Propane–Propylene Binary Adsorption on Zeolite 4A

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Abstract. In this work we report new experimental data of pure and binary adsorption equilibrium of propane and propylene on zeolite 4A at 423 and 473 K. The pressure range studied was 0–500 kPa, which is the entire pressure range used in PSA–VSA (Pressure–Vacuum Swing Adsorption) units. The amount adsorbed of propane is much higher than that reported in previous literature. Propane diffusivity was estimated from uptake curves in the linear isotherm region. Adsorption of propane was extremely slow and equilibrium was established only after three days of adsorbate–adsorbent contact. The IAST (Ideal Adsorbed Solution Theory) using the Generalized Dubinin model to describe the pure propylene equilibrium and the Langmuir model for propane predicted with acceptable accuracy the binary adsorption data. Alternatively, the multisite model of Nitta was used to fit pure component isotherms and used in the IAST. Predictions were worse than those with the other strategy.

Introduction

The propane–propylene separation by distillation is the most energy consuming separation in petrochemical industry. Adsorption is a suitable alternative because the adsorbent can increase the separation factor several times diminishing cost demands. Many commercial adsorbents have been already tested but the selectivity to propylene was not good enough (Grande and Rodrigues, 2001; Grande et al., 2002; Ghosh et al., 1993). Chemical deposition of some transition metals, π-complexation adsorption, was also considered (Rege et al., 1998; Padin et al., 2000).

Adsorption equilibrium of propane and propylene on zeolite 4A has been previously reported in literature (Da Silva and Rodrigues, 1999; Rege et al., 1998; Järvelin and Fair, 1993). The loading capacity of both

gases in these works is similar and in all of them propane is adsorbed only in minor quantities. Zeolite 4A has already been tested as a possible adsorbent to separate propane/propylene by Pressure–Vacuum Swing Adsorption, PSA–VSA obtaining propylene purity of 96% (Ramachandran et al., 1994). The simulated results predicted higher purity. The discrepancy can be due to erroneous propane equilibrium or diffusivity parameters, or a combination of both.

In this paper we present pure and binary equilibrium data of propane and propylene at 423 and 473°K and 0–500 kPa measured by a manometric–chromatographic method. Following the adsorption uptakes in the lower pressures (linear isotherm) propane diffusivity was estimated. Pure propylene equilibrium was fitted with the Generalized Dubinin equation while propane equilibrium was fitted with the Langmuir model. Binary equilibrium was predicted with the IAST (Ideal Adsorbed Solution Theory) and predicted very well the experimental data. An alternative analysis using the multisite model (Nitta et al., 1984) for pure component

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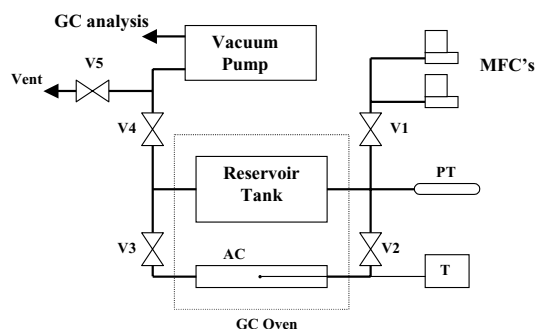†To whom correspondence should be addressed.

Figure 1. Experimental set-up of the manometric–chromatographic unit.

fitting and the IAST for binary predictions was performed.

Experimental

All the measurements were made in a manometric–chromatographic equipment operated in closed system. The pressure transducer used for total amount adsorbed measurements is Lucas Schaevitz 9000 series from 0 to 500 kPa, with an error of ± 0.04 kPa. The scheme of the equipment is shown in Fig. 1. The system was called manometric and not volumetric because the real variable measured is the pressure (Rouquerol et al., 1999). Propane–propylene composition was determined by FID (Flame Ionization Detector) in a Chrompack 9001 gas chromatograph with a 12 port Valco multivalve system collecting samples for later analysis. The capillary column is J&W Scientific (serial 4597223, USA) used at 353°K with 10 ml/min of nitrogen. The multivalve configuration is described elsewhere (Valco homepage). With the volume in the reference tank (retired with the vacuum pump to fill the loops for GC analysis) at least four chromatograms per equilibrium point were measured. We analyzed the molar fraction of each hydrocarbon in the gas phase and by a mass balance the adsorbed phase concentration of each compound was determined.

