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EFFECTIVE DIFFUSIVITIES OF WATER VAPOURS AND HEPTANE VAPOURS IN PARTICLES OF MOLECULAR SIEVES 4A AND 5A

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Abstract. *In the presented work we described an apparatus for the determination of effective diffusion coefficients of vapours of compounds in the presence of an inert gas in both spherical and cylindrical adsorbent particles at ambient temperatures. The determined values of effective diffusion coefficients of water vapours in the presence of air at 30 °C are: 1.99 .*10^{-11} m^2s^{-1} *and 1.73* 10^{-11} m^2s^{-1} *for the particles of 5A molecular sieves UC and VURUP, respectively, and 4.10* 10^{-11} m^2s^{-1} *and 7.55* 10^{-11} m^2s^{-1}*, for 4A molecular sieves UC and VURUP respectively. The effective diffusion coefficients of n-heptane vapours in the presence of air at 30 °C are 0.913* 10^{-11} m^2s^{-1} *and 3.71* 10^{-11} m^2s^{-1} *for molecular sieves UC and VURUP, respectively. The obtained values of* D_e *correspond to data published for similar systems.*

Key words: *diffusion, effective diffusivity, water, n-heptane, molecular sieve 4A, molecular sieve 5A.*

Introduction

All methods for the design of adsorption equipment basing on an adequate physical description of the adsorption process assume that the overall mass transfer resistance can be divided at least into two partial resistances: the partial resistance in the fluid phase surrounding the adsorbent particles, and the partial resistance in the pores of the adsorbent particle. It is obvious that both resistances can play a significant role and their values should be known in the calculation of the basic dimensions of an adsorber. The partial mass transfer resistance in the flowing fluid phase is relatively well described for various arrangements of the system. The values of the partial mass transfer coefficients in the fluid phase can be calculated from available dimensionless equations. The problem of determination of the partial mass transfer resistance in the pores of the adsorbent particle cannot be considered to be solved, despite the fact that numerous publications devoted to this topic has recently appeared in the literature. This is connected with the complicated structure of pores in the solid phase, their characterization and the description of transport within the pores. In spite of the existence of various mechanisms, the mass transfer in the pores of the adsorbent particles occurs via unsteady diffusion and is described by the Fick's second law of diffusion and characterized by only one parameter - the effective diffusion coefficient. Different transport mechanisms often take place parallel, whereby also in one system the prevailing mechanism and thus, also the values of determined effective diffusion coefficients, can change according to the experimental conditions.

The diffusion of substances in solid porous bodies is described in details in the monographs of Barrer [1], Jost [2], Aris [3], Cunnigham [4], and Kärger and Ruthven [5]. The solutions of the equation of unsteady diffusion for the basic forms of a porous material and chosen initial and boundary conditions are given in the work of Crank [6] or we can obtain them by the solution of an unsteady heat transfer in a solid material [7]. A lot of attention is devoted to the mass transfer in solid porous sorbents in the books of Timofeev [8], Ruthven [9], Keltsev [10], Kast [11], Suzuki [12], Satterfield [13] and other authors.

In the study of cyclic adsorption and desorption at pressure swing, Sundram and Yang [14] described the diffusional mass transfer in the solid phase. These authors suggested that the values of the effective diffusion coefficients do not vary with the adsorbate concentration and pressure over the given range of parameters. Al-Duri and Mc Kay [15] investigated the parallel diffusion and adsorption of high molecular colored organic substances in the particles of activated carbon in a batch system. They drew the following conclusion: The values of the effective diffusion coefficients depend on the adsorptive concentration in the batch exponentially. In studying the drying of solid particles Levy et al. [16] described the transport of vapors in the pores of a solid phase. Models for the diffusion in the pores of solid catalysts are given in the papers of Haugaard and Livbjerg [17]. The dependence of the surface diffusion on the concentration of adsorbate and the porous structure of the adsorbent was reported by Do and Do [18]. Chen and Yang [19] investigated the diffusion in the adsorbed phase during the multilayered adsorption. The mass transfer in the absence of an inert in the pores of certain size was described by Mac Elroy and Suh [20]. Cracknell et al. [21] studied the diffusion of methane in micropores of graphite having a slot form. Pore diffusion of substances within crystals of zeolites was investigated in the works [22] - [25]. In studying sorption Park and Do [26] used for the description of mass transfer unsteady diffusion within adsorbent particles with a bidisperse structure. Silva and Rodrigues [27] investigated the kinetics of sorption of n-hexane within 5A zeolite pellets. These authors reported following values of diffusion coefficients in the pores for the N_2 - n-C_6 system: 0.06 cm^2s^{-1} at 200 °C, 0.07 cm^2s^{-1} at 250 °C and 0.08 cm^2s^{-1} at 300 °C. Corresponding values of tortuosities were: 1.7; 1.6 and 1.6. Krishnan et al. [28] proposed a mathematical model for the adsorption of cyclopropane in modified zeolites X. Talu et al. [29] published measured data of effective diffusion coefficients of n-alkanes in silikalite based on steady measurements in a crystal mebrane. Schumacher and Karge [30] performed a study of adsorption kinetics of ethylbenzene in H-ZSM-5 zeolite. An improvement of the method used in determining effective diffusion coefficients from measurements in a thin layer of crystals proposed Loos et al. [31].

