculate the mixed-gas adsorption equilibria. Rudzinski et al. [6] proposed the following expression:

$$X_{ii} = p_i K_i' \cdot \left[ \frac{\gamma_i^s N_\Sigma M_i}{M_\Sigma} \left( \lim_{N_\Sigma \rightarrow 0} \frac{1}{\gamma_i^s} \right) \exp\left\{ \left( \frac{M_i - M_\Sigma}{N_\Sigma} - 1 \right) \left( \ln \gamma_i^s + \frac{c_i}{kT} \ln x_v^s - \Pi_i^m \right) \right\} \right]^{-1} \quad (4)$$

where  $X_{it}$  is the mole fraction of component  $i$  in the adsorbed phase,  $\Pi_i^m$  is the parameter whose value depends on the definition of the limits of adsorption energies (when infinite limits are assumed  $\Pi_i^m = 0$ ),  $\gamma_i^s$  are the activity coefficients:

$$\ln \gamma_1^s = \frac{W_{12}}{kT} (\theta_{2t})^2 + \frac{W_{1v}}{kT} (1 - \theta_{1t} - \theta_{2t})^2 + \frac{W_{12} + W_{1v} - W_{2v}}{kT} \theta_{2t} (1 - \theta_{1t} - \theta_{2t}) \quad (5)$$

$$\ln \gamma_2^s = \frac{W_{12}}{kT} (\theta_{1t})^2 + \frac{W_{2v}}{kT} (1 - \theta_{1t} - \theta_{2t})^2 + \frac{W_{12} + W_{2v} - W_{1v}}{kT} \theta_{1t} (1 - \theta_{1t} - \theta_{2t}) \quad (6)$$

$$\ln \gamma_v^s = \frac{W_{1v}}{kT} (\theta_{1t})^2 + \frac{W_{2v}}{kT} (\theta_{2t})^2 + \frac{W_{1v} + W_{2v} - W_{12}}{kT} \theta_{1t} \theta_{2t} \quad (7)$$

and the subscript 'v' is used to denote the 'vacancy' (3<sup>rd</sup> component).  $W_{ij}$  is the 'interchange energy' defined as follows:

$$W_{ij} = \omega_{ii} + \omega_{jj} - 2\omega_{ij} \quad (8)$$

where  $\omega_{ij}$  is the interaction energy between the two molecules  $i$  and  $j$  adsorbed on two neighbouring adsorption sites. In the case of 'third component' i.e. 'vacancy' the interaction parameters vanish ( $\omega_{iv} = 0$  and  $\omega_{vv} = 0$ ).

The case when  $W_{ij} = 0$  refers to 'ideal solution' when  $\omega_{ij}$  is simply the arithmetic average of  $\omega_{ii}$  and  $\omega_{jj}$ .

The mole fractions in the vacancy solution formalism can be calculated from the following relations

$$x_i^s = N_{it} \left[ \frac{N_{1t} + N_{2t}}{N_{1t}M_1 + N_{2t}M_2} \right], \quad i = 1, 2 \quad \text{and} \quad x_v^s = 1 - x_1^s - x_2^s \quad (9)$$

$N_\Sigma$  and  $M_\Sigma$  are defined as follows:

$$N_\Sigma = N_{1t} + N_{2t} \quad (10)$$

$$M_\Sigma = X_{1t}M_1 + X_{2t}M_2 \quad (11)$$

where  $N_{it}$  is the adsorbed amount of component  $i$  and  $M_i$  is the maximum loading.

The calculation of  $\lim_{N_\Sigma \rightarrow 0} 1/\gamma_i^s$  leads to the following result:

$$\lim_{N_\Sigma \rightarrow 0} \frac{1}{\gamma_i^s} = \exp\left\{-\frac{W_{iv}}{kT}\right\} \quad (12)$$

All other symbols in eq. (4) can be determined from the single-gas adsorption isotherms by adopting eq. (1).

The main idea used in our theoretical studies is the possibility to calculate the isosteric heats of adsorption in the mixed system by analyzing only the single-gas adsorption system. In other words, the theoretical expressions can include such best-fit parameters what were determined from isotherms and isosteric heats of single-gas adsorption. So the use of eqs (1) and (3) to the experimental data gives the complete information about 2-component system.