The activation of the samples was made in vacuum at 593°K for periods of 24 hours. For multicomponent adsorption, activation was carried out before each measurement. Note that in the experimental set-up there is no re-circulating pump. To determine the time required for a complete mixing of the gases, experiments without any adsorbent in the chamber at three different molar relations and three different

times (8, 16 and 24 hours) were performed. In all the cases, equilibration was completely ensured at 16 hours.

In all the binary experiments propylene was initially adsorbed alone and only after equilibrium was reached propane was injected to the system.

For all the experiments reported in this paper, we assume that the initial calibration procedure with helium is valid and that helium is not adsorbed on zeolite 4A at ambient temperature. The results of the calibration at higher temperatures (373, 423 and 473°K) are consistent with this assumption.

All gases used in this report were provided by Air Liquide: propane N35 and propylene N24 (purity greater than 99.95 and 99.4 respectively). Helium N50 was used for the calibration procedure. Zeolite 4A was kindly provided by CECA (France).

Pure Component Adsorption Equilibrium

The pure component adsorption equilibria can be described by numerous models (Yang, 1987). In this case we choose the generalized Dubinin equation (Jaroniec, 1997)

$$q = q_m \cdot \exp\left[-\left(\frac{RT \ln \frac{P^0}{P}}{E_o}\right)^d\right] \qquad (1)$$

where q_m is the maximum loading, E_o is the characteristic energy of adsorption, d is the third fitting constant of the equation and P^0 is the pressure of the saturated gas. The constant d was initially assumed as integer. Its physical meaning has been attributed to the number of degrees of freedom that the adsorbed molecules lost (Suzuki, 1990).

It has to be pointed out that the generalized Dubinin model is not thermodynamically correct, predicting a Henry slope of zero. This problem is presented by all the exponential isotherms (Jaroniec, 1984).

Binary Adsorption Equilibrium

The Ideal Adsorbed Solution Theory (IAST) is a traditional model used to describe multicomponent equilibria because is thermodynamically consistent and uses only pure-component adsorption parameters (Myers and Prausnitz, 1965). This theory states that the adsorbed phase constituted by N-components is ideal setting to unity the activity coefficients. This adsorbed phase is created mixing pure adsorbed gases at constant

surface potential. The mathematical framework of this theory is

$$\frac{\phi_i}{RT} = \int_0^{P_i^0} \frac{q_i}{P}\, dP \qquad (2)$$

$$\phi_i^0\big(P_i^0, T\big) = \phi(P, T, y_i) = \text{constant} \qquad (3)$$

$$x_i = \frac{P}{P_i^0} y_i \qquad (4)$$

$$\left(\frac{1}{q_t}\right) = \sum_i \frac{x_i}{q_i\big(P_i^0\big)} \qquad (5)$$

where ϕ_i is the surface potential, q_i is the amount adsorbed, q_t is the total amount adsorbed, P is the total pressure of the system, y_i and x_i are the gas and adsorbed molar fractions of component i, and P_i^0 is the pressure equilibrium of the pure component at the surface tension of the mixture.

Other advantage of this model is that it puts no restrictions on the description of pure component equilibrium. So different models can describe equilibrium of the different gases. This is important because a good description of pure component adsorption equilibrium (particularly at low pressures) is very important to predict well the multicomponent behavior (Richter et al., 1989).

Propane Diffusivity

The pressure signal was recorded in all the measurements till equilibrium was reached. Following the evolution of the amount adsorbed with time, the diffusivity coefficient can be estimated by means of the uptake curve. In the pressure range used for the measurements the adsorption of propane is in the linear zone (Henry law is valid). We assumed that the process is isothermal, that resistance in the micropores controls the diffusion process and that Fick's law is valid.