The purpose of this study was to investigate the effective diffusivity of water vapours in molecular sieves particles and the effective diffusivity of n-heptane vapours in molecular sieve 5A particles.

Mass Transfer within Solid Phase Pores.

For unsteady mass transfer in solid porous media the following equation can be derived from the balance of substance A:

$$\beta \frac{\partial c_A}{\partial \tau} - R_A = \nabla . D'' \nabla c_A \tag{1}$$

where c_A is the adsorptive concentration, D'' is the equivalent diffusion coefficient, R_A is the rate of production of substance A in the balanced volume, â is the adsorbent porosity, ô is time. The equivalent diffusion coefficient is defined by

$$D'' = D' + D_s \Gamma \tag{2}$$

where D' is the diffusion coefficient in the porous medium, D_s is the coefficient of surface diffusion and Ã is the equilibrium constant given by

$$q_A = \Gamma c_A \tag{3}$$

where q_A is the adsorbate concentration.
If mass transfer is performed by combination of molecular and surface diffusion, Eq. (2) can be rewritten into the following form:

(4)

where D_{AB} is the coefficient of molecular diffusion, k is the coefficient of waving of pores and T is tortuosity. If mass transfer is performed via a combination of Knudsen and surface diffusion, Eq. (2) is modified into the form

$$D'' = D_K \frac{\beta}{k^2} + D_s \Gamma = D_K \frac{\beta}{T} + D_s \Gamma \tag{5}$$

where D_K is the coefficient of Knudsen diffusion.
For simultaneous diffusion and adsorption in a porous medium R_A represents a negative change of the adsorption rate with respect to the volume of porous medium If the diffusion coefficient is equal in all directions, i. e. the porous material is isotropic in terms of mass transport, Eq, (1) can be written as:

$$\beta \frac{\partial c_A}{\partial \tau} + \frac{\partial q_A}{\partial \tau} = D'' \nabla^2 c_A \tag{6}$$

If one assumes the validity of a linear isotherm in the form of Eq. (3), and an infinitely rapid trapping of the adsorptive from the close vicinity on the adsorption surface, then one can rewrite Eq. (6) into the following form

$$\frac{\partial c_A}{\partial \tau} = D_e \nabla^2 c_A \tag{7}$$

where the effective diffusion coefficient D_e is given by the relation

$$D_e = \frac{D''}{\beta + \Gamma} \tag{8}$$

In the case of performing the study of diffusion within spherical or cylindrical adsorbent particles Eq. (7) can be transformed for spherical or cylindrical coordinates. For symmetric diffusion in spherical particles Eq. (7) has the following form:

$$\frac{\partial c_A}{\partial \tau} = D_e \left[\frac{\partial^2 c_A}{\partial r^2} + \frac{2}{r} \frac{\partial c_A}{\partial r} \right] \tag{9}$$

where r is the radial coordinate.
For symmetric diffusion in a cylindrical particle Eq. (7) is given by

$$\frac{\partial c_A}{\partial \tau} = D_e \left[\frac{\partial^2 c_A}{\partial r^2} + \frac{1}{r} \frac{\partial c_A}{\partial r} + \frac{\partial^2 c_A}{\partial z^2} \right] \tag{10}$$

