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Modeling of gas transport in a microporous solid using a slice selection procedure: Application to the diffusion of benzene in ZSM5

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ABSTRACT

The analytical solution of the equations of gas diffusion in a heterogeneous zeolite bed is presented. The problem is handled by assuming that the bed consists of a large number of very thin layers of solid, perpendicular to the direction of propagation of the gas. Mass transfer by diffusion in such a material is determined by a system of differential equations with boundary and interface conditions. The results allow us to make the theoretical determination of the time dependence of the concentration profiles and the inter- and intracrystallite diffusion coefficients of a gas in each layer of the bed. A numerical application concerns the diffusion of benzene in a cylindrical bed of ZSM5 displaced vertically and rapidly, step-by-step, inside the NMR probe. Thus, the time dependence of the concentration of gas absorbed at the level of each slice and each crystallite can be obtained. These coupled investigations give a better understanding of the diffusion process in this multilayer material.

1. Introduction

Mathematical modeling of mass transfer by diffusion in zeolite beds or other solids and the methods for finding the analytical solutions have been extensively studied by several authors [1–19]. Molecular transport in a bed of zeolite involves two processes: diffusion in the macropores formed by the space between the crystallites (intercrystallite diffusion) and diffusion in the micropores within the crystallites (intracrystallite diffusion). To determine the contribution of each of these processes to the overall diffusion process, one has to know the values of certain parameters, such as the pressure in the gas phase, the dimensions of the crystallite bed, the adsorption isotherms, etc. In the present work we assume that the bed consists of a large number of very thin layers of solid, perpendicular to the direction of propagation of the gas.

As an application of the theoretical results we present a study dealing with the penetration of a gas (benzene) in a zeolite catalyst (ZSM5) bed using the technique described in [20]. The proposed experimental method relies on the vertical displacement, step-by-step, of the bed during the adsorption of the gas, the NMR detection using a very thin coil. In this way, the region effectively probed is limited to a very thin slice. Thus we can obtain the variation as a function of time of the concentration of gas absorbed at the level of each slice. This dual approach enables us for the first time to determine the diffusion coefficient profiles at every position in the bed. But it should be noted even now that the main objective of this study will concern the co-diffusion of several gases in a complex microporous solid and its influence on a heterogeneous catalytic reaction.

2. Experiments

2.1. NMR apparatus

Our aim was to determine the evolution of the NMR spectrum along the length of a heterogeneous sample in the *z* direction of the magnetic field B_0. This original method of imaging has been presented in Ref. [20]. The idea is to select successively several sections at different positions of the sample along the *z*-axis (Fig. 1). For this purpose a mechanical device (NMR lift) was built to displace the sample tube (external diameter 5 mm) vertically step-by-step inside the NMR probe with an accuracy of 1 μm. In this way one obtains for each position a spectrum corresponding to the composition of the sample at this point. The experiment presented here concerns proton NMR (at 200 MHz) of adsorbed benzene performed at ambient temperature with a home-made console operated in conjunction with a wide-bore 4.7 T magnet.

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Nomenclature

c	adsorbate concentration in macropores
c_∞	adsorbate equilibrium concentration in macropores
$C = c/c_\infty$	dimensionless adsorbate concentration in macropores
D_{inter}	macropore diffusion coefficient ($\text{m}^2\,\text{s}^{-1}$)
D_{intra}	micropore diffusion coefficient ($\text{m}^2\,\text{s}^{-1}$)
$k = \overline{1, n+1}$	layer number; subscript k will be added to all the following symbols to specify that they are characteristic of the k layer
K	adsorption equilibrium constant
l	bed length (mm)
$\Delta l = l_k - l_{k-1}; k = \overline{1, n+1}$	layer thickness (we assume that all layers have the same thickness)
L	dimensionless bed length
M_{m}	micropore uptake
M_{M}	macropore uptake
M_t	total uptake at time t
M_∞	total uptake at equilibrium
p_{inter}	relative adsorbed gas in macropores in equilibrium condition
p_{intra}	relative adsorbed gas in micropores in equilibrium condition
q	adsorbate concentration in micro- and nanopores
q_∞	equilibrium adsorbate concentration in micropores
$Q = q/q_\infty$	dimensionless adsorbate concentration in nanopores
r	distance from crystallite center (mm)
R	mean crystallite radius (mm) (we assume that the crystallites are spherical)
$X = r/R$	dimensionless distance from crystallite center
z	distance from bottom of crystallite bed (mm)
$Z = z/l$	dimensionless distance from bottom of the crystallite bed