The following expression (Ruthven, 1984; Kärger and Ruthven, 1992) is the solution to the diffusion equation for spherical crystals and is valid for the assumptions mentioned above

$$\frac{q}{q_{eq}} = 1 - 6 \sum_{n=1}^{\infty} \frac{\exp\big(-D_c \alpha^2 t / r_c^2\big)}{9\Lambda/(1-\Lambda) + (1-\Lambda)\alpha^2} \qquad (6)$$

where q and q_{eq} are the adsorbed phase concentration varying with time and in equilibrium respectively,

D_c is the crystal diffusivity, r_c is the crystal radius and $\Lambda = (C_{ini} - C_{eq})/C_{ini}$ with C_{ini} being the initial concentration and C_{eq} the concentration of the gas phase when equilibrium is reached. Roots α_n are calculated by $\tan(\alpha_n) = 3\alpha/[3 + (1/\Lambda - 1)\alpha_n^2]$.

Multisite Langmuir and IAST

An alternative way to fit the pure component and binary data was evaluated using a thermodynamically correct model. The multisite Langmuir model for homogeneous adsorbents derived by Nitta using statistical thermodynamic arguments (Nitta et al., 1984) proved its consistency for treatment of binary equilibrium data. This model has also been capable to fit correctly data of paraffins in zeolite 5A (Silva and Rodrigues, 1999). A more general theory based on the mass-action law, where the Nitta model is a special case, has been recently proposed (Bhatia and Ding, 2001).

If we neglect adsorbate–adsorbate interactions, the model can be expressed as

$$\theta_i = K_i P (1 - \theta_i)^{ai} \qquad (7)$$

where $\theta_i = q_i/q_{mi}$ is the fractional amount of component i in the adsorbed phase, q_m is the saturation capacity of component i, P is the equilibrium pressure and a_i is the number of neighboring sites occupied by component i. The equilibrium constant K_i is described by an Arrhenius law of the form

$$K_i = K_i^0 \exp(-\Delta H/RT) \qquad (8)$$

where K_i^0 is the adsorption constant at the limit of $T \to \infty$. When the multisite model is used for the description of pure component adsorption and then introduced in the IAST for binary predictions (Eqs. (2–5)), the amount adsorbed of each component and the molar fractions can be calculated by a theoretical solution expressed by (Sircar, 1995)

$$\theta_1 = \frac{a_1 K_1 P y_1 \theta_1^0 \big(\theta_2^0\big)^2 \big(1 - \theta_1^0\big)^{a1}}{a_1 K_1 P y_1 \theta_1^0 \big(\theta_2^0\big)^2 \big(1 - \theta_1^0\big)^{a1} + a_2 K_2 P y_2 \theta_2^0 \big(\theta_1^0\big)^2 \big(1 - \theta_2^0\big)^{a2}} \qquad (9)$$

$$\theta_2 = \frac{a_2 K_2 P y_2 \theta_2^0 \big(\theta_1^0\big)^2 \big(1 - \theta_2^0\big)^{a2}}{a_1 K_1 P y_1 \theta_1^0 \big(\theta_2^0\big)^2 \big(1 - \theta_1^0\big)^{a1} + a_2 K_2 P y_2 \theta_2^0 \big(\theta_1^0\big)^2 \big(1 - \theta_2^0\big)^{a2}} \qquad (10)$$

$$a_2(a_1 - 1)\theta_1^0 + a_1 a_2 \ln\left(1 - \theta_1^0\right)$$
$$= a_1(a_2 - 1)\theta_2^0 + a_1 a_2 \ln\left(1 - \theta_2^0\right) \quad (11)$$

$$K_1 y_1 \frac{\left(1 - \theta_1^0\right)^{a1}}{\theta_1^0} + K_2 y_2 \frac{\left(1 - \theta_2^0\right)^{a2}}{\theta_2^0} = \frac{1}{P} \quad (12)$$

$$x_1 = \frac{a_2 \theta_1}{a_2 \theta_1 + a_1 \theta_2} \quad (13)$$

Results and Discussion

In previous reports, propane was reported as a weakly adsorbed gas on zeolite 4A having isotherms with small or no temperature dependence, ascribed to a small adsorption on the zeolite binder.

