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Equilibrium adsorption analysis of microporous adsorbents in propene/propane binary mixture separation

Hafez Maghsoudi[1,2]

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Abstract Diverse adsorbents including zeolites and MOFs have different capacities with various ideal selectivities for propene/propane separation. Among them, a comprehensive comparison should be made to find the more appropriate adsorbent for a desired process. In this paper, ideal adsorption solution theory (IAST) is utilized to compare binary gas adsorption performances (equilibrium selectivities and capacities) of all adsorbents. IAST model is accomplished at different gas compositions (0.1–0.9 propene mole fractions) and pressures (1–100 kPa). The results revealed that zeolites (i.e. DDR and ITQ-32) and MOFs (CuBTC or Mg-MOF-74) have higher equilibrium adsorption selectivities and capacities, respectively. Among them, DDR has the highest selectivity (1037 at 100 kPa and 418 K for a 50/50 mixture) while CuBTC has the highest capacity ($\approx$8.1 mmol/g at 100 kPa and 298 K for a 50/50 mixture). DDR selectivity is almost 100 times higher than that of CuBTC or Mg-MOF-74 while its adsorption capacity is lower than them by a factor of about 10. Finally, investigation shows that Mg-MOF-74 and CuBTC are appropriate for a process in which the adsorption capacity is more concerned. On the other hand, DDR and ITQ-32 zeolites are suitable for membrane applications where the adsorption selectivity is much more important than capacity.

Keywords Adsorption · Olefin · Ideal adsorption solution theory (IAST) · Zeolite · Metal–organic framework (MOF)

List of symbols

A	Adsorption surface (m^2)
b	Affinity parameter of Langmuir, Toth and Sips isotherms (kPa^{-1})
n	Heterogeneity parameter in Sips isotherm (–)
p	Pressure (kPa)
p^0	Hypothetical pressure of the pure component (kPa^{-1})
q^{sat}	Saturation adsorption capacity of adsorbent ($mmol\ g^{-1}$)
q	Amount adsorbed ($mmol\ g^{-1}$)
R_g	Universal gas constant ($J\ K^{-1}\ mol^{-1}$)
T	Temperature (K)
t	Heterogeneity parameter in Toth isotherm (–)
x	Mole fraction of a pure component at the adsorbed phase (–)
y	Mole fraction of a pure component at the gas phase (–)
z	Reduced spreading pressure ($mol\ cm^{-3}$)
π	Spreading pressure ($J\ m^{-3}$)

1 Introduction

Propene/propane gas separation is of vital importance in the petrochemical complexes to produce high purity propene with chemical (Purity > 95 mol %) and polymer grades (Purity > 99.5 mol %) (Agarwal et al. 2010; Da Silva and Rodrigues 1999; Grande et al. 2006). Energy intensive cryogenic distillation process using large number of trays is

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✉ Hafez Maghsoudi
hmaghsoudi@sut.ac.ir

[1] Chemical Engineering Department, Sahand University of Technology, P.O. Box: 51335-1996, Tabriz, Iran

[2] Nanostructure Materials Research Center (NMRC), Sahand University of Technology, P.O. Box 51335-1996, Tabriz, Iran

the common method for separation of light olefin/paraffin as their relative volatility lies between 1.0 and 1.1 at temperatures of 244–327 K and total pressures of 1.7–22 bar (Da Silva and Rodrigues 1999). For instance, ethene/ethane separation is achieved at about—25 °C and 320 psig (2.306 MPa) within a column with more than 100 trays, and propene/propane distillation column works at −30 °C and 30 psig (0.308 MPa)(Rege et al. 1998; Keller et al. 1992).

The increasing demand for propene based polymers confirms the need for an energy efficient process for propene/propane separation. Thus, development of alternatives based on adsorption, absorption and reactive distillation (Safarik and Eldridge 1998; Azizi et al. 2015), membrane separation (Faiz and Li 2012; Nymeijer et al. 2004b, 2004a; Kim et al. 2000; Huang et al. 2008; Feiring et al. 2015) and membrane-distillation hybrid processes (Xu et al. 2012) has been proposed. Among the potential alternatives, hybrid methods combining common distillation and adsorption processes have been proposed as an effective method (Kumar et al. 1992; Eldridge 1993; Ghosh et al. 1993).

The successful adsorption process can be achieved when a highly selective adsorbent based on equilibrium or kinetic separation is found. Recently, designing of highly selective microporous adsorbents (metal organic frameworks (MOFs) and zoelites) made progress in the development of adsorptive separation process for light olefin separation.