Similarly to the case of single-gas adsorption, we can use eq. (4) to calculate the isosteric heat of adsorption  $Q_i^{st}$  of a given component by the following:

$$Q_i^{st} = -k \left[ \frac{\partial \ln p_i}{\partial (1/T)} \right]_{\{\theta_n\}}, i=1,2 \quad (13)$$

The differentiation leads to the following expression [15]:

$$Q_i^{st} = q_i^{st0} - k \frac{\partial \ln \gamma_i^s}{\partial (1/T)} - k \left[ \frac{\partial}{\partial (1/T)} \ln \left( \lim_{N_\Sigma \rightarrow 0} \frac{1}{\gamma_i^s} \right) \right] + \left( \frac{M_i - M_\Sigma}{N_\Sigma} - 1 \right) \left( k \frac{\partial \Pi_i^m}{\partial (1/T)} - c_i \ln x_v^s - k \frac{\partial \ln \gamma_i^s}{\partial (1/T)} \right) \quad (14)$$

In the above equation some simplification can be done. Namely, we can substitute the logarithm of the limit by the limit of the logarithm [15]:

$$\ln \left( \lim_{N_\Sigma \rightarrow 0} \frac{1}{\gamma_i^s} \right) = - \lim_{N_\Sigma \rightarrow 0} (\ln \gamma_i^s) \quad (15)$$

$$-k \frac{\partial}{\partial (1/T)} \left( \lim_{N_\Sigma \rightarrow 0} (\ln \gamma_i^s) \right) = -k \lim_{N_\Sigma \rightarrow 0} \left( \frac{\partial \ln \gamma_i^s}{\partial (1/T)} \right) \quad (16)$$

and then

$$-k \frac{\partial}{\partial(1/T)} \ln \left( \lim_{N_{\Sigma} \rightarrow 0} \frac{1}{\gamma_i^s} \right) = k \lim_{N_{\Sigma} \rightarrow 0} \frac{\partial \ln \gamma_i^s}{\partial(1/T)} \quad (17)$$

Such mathematical transformations can be verified in the case of RAS when the expression  $\frac{\partial}{\partial(1/T)} \left( \lim_{N_{\Sigma} \rightarrow 0} (\ln \gamma_i^s) \right)$  in eq. (14) can be calculated directly from eq. (12). In both cases it leads to the same result [15]:

$$k \frac{\partial}{\partial(1/T)} \left( \lim_{N_{\Sigma} \rightarrow 0} (\ln \gamma_i^s) \right) = -W_{iv} \quad (18)$$

The derivatives of the activity coefficients  $\gamma_i^s$  have the following forms:

$$k \left( \frac{\partial \ln \gamma_1^s}{\partial(1/T)} \right)_{\{X_i\}} = W_{12} (\theta_{2r})^2 + W_{1v} (1 - \theta_{1r} - \theta_{2r})^2 + (W_{12} + W_{1v} - W_{2v}) \theta_{2r} (1 - \theta_{1r} - \theta_{2r}) \quad (19)$$

$$k \left( \frac{\partial \ln \gamma_2^s}{\partial(1/T)} \right)_{\{X_i\}} = W_{12} (\theta_{1r})^2 + W_{2v} (1 - \theta_{1r} - \theta_{2r})^2 + (W_{12} + W_{2v} - W_{1v}) \theta_{1r} (1 - \theta_{1r} - \theta_{2r}) \quad (20)$$

Because of a large number of mathematical expressions presented, we summarize the theoretical considerations for the reader's convenience. At first, eq. (1) can be used to analyze the experimental single-gas isotherms and eq. (3) to fit the isosteric heats of single-gas adsorption. As a result, we determine the best-fit single-gas parameters. Then, while studying the mixed-gas adsorptions, eq. (4) should be used whereas to calculate the isosteric heats of adsorption of a given component in mixture, eq. (14) can be applied.  $N_{\Sigma}$  and  $M_{\Sigma}$  in eqs (4) and (14) are defined by eqs (9,10), the activity coefficients and the mole fractions in the vacancy solution are shown in (5-8). The 'interchange energy'  $W_{ij}$  appearing in  $\gamma_i^s$  can be calculated by (11) (assuming ideal solution). The limits appearing in (4, 14) are defined by eq. (12) and the other parameters can be determined from single-gas adsorption systems. So, there are only five best-fit parameters for each component:  $M_i$ ,  $c_i/kT$ ,  $K_i'$ ,  $\omega_{ii}$  and  $q_i^{st0}$  necessary for theoretical calculations of adsorption phase diagrams and isosteric heats of adsorption of a given component in the mixture system.