Greek letters

$\varepsilon_{\text{inter}}$	bed porosity
τ_{M}	diffusion time required for a molecule to penetrate the crystallite bed from top to bottom (s)
τ_{m}	diffusion time required for a molecule to penetrate a crystallite from the external surface to the center (s)
τ_{inter}	time constant of diffusion in intercystallite space (s)
τ_{intra}	time constant of diffusion in intracrystallite space (s)
Γ	dynamic parameter

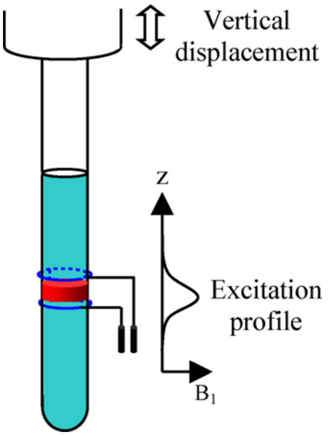


Fig. 1. Principle of experiment: blue, sample; red, zone of excitation (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.).

2.2. Adsorption measurement

The gas to be adsorbed is in equilibrium with the liquid, in the upper part of the ampoule (Fig. 2). It starts to diffuse into the zeolite bed when the wall separating the two parts is broken by means of the glass hammer. In accordance with the principle mentioned above, the zeolite sample is displaced vertically in the magnet during the adsorption, a few micrometers every time. The signal of the gas is detected for each position, rapidly so as to obtain the best possible precision. When the sample reaches the uppermost or the lowest position it starts again in the opposite direction, and continues in this way until adsorption equilibrium is reached. By this means one obtains a curve of gas adsorption as a function of time for each level in the adsorbent. This makes it possible to determine a diffusion coefficient at each point of the solid. This is essential for the planned studies (i) on the adsorption of gas in beds consisting of layers of different solids and (ii) on the competitive diffusion of several gases. The latter case will be assisted by the fact that one detects directly the real characteristic NMR signals.

In the present case we have studied the adsorption of benzene at 25 °C in ZSM5 zeolite. In the upper part of the ampoule the vapor pressure of benzene corresponds to the saturation vapor pressure in equilibrium with the liquid at 25 °C. It is clear that in such an experiment we cannot control all the physical parameters. In order to minimize the temperature variation when the glass wall is broken and the gas comes into contact with the zeolite, the volume under vacuum above the solid is very small and practically negligible compared to that much greater of the upper ampoule containing the liquid or gaseous benzene (Fig. 2). Moreover, the

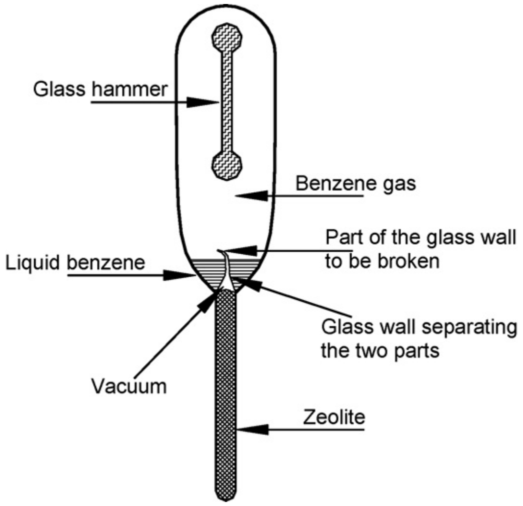
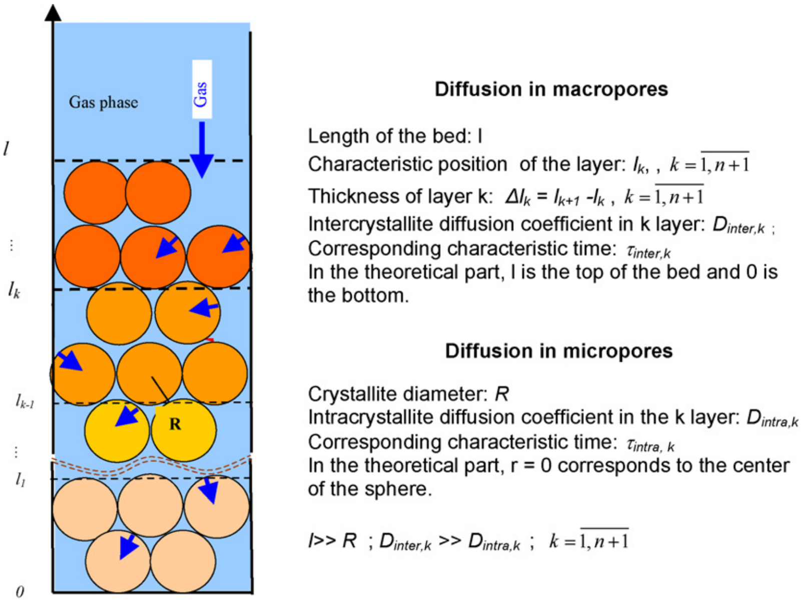