In the open literature, various zeolites including 4A (Da Silva and Rodrigues 1999; Granato et al. 2007a; Grande et al. 2006, 2003; Jarvelin and Fair 1993; Padin et al. 2000; Rege et al. 1998; Ruthven and Loughlin 1972; Ruthven and Reyes 2007), 5A (Derrah et al. 1972; Grande et al. 2002; Jarvelin and Fair 1993; Ruthven and Loughlin 1972; Ruthven and Reyes 2007; Shah and Ruthven 1977), 13X (Calleja et al. 1994; Campo et al. 2013; Costa et al. 1991; Da Silva and Rodrigues 1999; Dzhigit et al. 1979; Granato et al. 2010, 2007b; Grande et al. 2010; Jarvelin and Fair 1993; Lamia et al. 2007; Narin et al. 2014; Ruthven and Reyes 2007; Silva and Rodrigues 2001), DDR (Gascon et al. 2008; Krishna and van Baten 2006; Ruthven and Reyes 2007; Ter Horst et al. 2002; Vidoni 2011; Zhu et al. 1999; 2000), Si–CHA (Combariza et al. 2009; Krishna and van Baten 2006; Olson 2002; Olson et al. 2004; Ruthven and Reyes 2007; Strohmaier et al. 2003), ITQ-3 (First et al. 2011; Olson 2002; Olson et al. 2004), ITQ-12 (Gutiérrez-Sevillano et al. 2010), ITQ-32 (Palomino et al. 2007), SAPO-34 (Agarwal et al. 2010), and MOFs including Ni-MOF-74 (Chen et al. 2014), Mg-MOF-74 (Bao et al. 2011), Co-MOF-74 (Bae et al. 2012) and CuBTC (Lamia et al. 2009; Ferreira et al. 2011; Plaza et al. 2012a, b) have been utilized for olefin/paraffin separations. These adsorbents showed different adsorption capacities with various ideal selectivities. However, a comparison should be made between all the adsorbents to find the appropriate adsorbent for a desired process. Therefore, binary gas adsorption performances of all adsorbents must be compared. In the literature, binary equilibrium adsorption of propene/propane are experimentally studied for zeolites 4A (Grande et al. 2003) and 13X (Costa et al. 1991; Calleja et al. 1994). But, for the majority of the adsorbents, only single gas isotherms are reported. However, using dynamic/breakthrough experiments, the performances of some adsorbents including 13X (Silva and Rodrigues 2001; Grande et al. 2010; Campo et al. 2013; Jarvelin and Fair 1993), DDR (Gascon et al. 2008), Co-MOF-74 (Bae et al. 2012), ZIF-8 (Böhme et al. 2013), and Ni-MOF-74 (Chen et al. 2014) are investigated for binary propene/propane mixtures.

The main objective of this paper is to compare all adsorbents (MOFs and zeolites) with respect to their equilibrium adsorption selectivities and capacities in propene/propane separation. To do this issue, binary equilibrium adsorptions are obtained by ideal adsorption solution theory (IAST) at different gas compositions (0.1–0.9 propene mole fractions) and pressures (1–100 kPa).

1.1 Theory and modeling

The IAST of Myers and Prausnitz (1965) is a model applied to predict multicomponent equilibria using only pure-component adsorption isotherms. This theory assumes that the adsorbed phase consisting of N-components is ideal [no interactions in the binary systems (Ruthven 2008)]. Thus, all activity coefficients are set to unity. The main benefit of the IAST is its capability to calculate multicomponent adsorption equilibria based on the experimental data of the single-component adsorption (Alexander and Erling 2002).

The mathematical description of this theory is as follows:

$$z = \frac{A\pi}{R_g T} = \int_0^{p_i^0} \frac{q_i}{p} dp \tag{1}$$

$$x_i = \frac{p}{p_i^0} y_i \tag{2}$$

$$\frac{1}{q_t} = \sum \frac{x_i}{q_i^0} \tag{3}$$

where, A is adsorption surface, π is spreading pressure, z is reduced spreading pressure, p_i^0 is the hypothetical pressure of the pure component “i” that gives the same spreading pressure on the surface, p is the total pressure, q_i is the amount of pure component “i” adsorbed which may be presented by the isotherm, x_i is the mole fraction of pure component “i” at the adsorbed phase, y_i is the mole fraction of pure component “i” at the gas phase, q_t is the total amount adsorbed and q_i^0 is the amount of pure component “i” adsorbed at p_i^0.