In Fig. 2 we present new data of adsorption equilibrium of propane at 423 and 473°K where we obtain higher concentrations of propane on the adsorbed phase indicating some hydrocarbon adsorption on the zeolite structure and not on the binder. No desorption data was measured. Equilibrium measurements were extremely slow taking three days per equilibrium point for the lower temperature (423°K) measurements and two days for each measurement at 473°K. Equilibrium was assumed when the pressure signal does not change after six hours. Some of the equilibrium points were duplicated to verify the consistency of the data. The amount adsorbed was more than 1 mol/kg at 423°K and 100 kPa.

The measurements after three hours of contact adsorbent/adsorbate are also shown in Fig. 2 (points not in equilibrium). The difference with the amount adsorbed in equilibrium is large and this set of data is in agreement with other published works (Järvelin and Fair, 1993; Da Silva and Rodrigues, 1999). Note that
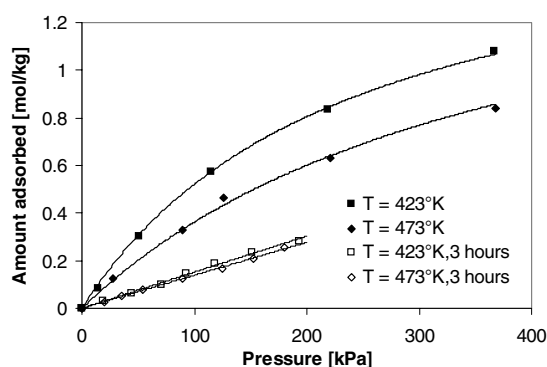
Table 1. Fitting parameters of the Dubinin model for propylene adsorption equilibrium and for Langmuir model for propane adsorption equilibrium on zeolite 4A.

C$_3$H$_6$–zeolite 4A		
q_m (mol/kg)	E_o (J/mol)	d
2.0779	21277	2.753

Propane equilibrium parameters: Langmuir model

C$_3$H$_8$–zeolite 4A		
q_m (mol/kg)	K^0 (mol/kg · kPa)	ΔH (J/mol)
1.7525	4.22×10^{-5}	16214.6

the dependence with temperature is weak, something that can be explained by a combination of equilibrium and kinetic effects.

When we consider the kinetic diameter of the propane molecule and the opening of the zeolite structure, we are assuming that the molecules as well as the zeolite channels are rigid (Xiao and Wei, 1992). With the equilibrium results shown in Fig. 2 is clear that propane pass through the zeolite channels, but we still do not known the mechanism of diffusion.

Data was fitted very well with the Langmuir model: $q = q_m KP/(1 + KP)$ where q_m is the maximum amount adsorbed and K is the equilibrium constant described by an Arrhenius expression like the one expressed by Eq. (8). The fitting parameters are listed in Table 1.

Propylene adsorption is shown in Fig. 3. An equilibrium isotherm was also measured in a lower temperature (373°K). This temperature was not used for propane measurements because the kinetics would
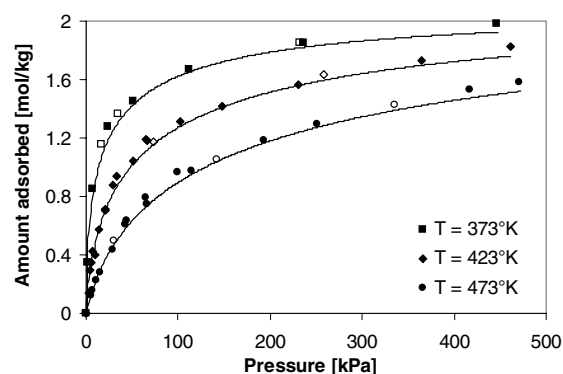
Figure 2. Adsorption equilibrium of propane on zeolite 4A CECA. Symbols: ■ $T = 423$°K, ♦ $T = 473$°K and solid lines–Langmuir model. Empty symbols are the loading measured after 3 hours.