Fig. 2. Experimental set-up.



Diffusion in macropores

Length of the bed: l
Characteristic position of the layer: l_k, , $k = \overline{1, n+1}$
Thickness of layer k: $\Delta l_k = l_{k+1} - l_k$, $k = \overline{1, n+1}$
Intercrystallite diffusion coefficient in k layer: $D_{inter,k}$;
Corresponding characteristic time: $\tau_{inter,k}$
In the theoretical part, l is the top of the bed and 0 is the bottom.

Diffusion in micropores

Crystallite diameter: R
Intracrystallite diffusion coefficient in the k layer: $D_{intra,k}$
Corresponding characteristic time: $\tau_{intra,\,k}$
In the theoretical part, r = 0 corresponds to the center of the sphere.

$l \gg R$; $D_{inter,k} \gg D_{intra,k}$; $k = \overline{1, n+1}$

Fig. 3. The process of diffusion in the zeolite bed.

area of liquid benzene is relatively high, and the diameter of the glass wall to be broken is not small, so as to avoid perturbing the diffusion of the gas.

3. Mathematical modeling

The model developed here is similar to that of the bipore model developed in Refs. [2–12,15–19,21,22]. A cylindrical bed of microporous zeolite crystallites, assumed to be spherical (radius R), is exposed to a constant concentration of adsorbate in the gas phase (Figs. 2 and 3). One face of this bed is permeable to the gas. In this case one can consider that gas diffusion is axial in the macropores (z direction along the height, l, of the bed) and radial in the micropores. We assume that the zeolite bed consists of a large number, n, of very thin layers of solid, of thickness $\Delta l_k = l_{k+1} - l_k$, perpendicular to the propagation of the gas in the z direction. We have made the following assumptions: (i) during the evolution of the system towards equilibrium there has to be a concentration gradient in the macropores and/or in the micropores; (ii) the effect of heat is negligible; (iii) diffusion occurs in Henry's law region of the adsorption isotherm; (iv) all solid particles are spherical; (v) all solid particles are of the same size; uniform packing through the particle bed is assumed.

The mathematical model of gas diffusion kinetics in the zeolite bed (which we consider to be a heterogeneous and multilayer porous medium) is defined by the solutions of the system of differential equations:

$$\varepsilon_{\text{inter},k}\frac{\partial c_k}{\partial t} = D_{\text{inter},k}\varepsilon_{\text{inter},k}\frac{\partial^2 c_k}{\partial z^2} - \frac{3(1-\varepsilon_{\text{inter},k})}{R}\left(D_{\text{intra},k}\frac{\partial q_k}{\partial r}\right)\bigg|_{r=R} \quad (1)$$

$$\frac{\partial q_k}{\partial t} = D_{\text{intra},k}\left(\frac{\partial^2 q_k}{\partial r^2} + \frac{2}{r}\frac{\partial q_k}{\partial r}\right) \quad (2)$$

in the domain:

$$I_n = \left\{ t>0, r\in(0,R), z\in\bigcup_{k=1}^{n+1}(l_{k-1}, l_k); l_0 = 0; l_{n+1} \equiv l < \infty \right\}$$

corresponding to the mass balance in the macropores (c_k) and in the micropores (q_k) for each k layer. The symbols of all notations are given in the Nomenclature.