Table 1 Parameters of propane adsorption isotherms on adsorbents

Zeolite	Temperature (K)	Saturation adsorption capacity (mmol/g)		Affinity parameter (kPa^{-1})		Heterogeneity parameter (–)		Isotherm	Ref.
		q_1^{sat}	q_2^{sat}	b_1	b_2	n_1 (or t)	n_2		
4A	298	1.7525	–	0.029348	–	1	–	Langmuir	(Grande et al. 2003)
	298	0.226	–	0.09770	–	1	–	Langmuir	(Jarvelin and Fair 1993)
5A	298	1.919	–	1.00223	–	1	–	Langmuir	(Jarvelin and Fair 1993)
13X	293	2.1850	–	0.0934	–	1	–	Langmuir	(Costa et al. 1991)
	308	2.1578	–	0.0496	–	1	–	Langmuir	(Costa et al. 1991)
	298	2.2958	–	0.68507	–	0.7662	–	Toth	This work[a]
	293	2.185	–	0.70056	–	1	–	Langmuir	(Calleja et al. 1994)
	298	2.20	–	0.7348	–	0.892	–	Toth	(Lamia et al. 2007)
ITQ-3	353	1.46	–	0.01091	–	1	–	Langmuir	This work
ITQ-12	300	0.973	–	0.01549	–	1.710	–	Toth	This work
ITQ-32	298	1.222	–	0.02165	–	0.4879	–	Toth	This work
	333	0.736	–	0.2595	–	1	–	Langmuir	This work
Si-CHA	353	3.0561	–	19.27e-4	–	1	–	Langmuir	This work
DDR	318	0.78	0.02897	0.0717	4.38	1	1	Dual-site Langmuir	This work
SAPO-34	303	3.12	–	0.00277	–	1.1050	–	Sips	(Agarwal et al. 2010)
Ni-MOF-74	298	4.0	–	0.8762	–	1	–	Langmuir	(Chen et al. 2014)
Mg-MOF-74	298	6.67	1.8	0.3252	0.00243	0.8	1.44	Dual-site Sips	(Bao et al. 2011)
	318	6.67	1.8	0.14	0.00054	0.8	1.44		
CuBTC	298	6.21	1.14	0.1716	0.46427	0.82	0.32	Dual-site Sips	(Lamia et al. 2009)
	318	6.21	1.14	0.0828	0.19536	0.82	0.32		

[a] The experimental data of Jarvelin and Fair (1993) were extracted and well fitted with Toth model

To find p_i^0, an initial guess for reduced spreading pressure (z) is estimated according to Eq. 4

$$z = \frac{A\pi}{R_g T} = \sum y_i \int_0^p \frac{q_i}{p} dp \tag{4}$$

Using Eq. 1 and the initial guess of reduced spreading pressure, p_i^0 can be determined either analytically or numerically depending on the isotherm types used to describe the pure component equilibria. This value of p_i^0 is an initial guess which must be used to find the exact value from nonlinear equation (Eq. 5)

$$\sum x_i - 1 = \sum \frac{p}{p_i^0} y_i - 1 = 0 \tag{5}$$

While the exact value is obtained, corrected value of reduced spreading pressure can be obtained from Eq. 1. This trial and error procedure is continued to find all converged values of z and p_i^0. Then, Eqs. 1 and 2 are utilized to obtain the mole fractions at adsobed phase and total amount adsobed, respectively.

In this paper, a C^{++} code was devepoled to perform all computations. In that program, integration (Eq. 1) was computed numerically and all nonlinear equations were solved by Newton–Ralphson method.

2 Isotherms data

For binary adsorption calculations, single component adsorption isotherms should be known. In this regard, equilibrium adsorption isotherms of propane and propene on different zeolites and MOFs have been reported in the open literature. They have been measured at different temperatures usually fitted by Langmuir (Eq. 6), Toth (Eq. 7) and Sips (Eq. 8) isotherms in the form of one or dual-site models.

$$q = q_1^{sat} \frac{b_1 p}{1 + b_1 p} + q_2^{sat} \frac{b_2 p}{1 + b_2 p} \tag{6}$$

$$q = q^{sat} \frac{bp}{\left(1 + (bp)^t\right)^{1/t}} \tag{7}$$

$$q = q_1^{sat} \frac{(b_1 p)^{1/n_1}}{1 + (b_1 p)^{1/n_1}} + q_2^{sat} \frac{(b_2 p)^{1/n_2}}{1 + (b_2 p)^{1/n_2}} \tag{8}$$