where z is the axial coordinate. Eqs. (9) and (10) are solved for the required initial and boundary conditions.
If at the beginning of adsorption the adsorbent is supposed to be without adsorbate and adsorptive and, from certain time a constant adsorptive concentration c_{Ao} is kept on the particle surface, one can define both initial and boundary conditions by

$$c_A = 0; \qquad 0 \le r \le r_o; \qquad \tau = 0$$

$$; \qquad r = r_o; \tag{11}$$

By solving Eq. (9) for conditions (11) one obtains the dependence $c_A = f(z,ô)$, which makes it possible to calculate the adsorptive concentration in an arbitrary place of the spherical adsorbent particle at an arbitrary time. The relation required for the purpose of determining D_e is derived from the solution of Eq.(9) by transformation into adsorbate concentration at a chosen time. Then, the final form of solution is given by [1, 6, 8]:

$$\gamma_\tau = \frac{\Delta q_\tau}{\Delta q_\infty} = \frac{\Delta m_\tau}{\Delta m_\infty} = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp\left(- \frac{n^2 \pi^2 D_e \tau}{r_o^2} \right) \tag{12}$$

where Δm_τ, Δq_τ, Δm_∞, Δq_∞ is the increment of the amount of sorbate and/or adsorbate concentration at time τ and the increment of the amount of sorbate and/or the equilibrium adsorbate concentration, respectively.
Eq. (12) is recommended for higher adsorption times when the series rapidly converges. For low values of adsorption time Crank [6] derived the following relation

$$\gamma_\tau = 6\sqrt{\frac{D_e\tau}{r_o^2}}\left[\frac{1}{\sqrt{\pi}} + 2\sum_{n=1}^{\infty}\operatorname{ierfc}\left(\frac{nr_o}{\sqrt{D_e\tau}}\right)\right] - 3\frac{D_e\tau}{r_o^2} \tag{13}$$

For equal adsorption conditions in cylindrical particles initial and boundary conditions can be written by:

$$c_A(r,z,0) = 0 \; ; \quad c_A(r_o,z,\tau) = c_{A_o} \; ; \quad c_A(r,\pm l/2,\tau) = c_{A_o}$$

$$\frac{\partial c_A(0,z,\tau)}{\partial r} = 0 \; ; \quad \frac{\partial c_A(r,0,\tau)}{\partial z} = 0 \tag{14}$$

Then, the final form of solution suitable in determining D_e has the following form:

$$\gamma_\tau = \frac{\Delta q_\tau}{\Delta q_\infty} = \frac{\Delta m_\tau}{\Delta m_\infty} = 1 - \frac{32}{\pi^2}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{1}{\mu_n^2(2m-1)^2}\exp\left[-\left(\frac{\mu_n^2}{r_o^2} + \frac{(2m-1)^2\pi^2}{l^2}\right)D_e\tau\right] \tag{15}$$

where l is the length of the cylindrical particle.

Eqs. (12), (13) and (15) can be used in determining D_e from kinetic measurements.

Experimental Part

Materials.

Two samples of 5A molecular sieves (MS):

1. Spherical particles with a mean diameter of 1.12 mm, produced by Union Carbide (UC) for the separation of n-alkanes
2. Spherical particles with a mean diameter of 1.12 mm developed by the Research Institute of Petroleum and Gas (VURUP), Bratislava

Two samples of 4A zeolite molecular sieves in the form of cylinders:

1. with a mean diameter of 1.15 mm and a mean length of 4.65 mm, produced by Union Carbide
2. with a mean diameter of 1.63 mm and a mean length of 4.15 mm, produced by the Research Institute of Petroleum and Gas, Bratislava

Water used for measurements was twice distilled.

n-Heptane was purified by rectification and contained 99.5 wt. % n-heptane, 0.2 wt % and 0.3 wt % lower and higher boiling substances, respectively.