### 3. FURTHER REMARKS

Although the presented equations are complicated, some simplifications applied lead to relatively simple calculations. Namely, we used the case named ‘ideal solution’ and we assumed infinite values of adsorption energies. Such brief assumptions lead to important simplifications:  $\Pi_i^m = 0$  and  $k(\partial \Pi_i^m / \partial(1/T)) = 0$ . All ‘interchange energies’  $W_{ij}$  are equal to 0 and it causes:

$$\ln \gamma_i^s = 0, \quad k(\partial \ln \gamma_i^s / \partial(1/T)) = 0, \quad k \frac{\partial}{\partial(1/T)} \ln \left( \lim_{N_\Sigma \rightarrow 0} (1/\gamma_i^s) \right) = 0 \quad \text{and} \quad \lim_{N_\Sigma \rightarrow 0} (1/\gamma_i^s) = 1.$$

So the theoretical phase diagram (4) is of the following form:

$$p_i K_i \exp \left\{ \frac{\varepsilon_i^0}{kT} \right\} = X_{ii} N_\Sigma \frac{M_i}{M_\Sigma} \exp \left\{ \left( \frac{M_i - M_\Sigma}{N_\Sigma} - 1 \right) \left( \frac{c_i}{kT} \ln x_v^s \right) \right\} \quad (21)$$

and the theoretical isosteric heat of adsorption (14) simplifies:

$$Q_i^{st} = q_i^{st0} + c_i \left( \frac{M_i - M_\Sigma}{N_\Sigma} - 1 \right) \ln x_v^s \quad (22)$$

In all the above equations the interaction parameter  $\omega_{ii}$  does not occur. Thus, this best-fit parameter only improves agreement between the single-gas isotherms and the single-gas isosteric heats.

The theoretical phase diagram (4) and the isosteric heat of adsorption of a given component in mixture (14) presented in forms (22) and (23) show how numerical calculations can be simple. Using eqs (4) and (14) without any simplifications would probably bring to better agreement but produces additional best-fit parameters.

### 3. CALCULATIONS

Now we examine the presented set of theoretical expressions describing single- and mixed-gas adsorption equilibria and heat effects accompanying them. As we mentioned previously, the theoretical analysis of single-gas isotherms and isosteric heats of single-gas adsorption gives enough knowledge to predict the behaviour of mixed adsorption system. To carry out the numerical exercises we use the experimental data by Dunne et al. [7-9] and Siperstein et al. [10]:  $C_2H_6+CH_4$  on MFI at 23<sup>0</sup>C and  $CO_2+C_2H_6$  on NaX (32<sup>0</sup>C) and  $SF_6+CH_4$  on MFI. Although our model of calculations requires the same temperature of all single-

and mixed-gas experiments, because of small differences between measurement temperatures we neglect them. We used these experimental data in our previous studies [11] and one of the conclusions is that adsorption of  $C_2H_6$  and  $CH_4$  on MFI takes place like on the homogeneous surface i.e. the heterogeneity parameter  $kT/c_i = 1$ . Then, the homogeneous character of adsorption processes in the case of MFI justifies simplification of eq. (3):

$$q_i^{st} = q_i^{st0} + \omega_{ii}\theta_{ii} \quad (23)$$

where, in comparison to eq. (3), the logarithmic term vanishes.

In the adsorption system  $CO_2+C_2H_6$  our numerical studies suggest that the strong interaction effects between the adsorbed molecules exist. Although the results of the analysis of isotherms and isosteric heats of single-gas adsorption were presented in our previous paper [11] we show them again in Table 1 and Figure 1 for the reader's convenience.

Tab. 1. Values of the parameters obtained by applying equation (1) to the experimental isotherms of  $C_2H_6$  and  $CH_4$  adsorbed on MFI,  $CO_2$  and  $C_2H_6$  adsorbed on NaX, reported by Dunne et al. [7-9] and  $SF_6$  and  $CH_4$  adsorbed on MFI, reported by Siperstein et al. [10]. In the last but one column the best-fit values obtained from adopting the theoretical equation for heat of adsorption (3) and (23) were inserted. We also present the Error values corresponding to fitting quality, defined as the residual sum of squares [11].