Table 2 Parameters of propene adsorption isotherms on adsorbents

Zeolite	Temperature (K)	Saturation adsorption capacity (mmol/g)		Affinity parameter (kPa^{-1})		Heterogeneity parameter (−)		Isotherm	Ref.
		q_1^{sat}	q_2^{sat}	b_1	b_2	n_1 (or t)	n_2		
4A	298	2.092	–	0.95096	–	1	–	Langmuir	(Jarvelin and Fair 1993
5A	298	2.436	–	1.4726	–	1	–	Langmuir	(Jarvelin and Fair 1993)
13X	293	2.2855	–	1.3205	–	1	–	Langmuir	(Costa et al. 1991)
	308	2.3083	–	0.4626	–	1	–	Langmuir	(Costa et al. 1991)
	298	2.7563	–	8.0618	–	0.5627	–	Toth	This work
	293	2.2855	–	9.90456	–	1	–	Langmuir	(Calleja et al. 1994)
	298	2.59	–	6.7647	–	0.658	–	Toth	(Lamia et al. 2007)
ITQ-3	353	1.460	–	0.03338	–	1	–	Langmuir	(Olson et al. 2004)
ITQ-12	300	1.2887	–	0.1290	–	1.997	–	Toth	This work
ITQ-32	298	1.222	–	0.94537	–	0.8866	–	Toth	This work
	333	1.1482	–	0.2900	–	1	–	Langmuir	
Si-CHA	353	3.0561	–	0.02745	–	1	–	Langmuir	(Olson et al. 2004)
DDR	318	0.781	1.790	1.181	0.00394	1	1	Dual-site Langmuir	(Gascon et al. 2008)
SAPO-34	303	2.25	–	0.1966	–	2.9586	–	Sips	(Agarwal et al. 2010)
Ni-MOF-74	298	4.85	–	3.1087	–	1.667	–	Sips	(Chen et al. 2014)
Mg-MOF-74	298	6.38	2.86	4.3093	0.02770	0.82	1.31	Dual-site Sips	(Bao et al. 2011)
	318	6.38	2.86	1.04	0.013	0.82	1.31	Dual-site Sips	
CuBTC	298	7.09	1.22	1.5550	0.2605	1	0.8	Dual-site Sips	(Lamia et al. 2009)
	298	7.09	1.22	0.5368	0.0790	1	0.8	Dual-site Sips	

where, q in the amount adsorbed, b is the affinity parameter and n or t is the heterogeneity parameter.

The values of the parameters were taken from the literature and reported in Tables 1 and 2 for propane and propene, respectively. In those tables, zeolites 4A, 5A and 13X are commercial adsorbent in shaped form obtained from Union Carbide or CECA while the other sorbents are in form of powder synthesized in the laboratory. More detailed information about those commercial zeolites is presented in Table 3.

At some cases, different researchers have reported dissimilar and even conflicting isotherm data (i.e. 13X and 4A zeolite) and for some other zeolites, isotherms of propane have not been reported yet (i.e. ITQ-3 and Si-CHA).

The success of IAST depends strongly on how well the pure component data are fitted. An error in the isotherm parameters can cause a large error in the multicomponent computations (Do 1998). Thus, in the first step, a reasonable and accurate isotherm data should be selected or estimated. For zeolite 4A, Grande et al. (2003) reported Langmuir fitted isotherm of propane which is not in agreement with the data obtained by Jarvelin and Fair (1993). They reported the propane isotherm much less than the amount measured by Grande et al. On the other hand, Granato et al. (2007a) utilized molecular simulations to calculate the pure and binary adsorption equilibria of propane and propylene over 4A zeolite. Their simulation results are in good agreement with the data of Grande et al. (2003). So, comparison of the data reveals that the data of Jarvelin and Fair (1993) was probably taken in non-equilibrium conditions because of the kinetic nature of propane adsorption on 4A.

Propane equilibrium adsorptions on Si-CHA and ITQ-3 zeolites have not been reported yet. The only data is the uptake rate measurement of propane at 80 °C and 600 torr which is available from the work of Olson et al. (2004). It means that, even with the assumption of equilibrium at the end of the uptake rate experiments, only one point of equilibrium adsorption does exist, at 80 °C and 600 torr. This one point is not adequate for obtaining the isotherm model. Thus, only Langmuir affinity parameter (b) can be taken if the saturation adsorption capacity of propane is known. In this regard, as the saturation adsorption capacity of propene is known and also propene and propane liquid densities at high pressures are almost the same, saturation adsorption capacity of propane is assumed to have the same value that reported for propene. Therefore, the values presented in Table 1 for Si-CHA and ITQ-3 zeolite are estimated on the base of the above assumptions.