Apparatus and Method of Measurement

A glass apparatus schematically drawn in Figure 1 was used for measuring the adsorption of water vapors or n-heptane vapors from air. Air entering the apparatus was purified in adsorbers 1 and 2 by adsorption of organic impurities and water on silicagel and 5A molecular sieve. The purified air was divided into two paths. The smaller flow of air was saturated with water vapors or vapors of n-heptane by evaporation from the free surface in saturators 6. The flow rate of air in the second flow measured by flowmeter 4 was adjusted in such a manner that mixing both flows ensured the required adsorptive concentration and the required flow rate of air before entering adsorbers 7, 8 or 9 (minimal 18 l/min). Prior to reaching steady conditions in saturators (about 20 min) air being saturated was released into the atmosphere. After reaching constant values of flow rates and adsorptive concentration the flow of saturated air was switched to adsorber 7 and adsorbers 10-12. After elapsing the required time the flow of air being saturated was switched to adsorber 8, and adsorber 7 was weighed. Adsorption times in adsorbers 7 and 8 were equal. After elapsing the adsorption time in adsorber 8 the flow of gas was switched again to adsorber 7 and the whole procedure was repeated. The adsorption times in adsorbers 7 and 8 were 1 min at the beginning and 5 minutes at the end. The measurement was finished when the increment of the adsorbed amount was negligible. The adsorptive concentration in air entering the adsorbers was estimated from the total increment of weights in adsorbers 7 – 12 and the amount of flowing air used during the adsorption. The results of measurements are represented by the set of data $\{\gamma_{\tau i}, \tau_i\}$ for one adsorption step.

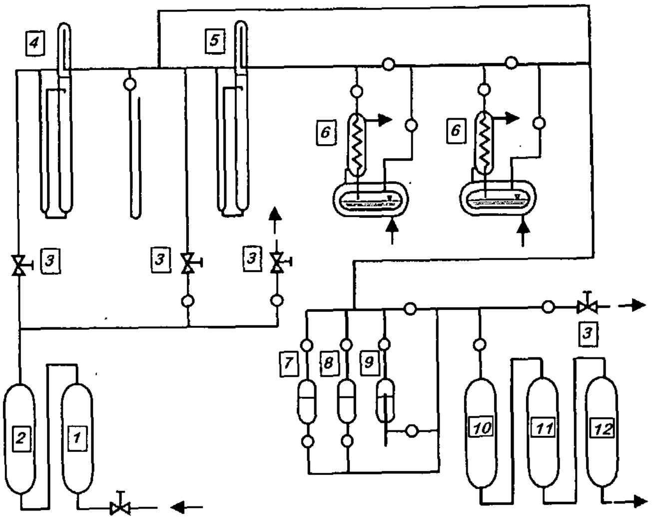

Figure 1. Diagram of the experimental apparatus.
1 – cleaning adsorber filled with silicagel, 2 – drying adsorber filled with molecular sieve, 3 – distribution valves, 4,5 – flowmeters, 6 – saturators, 7,8 – adsorbers containing differential bed of adsorbent, 9 – adsorbens containing differential bed of adsorbent with thermocouple, 10, 11, 12 – adsorber filled with silicagel and molecular sieve

Adsorbers 7 and 8 were equipped with a grid, which was fixed in their centers. This grid was made of a perforated sheet, on which an adsorbent bed with a height equal to the particle diameter was placed. Both the upper and the lower parts of the equipment were filled with hollow glass particles in such a manner that a uniform flow of gas pass around the adsorbent particles was ensured. Adsorber 9 is designed in the same manner as adsorbers 7 and 8. In addition, however, it is equipped with a thermocouple, which is inserted in the adsorbent particle. Thus, the temperature inside of the particle can be investigated during the adsorption process.

Adsorbers 10 - 12 were filled with silica gel and 5A molecular sieve. The amounts of the adsorbent were chosen in such a manner that the increment of the amount of adsorbate in adsorber 12 was zero or minimal during the adsorption.

Prior to measurement all adsorbents were activated. The adsorbers filled with molecular sieve heated in an oven at 400 °C in a small flow rate of dried air for about 3 h. Adsorbers filled with silica gel were heated in laboratory oven to a temperature of 150°C. For activation ovens designed for the given dimensions of adsorbers were used.

Results and Discussion

From the measured sets of data $\{\gamma_{\tau i}, \tau_i\}$ values of effective diffusion coefficients were calculated by the optimization method. As optimization function Eq. (16) was used:

$$F = \sum_{i=1}^{N} \left[(\gamma_{\tau i})_{\exp} - (\gamma_{\tau i})_{calc} \right]^2 \qquad (16)$$

Values $(\gamma_{\tau i})_{calc}$ calculated for the respective experimental adsorption time in spherical or cylindrical particles using Eq. (12) and Eq. (15), respectively are plotted along with the experimentally measured data in Figures 2 - 4 for the chosen systems. The results of calculation for the adsorption of water on 4A molecular sieves (VURUP) are listed in Table 1 and plotted in Figure 2.