Figure 3. Adsorption equilibrium of propylene on zeolite 4A CECA. Symbols: ■ $T = 373$°K, ♦ $T = 423$°K, ● $T = 473$°K and solid lines–Dubinin model. Empty symbols are desorption points.
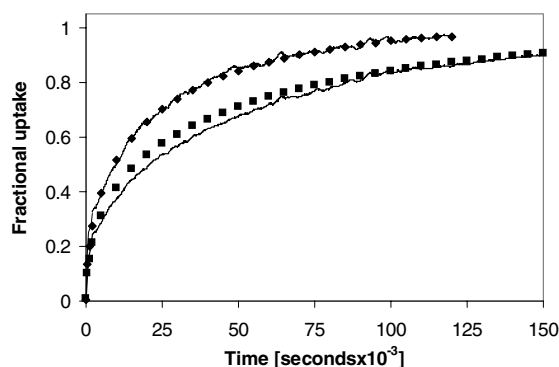
Figure 4. Fractional uptake curves of propane on zeolite 4A. Symbols: $\nu T = 423°$K and $\upsilon T = 473°$K.

Figure 5. x–y diagrams at $423°$K of propane–propylene equilibrium. Solid line—IAST with Dubinin (propylene) and Langmuir (propane) models and dashed line—IAST with Nitta model for both gases.

be extremely slow. In the lower pressure range (0–100 kPa), these data are in agreement with other published data (Järvelin and Fair, 1993; Da Silva and Rodrigues, 1999). These isotherms were fitted with the Generalized Dubinin equation with a good quality in all the pressure range. Equilibrium parameters for propylene are also detailed in Table 1. Langmuir and Toth models give poor fits in the high-pressure range.

For the low-pressure equilibrium points, the pressure decrease was monitored in all the equilibration time. Making a material balance the amount adsorbed at each moment can be calculated (Sircar, 2001) to obtain the uptake curves. The crystal diffusivity of propane was estimated from the fractional uptake curves by matching the experimental data to Eq. (6). The average crystal radius of the zeolite crystals is 1.9 μm determined by Scanning Electron Microscopy. The uptake curves at 423 and $473°$K used for kinetic measurements together with the fitting are plotted in Fig. 4. The crystal diffusivity is 2.7 and 5.5×10^{-18} m^2/s at 423 and $473°$K, respectively. This value is one order of magnitude different from other values previously reported of 1.7×10^{-17} m^2/s at $424°$K (Khodakov and Rees, 1995), although the activation energy of 23.7 kJ/mol is comparable with the 24.5 kJ/mol value also reported in that work. Similar discrepancies in diffusivity values with constancy in the activation energy were also reported for smaller molecules in this zeolite (Ruthven, 2001).

In Fig. 5 we plot the x–y (adsorbed vs. gas phase molar fractions) diagram for propane–propylene at $423°$K. The total pressure used for simulations was 100 kPa, although at the temperatures studied, total pressure has only a slight influence in the x–y diagram (solid lines). The experimental points are also plotted in this diagram and confirm the predictions. Complete information of
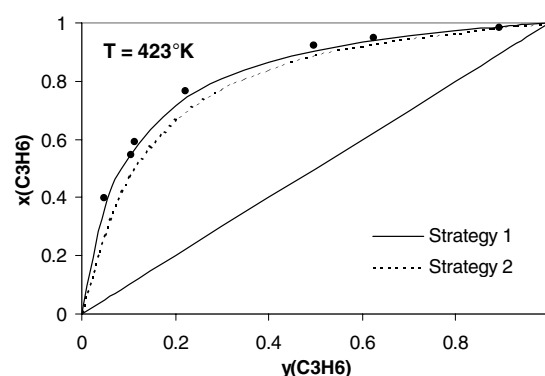
the binary results is detailed in Table 2 for data storage. Note that the total pressure of the points is scatter and in all the cases the IAST (when used with the Dubinin model for propylene and Langmuir model for propane) predicts very well the data. This indicates that the binary mixture in the conditions studied behaves like an ideal mixture. The corresponding data and predictions for $473°$K are plotted in Fig. 6 (experimental information is listed also in Table 2). The prediction of the theory is very good and the mixture is also ideal in these P-T conditions.