Table 3 Specifications of commercial zeolites utilized for propene/propane adsorption

Zeolite	Supplier	Form	Binder content	Ref.
4A	Union Carbide	Extrudate	Not reported	(Jarvelin and Fair 1993)
	CECA	Extrudate	Not reported	(Grande et al. 2003)
5A	Union Carbide	Extrudate	Not reported	(Jarvelin and Fair 1993)
13X	Union Carbide	Cylindrical Extrudate	20 %	(Costa et al. 1991)
	Union Carbide	Extrudate	Not reported	(Jarvelin and Fair 1993)
	Union Carbide	Cylindrical Extrudate	20 %	(Calleja et al. 1994)
	CECA	Extrudate	Not reported	(Lamia et al. 2007)

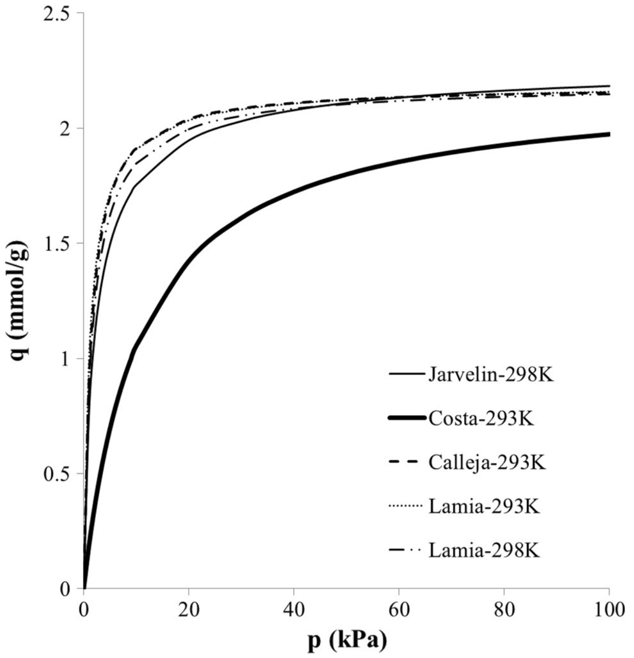


Fig. 1 Propane adsorption isotherms on 13X reported in the literature

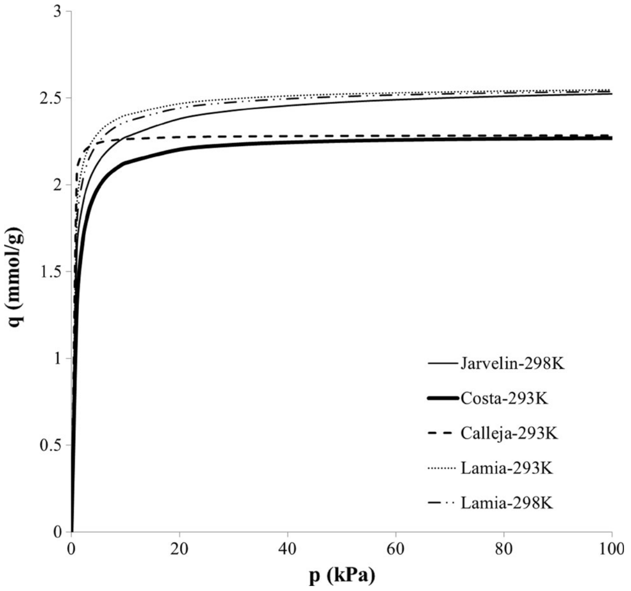


Fig. 2 Propene adsorption isotherms on 13X reported in the literature

According to Table 3, all 13X zeolites are commercial adsorbents having some extent of binder. In some references, the amount of the binder has not been reported. But, from the literature data and the published patents, it seems that both Union Carbide and CECA use 20 % binder in the fabrication of extruded zeolite adsorbents (Plee and Methivier 2008; Bouvier et al. 2011; Plee et al. 1922). Thus, it can be assumed that all mentioned commercial adsorbents have nearly the same content of binders.

For commercial zeolite 13X, more conflicting isotherm data have been reported in the literature so that it needs much more critical investigation on them. For this purpose, equilibrium isotherms of propane and propene on 13X zeolites are calculated and plotted (Figs. 1, 2) based the isotherm models reported in the literature.

Figure 1 shows that the propane adsorption isotherms proposed by the work of Costa et al. (1991) are not in agreement with the other works. Thus, for propane adsorption, the works of Jarvelin and Fair (1993), Calleja et al. (1994) and Lamia et al. (2009) are in good agreements and confirm each other. The lower adsorption isotherm of Costa et al. is reasonable if the utilized zeolite adsorbent has higher binder content than the others. But, according to Table 3, the commercial adsorbents utilized in the works of Costa et al. and Calleja et al. are the same while different results have been obtained.

Considering propene adsorptions in Fig. 2, reveals that the work of Calleja et al. (1994) is not supported by the other works. Calleja et al. (1994) reported parameters of Langmuir isotherm for propene which is not in agreement with their own experimental results. They obtained saturation adsorption capacity of 2.2855 mmol/g for Langmuir which is lower than their experimental (2.473 mmol/g at 538.4 torr). This means that their experimental are not well fitted with the isotherms parameters. Thus, only Jarvelin and Fair (1993) and Lamia et al. (2009) are utilized in this paper.