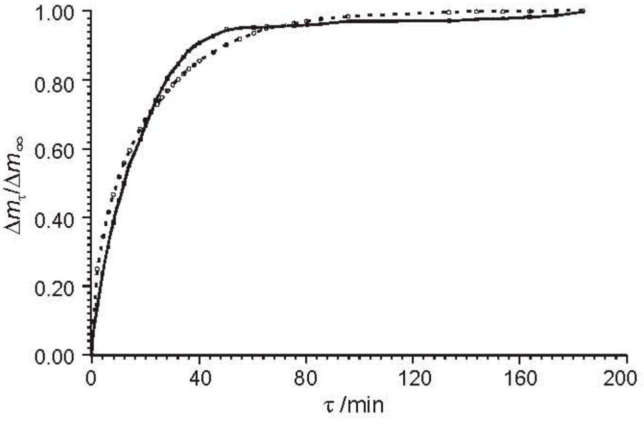

Figure 2. Kinetic curve of the adsorption of water vapour on MS 4A (VURUP). Full line: measured values □, dotted line: calculated values ○, shape of the adsorbent: cylindrical particles, l = 4.15, mm, d = 1.0 – 1.25 mm

The model used describes the investigated system relatively well. In the region of shorter times, the calculated values of γ, similarly as in the case of adsorption times higher than 75 min, are higher than experimental times. The calculated value of D_e = 7.55. 10^{-11}m^{2}s^{-1} is significantly higher than that found for MS 4A produced by Union Carbide (see Table 2). In the literature data on diffusion of water vapors in molecular sieves of type A are scarce. In the monograph [5] are reported kinetic curves of water vapors on the molecular sieve Zeosorb 4A (Laporte) at 303 K. Molecular sieve particles had a spherical form with a mean diameter of 2.93 mm. The concentration of water in the gas was 0.15 g.m^{-3}. The calculated value of the diffusion coefficient of water within the pores is D_p = 0.0397 cm^{2}s^{-1}. In accordance with the symbols used

$$D_e = \frac{\beta D_p}{\beta + (1-\beta)\Gamma} \qquad (17)$$

For the conditions of measurement of adsorption of water on MS 4A VURUP, $\hat{a}$ = 0.34 and the particle density of the molecular sieve is being 1.137 g cm^{-3}. Then, $\tilde{A}$ has the following value:

$$\Gamma = \frac{0{,}2377.1{,}137.10^6}{3{,}77} = 71\ 668{,}3$$

The value of the effective diffusion coefficient calculated from the relation (17) for the above mentioned conditions is :

$$D_e = \frac{0{,}34.0{,}0397}{0{,}34 + (1 - 0{,}34)71688{,}3} 2{,}85.10^{-7}\,cm^2 s^{-1} = 2{,}85.10^{-11}\,m^2 s^{-1}$$

The calculated value of the effective diffusion coefficient is of the same order of magnitude as values found for the systems water vapour - MS 4A. The fact, that the diffusion coefficient of water in MS Zeosorb 4A is lower, can be connected with the application of relatively large molecular sieve particles. The mutual difference between the values of the effective diffusion coefficient for MS 4A Union Carbide and VURUP is probably connected with the degree of exchange of the cation localized at the entering holes of the molecular sieve crystal.

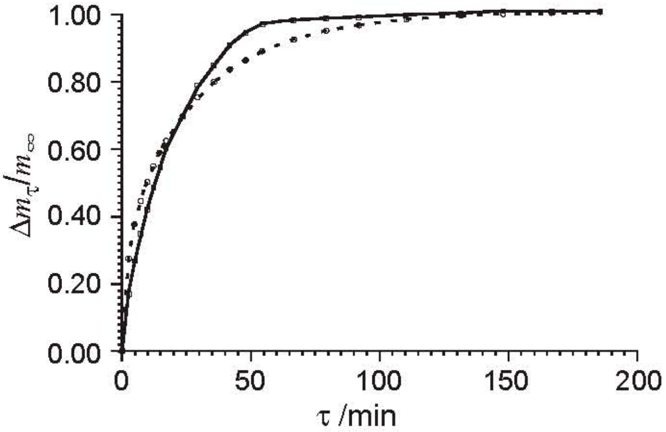

Figure 3. Kinetic curve of the adsorption of water on MS 5A (VURUP). Full line: measured values □, dotted line: calculated values ○, Shape of the adsorbent: spherical particles d = 1.0 – 1.25 m