Table 2. Propane–propylene binary adsorption equilibrium at 423 and $473°$K.

| P (kPa)	y	x	q_t (mol/kg)	q_{sim} (mol/kg)
		$T = 423°$K		
84.61	0.050	0.399	0.5731	0.5910
37.97	0.106	0.545	0.4503	0.4278
104.15	0.114	0.590	0.8192	0.7829
145.42	0.224	0.766	1.0924	1.0477
107.45	0.496	0.923	1.1420	1.1385
99.51	0.624	0.946	1.1657	1.1771
98.41	0.895	0.971	1.2716	1.2633
		$T = 473°$K		
102.93	0.062	0.284	0.4595	0.4358
90.84	0.117	0.403	0.4983	0.4455
94.26	0.282	0.661	0.5989	0.5780
99.39	0.414	0.789	0.6769	0.6747
106.35	0.589	0.906	0.8098	0.7864
118.99	0.957	0.993	0.9515	0.9691
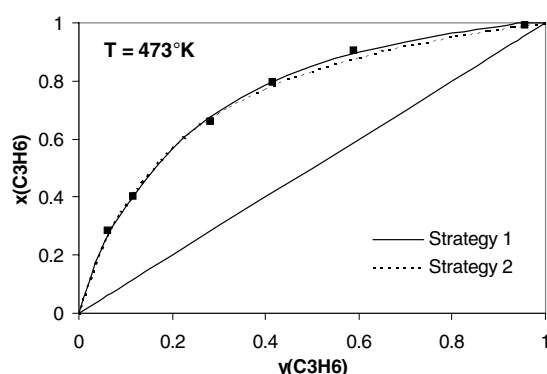
Figure 6.   x–y diagrams at 473°K of propane–propylene equilibrium. Solid line—IAST with Dubinin (propylene) and Langmuir (propane) models and dashed line—IAST with Nitta model for both gases.
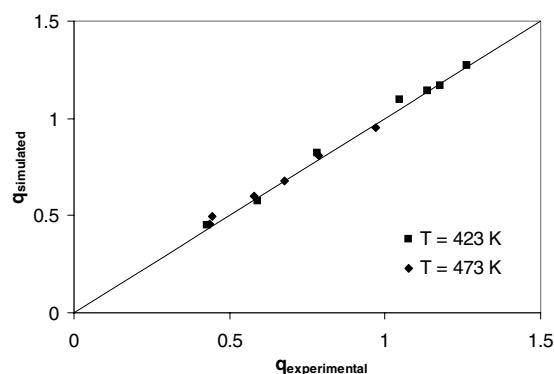

Figure 7.   Comparison of the experimental total amount adsorbed with the predicted by IAST with Dubinin (propylene) and Langmuir (propane) models.

As the total pressure in all the points is different, a plot of the adsorbed phase concentrations vs. the molar fractions is not possible to build, but the total adsorbed phase concentration predicted with the IAST is plotted against the experimental values in Fig. 7. Also, because of the non-isobaric nature of the data and the small number of points, the integral consistency test (Myers and Sircar, 1972) could not be performed. Although, the interception rule is obeyed at large propylene molar fractions (Valenzuela and Myers, 1989).

A second analysis was performed using the Nitta model to fit pure component adsorption and use in the IAST model. The multisite model is thermodynamically consistent model and fits well the data of propane and propylene. Propylene fitting can be observed in Fig. 8. The fitting of propane is the same as with the Langmuir model because the Nitta model is Langmuir reducible. The parameters are detailed in Table 3. The

Table 3.   Fitting parameters of the multisite Langmuir model of Nitta for propane and propylene adsorption equilibrium at 373, 423 and 473°K.