Experimental adsorption data for ITQ-12, ITQ-32 and DDR are extracted from the works of Gutiérrez et al. (2010), Palomino et al. (2007) and Gascon et al. (2008), respectively, and then fitted with an appropriate model.

3 Results and discussion

Binary equilibrium adsorption of a mixture of propane and propene with different gas phase compositions are obtained using IAST model. In the first step, the effect of binary mixture composition on the equilibrium adsorption selectivity is investigated. In this regard, all calculations are made at 100 kPa and the temperatures that the isotherms are reported. The results are plotted in Figs. 3 and 4 against propene mole fractions in the gas phase for adsorbents having selectivity below and above 20, respectively. These figures show that all adsorbents except SAPO-34 zeolite have higher selectivities at higher pressures. Thus, the higher the gas phase mole fraction the higher selectivity that can be achieved. Figure 3 reveals that the adsorbents with selectivities less than 20 are in the following order: Si-CHA > 13X > Mg-MOF-74 > Ni-MOF-74 > CuBTC > 5A > ITQ-3. According to Fig. 4 (i.e. 13X and Mg-MOF-74), usually the selectivity decreases with increase in temperature. Therefore, it should be noted that the selectivity of ITQ-3 at 298 K may be higher than the others like 5A and CuBTC. Additionally, Si-CHA and ITQ-3 selectivities don't change with the variation of propene mole fraction. This may be attributed to the procedure described before for estimation of Langmuir isotherm parameters; i.e. only one equilibrium point exists in the literature. Figure 4 obviously shows the supreme capability of DDR zeolite to separate propene from propane because it has a very high equilibrium selectivity, i.e. higher than 1000. However, IAST modeling of DDR has been performed at a higher temperature than the

Fig. 3 Propene/propane equilibrium adsorption selectivity at 100 kPa versus gas phase composition for adsorbents with low selectivities

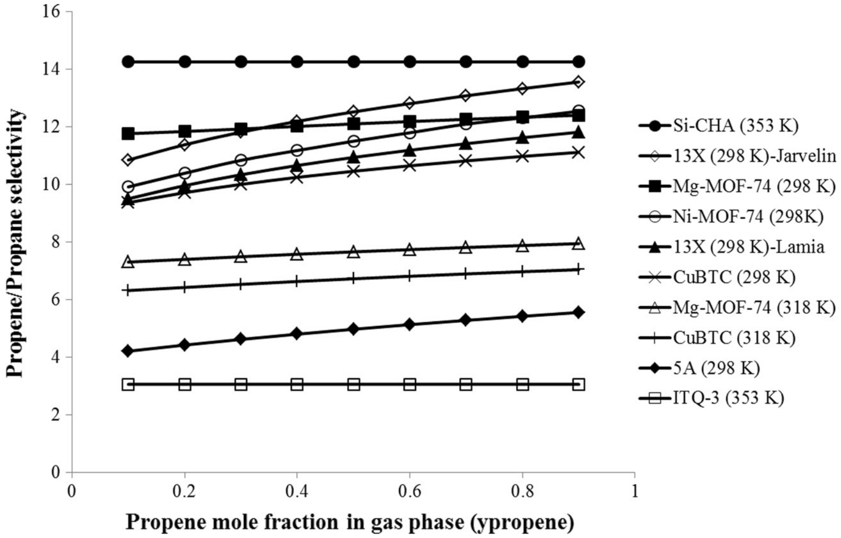
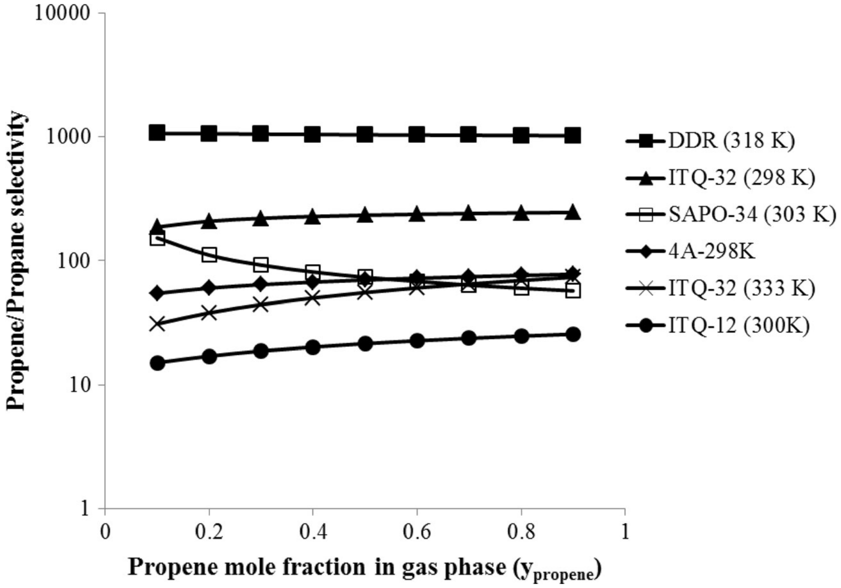