During adsorption of water on MS 5A Union Carbide and VURUP no differences in the determined values of effective coefficients were found, despite the fact that equilibrium values of adsorbate concentration are different. By comparison of effective diffusion coefficients of water in molecular sieves 4A and 5A one can see, that the values of D$_e$ of water in MS 5A are significantly lower than in the case of MS 4A, despite the fact that experimentally measured kinetic curves of adsorption of water on MS 4 A, Figure 2 and on MS 5A, Figure 3, are practically the same. Obviously, the affinity towards water has a more dominant influence than the size of the entrance windows of the molecular sieve crystal.

Post [22] reports dependences of the diffusion coefficient of n-alkanes within 5A zeolite crystals at 473 K obtained by various methods of measurement. For n-heptane the corresponding value is 10^{-13}m^{2}s^{-1}. A similar dependence for ZSM-5

Table 1 Results of calculation for the adsorption system water - MSA (VURUP)

Adsorbent : MS 4A (VURUP); cylinder, length 4.15 mm, diameter 1.63 mm
Sample of adsorbent : 1.0457 g
Temperature : 30°C

Measurement No.	τ [min]	Δm [g]	$(\Delta m_\tau/\Delta m_\infty)_{exp}$	$(\Delta m_\tau/\Delta m_\infty)_{calc}$	$(y_{\tau i})_{exp}$ - $(y_{\tau i})_{calc}$
0	0	0.0000	0.00000	0.00000	0.00000
1	2	0.0368	0.14803	0.25232	-0.10429
2	4	0.0595	0.23934	0.34703	-0.10769
3	6	0.0787	0.31657	0.41620	-0.09963
4	8	0.0964	0.38777	0.47203	-0.08426
5	10	0.1121	0.45093	0.51928	-0.06835
6	12	0.1250	0.50282	0.56036	-0.05755
7	14	0.1376	0.55350	0.59675	-0.04325
8	18	0.1566	0.62993	0.65888	-0.02896
9	20	0.1669	0.67136	0.68571	-0.01435
10	22	0.1755	0.70595	0.7102.1	-0.00426
11	24	0.1848	0.74336	0.73267	0.01069
12	26	0.1930	0.77635	0.75329	0.02305
13	28	0.2008	0.80772	0.77227	0.03546
14	30	0.2061	0.82904	0.78975	0.03930
15	32	0.2115	0.85076	0.80585	0.04492
16	34	0.2163	0.87007	0.82070	0.04937
17	36	0.2205	0.88697	0.83442	0.05255
18	38	0.2241	0.90145	0.84707	0.05438.
19	40	0.2267	0.91191	0.85875	0.05315
20	45	0.2313	0.93041	0.88420	0.04621
21	50	0.2353	0.94650	0.90506	0.04144
22	55	0.2368	0.95253	0.92216	0.03037
23	60	0.2368	0.95253	0.93618	0.01635
24	65	0.2376	0.95575	0.94769	0.00807
25	75	0.2383	0.95857	0.96485	-0.00628
26	80	0.2386	0.95977	0.97119	-0.01141
27	85	0.2393	0.96259	0.97638	-0.01379
28	95	0.2413	0.97064	0.98414	-0.01350
29	133	0.2416	0.97184	0.99652	-0.02468
30	143	0.2426	0.97586	0.99767	-0.02180
31c	153	0.2432	0.97828	0.99844	-0.02016
32	163	0.2442	0.98230	0.99895	-0.01665
33	173	0.2449	0.98512	0.99930	-0.01418
34	183	0.2486	1.00000	0.99953	0.00047