Adsorption system	T [°C]	$M_i$ [mmol/g]	$\frac{kT}{c_i}$	$\frac{\omega_{ii}}{kT}$	$K_i \exp\left\{\frac{\varepsilon_i^0}{kT}\right\}$	Linear Regression Error	$q_i^{st0}$ [kJ/mol]	
MFI	$C_2H_6$	23.31	1.97	0.991	0.404	$1.5 \cdot 10^{-2}$	$2.2 \cdot 10^{-5}$	31.05
	$CH_4$	23.07	1.96	0.987	0.304	$6.2 \cdot 10^{-4}$	$2.5 \cdot 10^{-4}$	21.17
NaX	$CO_2$	31.4	8.97	0.802	-4.488	$5.1 \cdot 10^{-2}$	$4.2 \cdot 10^{-2}$	38.98
	$C_2H_6$	32.4	3.78	0.98	1.225	$3.5 \cdot 10^{-3}$	$1.7 \cdot 10^{-3}$	28.44
MFI	$SF_6$	$\approx 24$	1.98	0.751	1.265	$1.4 \cdot 10^{-2}$	$4.2 \cdot 10^{-3}$	36.00
	$CH_4$	$\approx 23$	2.35	0.978	0.204	$5.0 \cdot 10^{-4}$	$3.1 \cdot 10^{-5}$	21.50

The best-fit parameters collected in Table 1 are sufficient for modelling mixed-gas adsorption system. It is the master rule of the proposed model of calculations because the single-gas isotherms and calorimetric data are relatively easy to determine and provide complete information necessary to calculate adsorption phase diagrams and the isosteric heats accompanying mixed-gas adsorption.

While performing calculations of the mixed-gas adsorption equilibria we must explain a certain property of the analysed experimental data. Namely,



probably due to technical complications the adsorption phase diagrams and the enthalpic effects accompanying them were determined with varied total pressure. Therefore the calculated theoretical adsorption phase diagrams and isosteric heats of adsorption are the collection of points calculated for each mole fraction of the gas phase determined during experiment. So, because the theoretical phase diagrams and isosteric heats of adsorption are not a continuous function for the readability we connected all theoretical points by line. It simplifies the comparison of the calculation results with experiment.

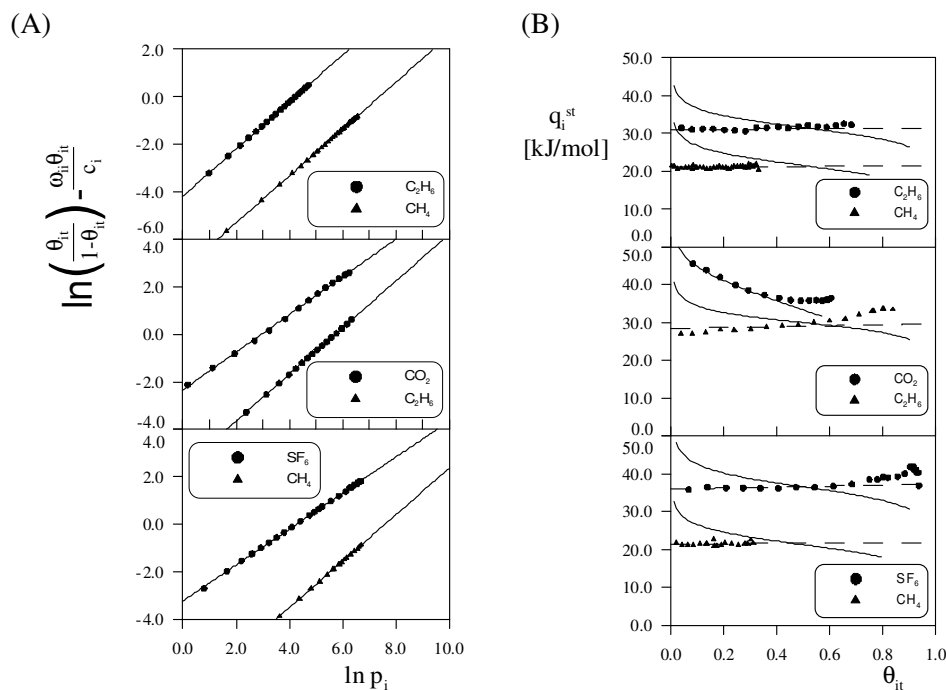


Fig. 1. (A) The application of the linear form of eq. (1) to the experimental data reported by Dunne et al. [7-9]:  $CH_4$  and  $C_2H_6$  adsorbed on MFI,  $CO_2$  and  $C_2H_6$  adsorbed on NaX; and Siperstein et al. [10]:  $SF_6$  and  $CH_4$  adsorbed on MFI. (B) The comparison between the isosteric heats of adsorption of pure components (3) (solid lines) and eq. (23) (dashed lines) with the analyzed experimental data reported by [7-10]. The presented results were shown in our previous studies [11].