Fig. 4 Propene/propane equilibrium adsorption selectivity at 100 kPa versus gas phase composition for adsorbents with high selectivities



other zeolites with higher selectivities. Additionally, Bae et al. (Bae et al. 2012) synthesized Co-MOF-74 which has a very high selectivity than the other MOF-74 s (Ni-MOF-74 and Mg-MOF-74). Its selectivity for an equimolar mixture of propene/propane is reported to be 46 with adsorption capacity of 6.8 mmol/g at 298 K and 100 kPa (Bae et al. 2012). Figure 4 along with the work of Bae et al. (2012) sorts the adsorbents in the following order with respect to their equilibrium selectivities: DDR > ITQ-32 > SAPO-34 > 4A > Co-MOF-74 > ITQ-12.

Additional investigation was conducted to find the effect of pressure on the selectivity of adsorbents studied. So, IAST modeling was done for a 50/50 mixture of propene/propane at different pressures in the range of 1-100 kPa. The results are graphically presented in Figs. 5 and 6 for adsorbents having selectivity below and above 20, respectively. All adsorbents show an increase in the selectivity with increase in pressure except for SAPO-34 and MOFs (Mg-MOF-74, Ni-MOF-74 and CuBTC). Pressure increase has totally adverse effect on SAPO-34 selectivity while MOFs generally show a minimum at lower pressures.

3.1 Equilibrium adsorption selectivity versus capacity

From economical and operational view points, not only the selectivity of adsorbent is important but also the adsorption capacity may take a crucial role in the selection for adsorption

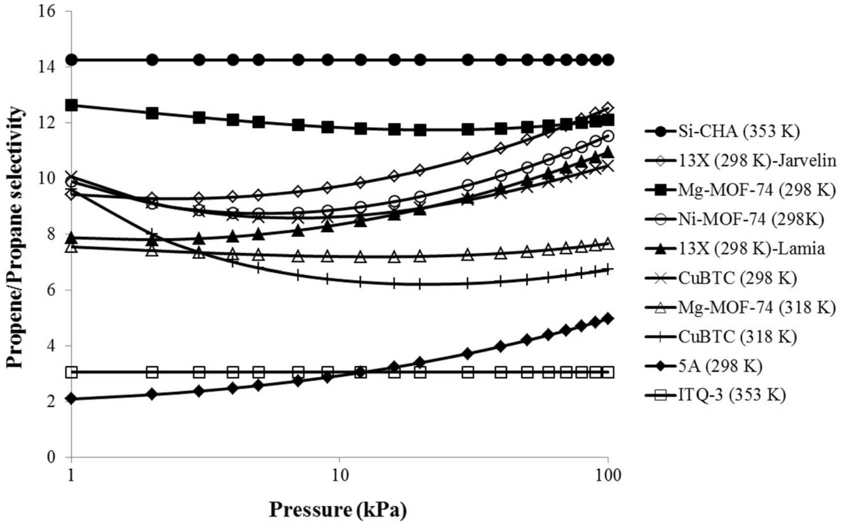


Fig. 5 Propene/propane equilibrium adsorption selectivity versus pressure for adsorbents with low selectivities