$D_e = 7{,}55.10^{-11}\ m^2s^{-1}$

at 334 K yields a value with the order of magnitude $10^{-12}\ m^2s^{-1}$. Diffusion coefficients of n-hexane within 5A molecular sieve pellets at temperatures of 573K, 523K and 473K published by Silva and Rodrigues [27] are given in the introductory part of this paper. Using these data in computing effective diffusion coefficients according to Eq. (17) at a temperature of 303K one obtains $D_e = 1.25.10^{-10} m^2s^{-1}$. Doetsch et al [32] investigated the kinetics of sorption and diffusion of n-heptane within crystals of molecular sieve 5A (Linde) with a mean size of the edge of cube 3.91 ì m at temperatures 409 and 491 K. The determined values of the diffusion coefficient of n-heptane depend on the adsorbate concentration and are ranging from $0.2.10^{-11}$ to $8.0.10^{-10} cm^2s^{-1}$. Though the published data were not determined under the investigated conditions, they document that the proposed method is convenient in determining D_e, which is the basic characteristic of the system in designing adsorbers.

Symbols

c_A	concentration of component *A* in the gas phase	$kg\,m^{-3}$
D'	diffusion coefficient in porous medium	$m^2\,s^{-1}$
D''	equivalent diffusion coeffient	$m^2\,s^{-1}$
D_{AB}	molecular diffusion coefficient	$m^2\,s^{-1}$
D_e	effective diffusion coefficient	$m^2\,s^{-1}$
D_K	diffusion coefficient of Knudsen diffusion	$m^2\,s^{-1}$
D_s	coefficient of surface diffusion	$m^2\,s^{-1}$
k	coefficient of wave of pores in Eq.(8)	

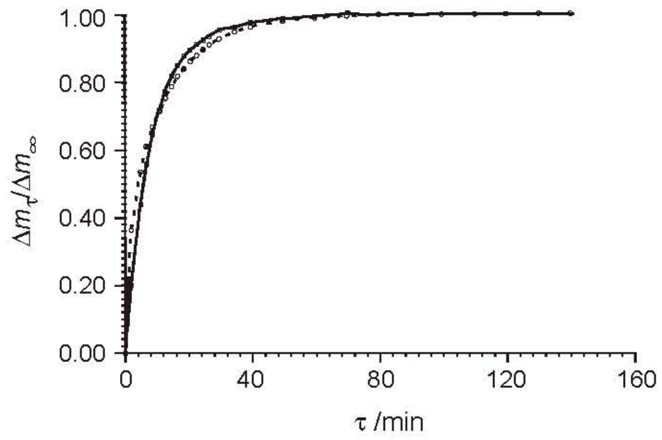

Figure 4. Kinetic curve of the adsorption of n-heptane on MS 5A (VURUP). Full line: measured values ☐, dotted line: calculated values ○, shape of the adsorbent: spherical particles d = 1.0 – 1.25 mm

Table 2. Evaluted values of D_e and measurement concitions

Adsorbent	Adsorptive	c_o [g m^{-3}]	a_∞.10^2 [g g^{-1}]	Temperature [°C]	D_e.10^{11}[m^{2}s^{-1}]
1. MS 5A UC	H_2O	3.81	16.60	30	1.99
2. MS 5A VURUP	H_2O	3,81	19,99	30	1,73
3. MS 4A UC	H_2O	3,77	18,45	30	4,10
4. MS 4A VURUP	H_2O	3,77	23,77	30	7,55
1. MS 5A UC	n-C_7	4,42	2,57	30	0,913
2. MS 5A VURUP	n-C_7	4,42	3,83	30	3,71

Äm_τ	increment of the adsorbed amount at time τ	kg
Äm_∞	increment of the adsorbed amount in equilibrium	kg
q_A	adsorbate concentration	kg m^{-3}
Äq_τ	increment of the adsorbate concentration in time τ	kg m^{-3}
Äq„	increment of the adsorbate concentration in equilibrium	kg m^{-3}
r	radial coordinate	m
r_o	the particle radius	m
R_A	rate of production of component A in the volume of the porous body	kg m^{-3}
s^{-1}		
T	tortuosity	
â	porosity	m^{3}m^{-3}
ã$_\tau$	dimensionless concentration defined by Eqs.(12) (13) or (15)	
Γ	equilibrium constant defined by Eq. (3)	
μ_n	roots of 1st type zero – order Bessel function	
τ	time	s

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