Figure 2 shows the comparison between the theoretically calculated and experimentally determined adsorption phase diagrams and isosteric heats accompanying them. Besides the case of the isosteric heats of ( $CO_2+C_2H_6$ ) adsorption we can observe satisfactory agreement between the theoretically

calculated curves and the experimental data. In all cases the predicted isosteric heats of the components in the mixture are slightly overestimated.

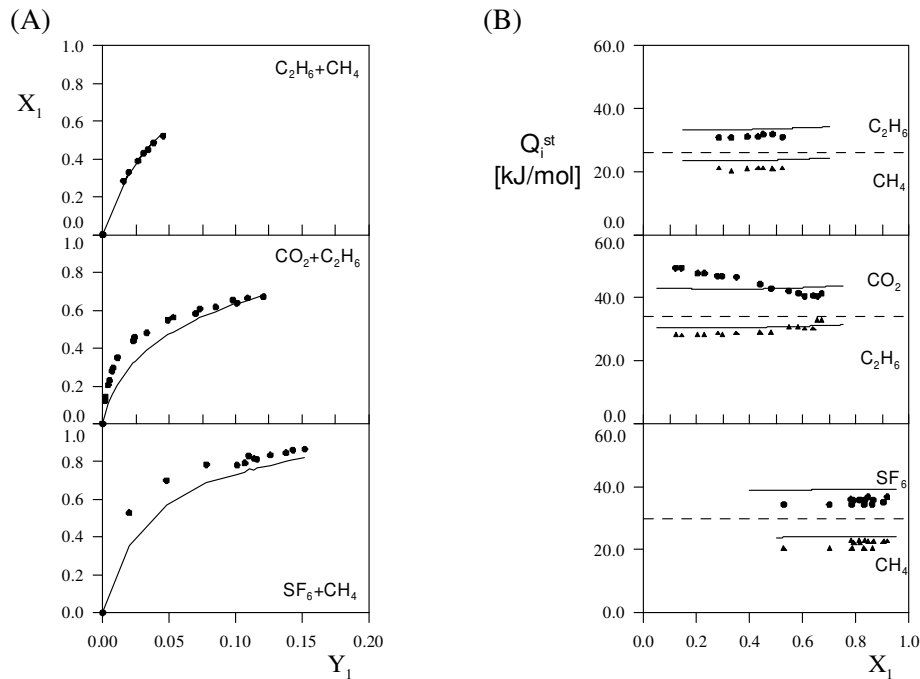


Fig. 3. (A) Adsorption from the: ( $\text{C}_2\text{H}_6+\text{CH}_4$ ), ( $\text{CO}_2+\text{C}_2\text{H}_6$ ) and ( $\text{SF}_6+\text{CH}_4$ ) gaseous mixtures reported by Dunne et al. [7-9] and Siperstein et al. [10]. Comparison with the experiment ( $\bullet$ ) of the X-Y composition phase diagrams calculated by applying eq. (4) (solid line). The theoretical, calculated points are hidden to raise clarity of the figure.  $Y_1$  is the mole fraction in the gas phase whereas  $X_1$  relates to the adsorbed phase. The theoretical phase diagrams were calculated with the assumption of infinite values of adsorption energies i.e.  $\Pi^m = 0$ . (B) Comparison of the individual theoretical isosteric heats of adsorption from the gaseous mixtures (marked in the figure) calculated by using eq. (14) [15]. Theoretical curves were calculated by using the parameters collected in Table 1. To separate the heat effects of components a thin slightly broken line divides the figures.

## 5. CONCLUSIONS

The results of this work demonstrate that the Vacancy Solution Theory, in general, provides a good quantitative description of the heat effects accompanying mixed-gas adsorption equilibria. Basing on the Vacancy Solution Theory we proposed relatively simple theoretical expression for the isosteric

heats in the mixed-gas adsorption system. By using some simplifications the theoretical adsorption phase diagrams and isosteric heats of a given mixture component reduce to simple mathematical expressions. The theoretical studies performed by us previously [11-13] when we studied other theories of mixed-gas adsorption equilibria (IE, IAS) indicate that the isosteric heat of adsorption in the mixed system always is the logarithmic function of the surface coverage.

Despite some drawbacks of the presented model, the unquestionable advantage is a simple form of equations.

## 5. REFERENCES

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## CURRICULUM VITAE



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