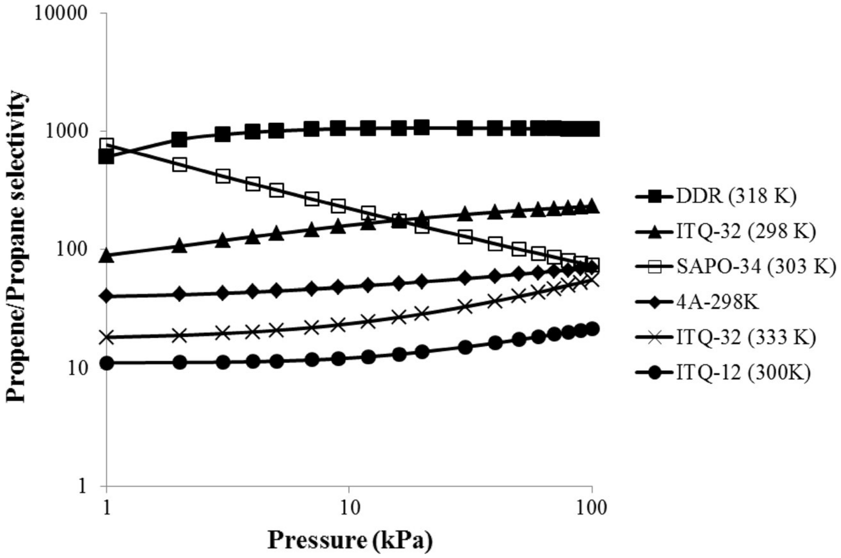
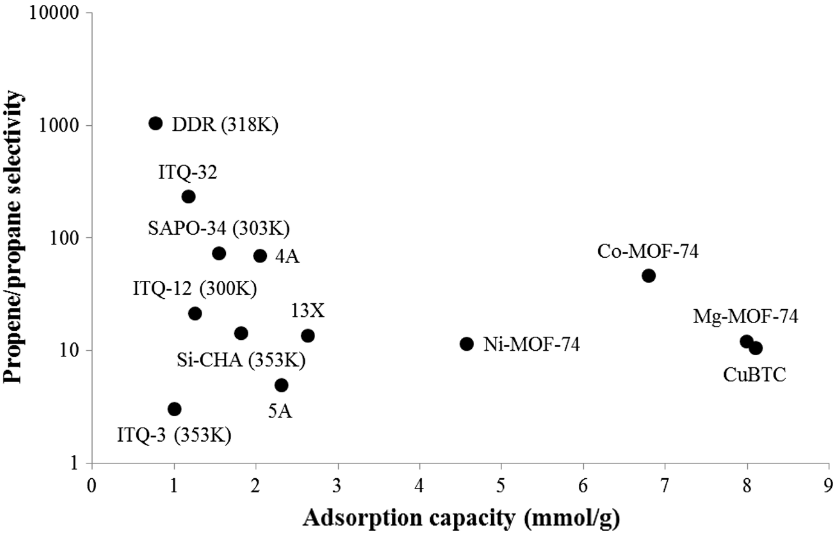


Fig. 6 Propene/propane equilibrium adsorption selectivity versus pressure for adsorbents with high selectivities

Fig. 7 Propene/propane equilibrium selectivity versus amount adsorbed at 298 K unless otherwise stated



based processes. In other words, an adsorbent is suitable which has higher selectivity and capacity, simultaneously. In the previous section, only the selectivity, the inherent capability, of zeolites and MOFs are compared and the equilibrium adsorption amount was not considered. Figure 7 shows simultaneously the selectivities and adsorption amounts of adsorbents at 100 kPa for 50/50 binary mixture. This figure indicates that MOFs have higher adsorption capacities. On the other hand, zeolites DDR, ITQ-32 separate propene from propane with high selectivities. Obviously, it can be stated that the higher selectivity is gained in the cost of decrease in the adsorption capacity. For instance, DDR selectivity is almost 100 times higher than that of CuBTC or Mg-MOF-74 while its adsorption capacity is lower than them by a factor of about 10. This figure is useful for selection of adsorbents, however, the selection of suitable sorbent needs some economic considerations where the importance of capacity or selectivity should be taken into account. But, generally, it may be stated that the MOFs especially M-MOF-74 and CuBTC are appropriate for a process where the adsorption capacity is more pronounced. On the other hand, DDR, ITQ-32 zeolites are suitable for membrane applications where the adsorption selectivity is much more important than capacity.

4 Conclusions

Binary adsorption of propene/propane mixtures using IAST model led to evaluate the capability of various microporous adsorbents (zeolites and MOFs) that have been utilized in the literature. Figure 7 may be a very useful graph that can be utilized for selecting the suitable adsorbent for a specified process. The results revealed that MOFs have higher adsorption capacity (~8 mmol/g) with a propene/propane equilibrium selectivity of about 10–12 at 100 kPa and 298 K for a 50/50 binary mixture. On the other hand, all-silica DDR zeolite showed a very high selectivity of more than 1000 with adsorption capacity of about 0.8 mmol/g. Additionally, the other silica zeolite, i.e. ITQ-32, is an alternative that has a selectivity of 230 and adsorption capacity of about 1.2 mmol/g. Generally, it may be said that the MOFs especially M-MOF-74 and CuBTC with higher capacity are appropriate choices for bulk separations based on equilibrium adsorption. On the other hand, DDR, ITQ-32, SAPO-34 and 4A zeolite are proper candidates for membrane applications where the adsorption selectivity is more important.

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