Gas	q_{mi} (mol/kg)	a_i (–)	K_i (373°K) (kPa^{-1})	K_i (423°K) (kPa^{-1})	K_i (473°K) (kPa^{-1})
C_3H_6	2.600	2.612	0.0714	0.0288	0.0103
C_3H_8	3.103	2.189	–	0.0024	0.0015
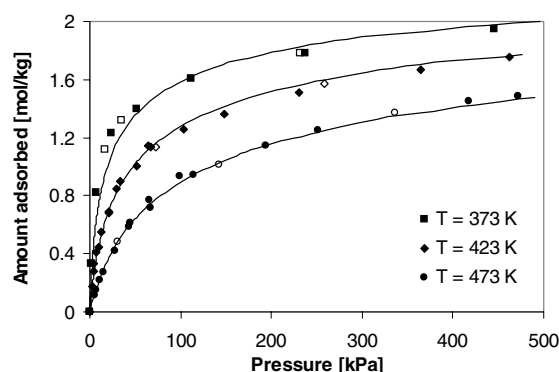
Figure 8.   Adsorption equilibrium of propylene on zeolite 4A CECA. Symbols: ■ $T = 373°K$, ♦ $T = 423°K$, ● $T = 473°K$ and solid lines–Nitta model.

saturation capacity of propane is imposed by the thermodynamic constraint $a_i q_{mi} =$ constant (Sircar, 1995). Relating the temperature dependence of the equilibrium constants by Eq. (8), the isosteric heat of both gases can be obtained. The values for propane and propylene are 15.5 and 28.2 kJ/mol. The values are constant with loading because we assume that the adsorbent is homogeneous by fitting the data with this model. Propylene value is little smaller than in other reports where was around 30 kJ/mol (Da Silva and Rodrigues, 1999).

We analyze the low-pressure range fitting of propylene in the Virial domain (Talu, 1998). This was made by plotting the isothermal data in the form $\ln(P/q)$ vs. q. We can see that in the low-pressure range the fitting is not very good. The Virial domain is plotted in Fig. 9. The solid line represents the Dubinin model and the dotted line the multisite model. The multisite model shows a good fitting at 473°K, a small deviation at 423°K and a large deviation at 373°K. The effect of these small deviations is shown in the dotted lines in Figs. 5 and 6.

The virial isotherm expressed as:

$$H = \frac{q}{P} \exp\left(2A_1q + \frac{3}{2}A_2q^2 + \frac{4}{3}A_3q^3 + \cdots\right) \quad (14)$$

Table 4. Fitting parameters of the Virial model for propylene adsorption equilibrium at 373, 423 and 473°K.

Temperature (°K)	H (mmol/g · kPa)	A_1 (g/mmol)	A_2 (g/mmol)^2
373	0.453	0.428	0.498
423	0.089	0.450	0.300
473	0.027	0.475	0.160
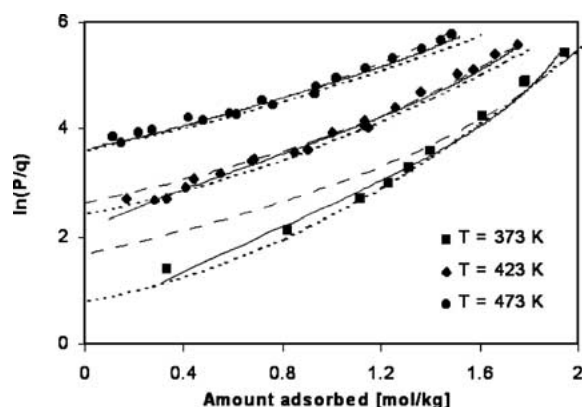
Figure 9. Virial domain plot of propylene adsorption equilibrium. Symbols: ■ $T = 373$°K, ♦ $T = 423$°K, ● $T = 473$°K, solid lines—Dubinin model, dashed lines—Nitta model and dotted lines—Virial model.

was also used to fit the propane and propylene equilibrium. The parameters of this fitting are shown in Table 4 and the propylene results are shown in Fig. 9. The Henry constant, H, followed exponential temperature dependence while and linear dependence was observed by the virial coefficients A_i. This model was not used for multicomponent prediction because it has six parameters to describe equilibrium as a function of pressure and temperature while the Dubinin and Nitta models have three and four parameters, respectively.

The zeolite sample was the same for all the experiments reported in this work. Near 3 grams of adsorbent were used. After three months of continuous exposition of propylene at high temperatures and pressures, the initial pure propylene experiment was completely reproducible indicating that no coke was formed.

Conclusions

Propane and propylene adsorption equilibrium was measured at 373, 423 and 473°K in the 0–500 kPa pressure range. Propane adsorption is much higher than in previous reports and is 1 mmol/g at 423°K and 100 kPa.

Propane can penetrate the zeolite cages but only after three days of contact equilibrium is reached. The diffusivity of propane estimated from the uptake curves is 2.7 and 5.5×10^{-18} m^2/s at 423 and 473°K, respectively. The energy of activation is 23.7 kJ/mol. The small value of the diffusivity together with a non-linear isotherm can affect seriously the PSA behavior by inherent difficulties of propane desorption.

The binary mixture adsorption equilibrium was measured at 423 and 473°K and the Ideal Adsorbed Solution Theory (IAST) predicts well the data when the Dubinin model is used for propylene and the Langmuir model for propane. When the Nitta model is used for the fitting of both pure gases the pure component fitting at lower pressures is poor at 423°K and this affect the binary predictions.

Binary data indicates that the mixture adsorption behaves as an ideal solution, at least in the pressure and temperature ranges studied.

Appendix

$T = 373$°K		$T = 423$°K		$T = 473$°K	
P (kPa)	q (mmol/g)	P (kPa)	q (mmol/g)	P (kPa)	q (mmol/g)
Propylene adsorption on zeolite 4A					
0.00	0.000	0.000	0.000	0.00	0.000
1.34	0.347	2.56	0.178	5.49	0.122
6.84	0.852	4.15	0.294	6.35	0.154
16.67	1.158	7.45	0.427	10.99	0.225
24.10	1.279	4.88	0.345	14.77	0.283
34.80	1.367	9.52	0.459	28.50	0.438
51.28	1.456	13.19	0.571	30.65	0.496
112.21	1.673	20.27	0.704	43.35	0.612
231.38	1.850	21.12	0.716	44.20	0.637
236.87	1.855	29.67	0.882	65.32	0.795
446.03	1.943	33.21	0.938	66.91	0.748
		51.16	1.044	98.90	0.968
		64.50	1.193	115.00	0.976
		66.34	1.180	142.49	1.056
		73.02	1.177	194.02	1.185
		102.69	1.310	251.53	1.296
		148.00	1.416	335.90	1.424
		230.40	1.569	417.70	1.527
		258.49	1.635	471.43	1.585
		364.22	1.729		
		461.90	1.824		
Propane adsorption on zeolite 4A					
		0.00	0.000	0.00	0.000
		14.41	0.085	27.25	0.124
		50.31	0.302	89.50	0.330
		114.41	0.576	126.37	0.465
		219.06	0.834	220.77	0.629
		366.39	1.080	367.89	0.842

Nomenclature

a_i	Number of neighboring sites occupied by component i
C_{ini}	Initial concentration of gas (mol/m^3)
C_{eq}	Concentration of gas when equilibrium is reached (mol/m^3)
d	Parameter of the generalized Dubinin model
D_c	Crystal diffusivity (m^2/s)
E_o	Characteristic adsorption energy (J/mol)
K_i	Equilibrium constant of component i (kPa^{-1})
K_i^0	Equilibrium constant of component i at the limit $T \to \infty$ (kPa^{-1})
P	Pressure (kPa)
P^0	Pressure of the saturated gas (kPa)
P_i^0	Equilibrium pressure of pure component i at the surface tension of the mixture (kPa)
q_i	Adsorbed phase concentration of component i (mol/kg)
q_m	Maximum adsorbed phase concentration (mol/kg)
q_{eq}	Equilibrium adsorbed phase concentration (mol/kg)
r_c	Crystal radius (m)
T	Temperature ($^\circ$K)
x_i	Adsorbed molar fraction of component i
y_i	Gas molar fraction of component i

Greek Letters

α_n	Roots of auxiliary equation for diffusivity calculations
θ_i	Fractional coverage of component i on the adsorbed phase
$-\Delta H$	Isosteric heat of adsorption (J/mol)
Λ	Concentration variation parameter
ϕ_i	Surface potential of component i

Acknowledgments

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