With the initial conditions:

$$c_k(t=0,z) = 0; \qquad q_k(t=0,r,z) = 0 \quad (3)$$

the boundary conditions:

$$c_{n+1}(t, z=l) = c_{\infty_{n+1}}; \qquad q_k(t, r=R, z) = K_k c_k(z,t) \quad (4)$$

$$\frac{\partial c_1}{\partial z}(t, z=0) = 0; \qquad \frac{\partial q_k(t, r=0, z)}{\partial r} = 0 \quad (5)$$

and the interface conditions between adjacent layers along the z-axis:

$$[c_k(t,z) - c_{k+1}(t,z)]|_{z=l_k} = 0; \qquad \left[\frac{\partial}{\partial z}c_k(t,z) - \frac{\partial}{\partial z}c_{k+1}(t,z)\right]\bigg|_{z=l_k} = 0, \quad k = \overline{1,n} \quad (6)$$

where

$$K_k = \frac{q_{\infty k}}{c_{\infty k}}, \quad k = \overline{1, n+1}$$

Using dimensionless quantities (except time):

$$C_k = \frac{c_k}{c_{\infty k}}; \qquad Q_k = \frac{q_k}{q_{\infty k}}; \qquad Z = \frac{z}{l}; \qquad X = \frac{r}{R}; \qquad L_k = \frac{l_k}{l}$$

in Eqs. (1) and (2), the problem becomes: to find the solution of the partial differential equations:

$$\tau_{Mk}\frac{\partial C_k}{\partial t} = \frac{\partial^2 C_k}{\partial Z^2} - \Gamma_k \frac{\partial Q_k}{\partial X}\bigg|_{X=1} \quad (7)$$

$$\tau_{mk}\frac{\partial Q_k}{\partial t} = \frac{\partial^2 Q_k}{\partial X^2} + \frac{2}{X}\frac{\partial Q_k}{\partial X} \quad (8)$$

in the domain:

$$D_n = \left\{ t>0, X\in(0,1), Z\in\bigcup_{k=1}^{n+1}(L_{k-1}, L_k); L_0 = 0; L_{n+1} \equiv 1 \right\}$$

with the initial conditions:

$$C_k(t=0,Z) = 0; \qquad Q_k(t=0,X,Z) = 0 \quad (9)$$

the boundary conditions:

$$C_{n+1}(t, Z=1) = 1; \qquad Q_k(t, X=1, Z) = C_k(t, Z) \tag{10}$$

$$\frac{\partial C_1}{\partial Z}(t, Z=0) = 0; \qquad \frac{\partial Q_k}{\partial X}(t, X=0, Z) = 0 \tag{11}$$

and interface conditions:

$$[C_k(t,Z) - C_{k+1}(t,Z)]|_{Z=L_k} = 0;$$
$$\left[\frac{\partial}{\partial Z} C_k(t,Z) - \frac{\partial}{\partial Z} C_{k+1}(t,Z)\right]\bigg|_{Z=L_k} = 0, \quad k = \overline{1,n} \tag{12}$$

here:

$$\Gamma_k = \frac{3}{P_{\mathrm{inter},k}} \frac{\tau_{M_k}}{\tau_{m_k}}; \qquad \tau_{M_k} = \frac{l^2}{D_{\mathrm{inter},k}}; \qquad \tau_{m_k} = \frac{R^2}{D_{\mathrm{intra},k}};$$
$$P_{\mathrm{inter},k} = \frac{\varepsilon_{\mathrm{inter},k} C_k}{\varepsilon_{\mathrm{inter},k} C_k + (1-\varepsilon_{\mathrm{inter},k}) Q_k} \approx \frac{\varepsilon_{\mathrm{inter},k}}{\varepsilon_{\mathrm{inter},k} + (1-\varepsilon_{\mathrm{inter},k}) \frac{Q_k}{C_k}},$$
$$k = \overline{1, n+1}$$

The adsorption constant K_k of molecules (e.g., hydrocarbons) in zeolites is usually very high. Therefore $\varepsilon_{\mathrm{inter}}$ is much smaller than $(1-\varepsilon_{\mathrm{inter}})K$ and can be neglected in the expression of $P_{\mathrm{inter},k}$ giving the relative amount of gas in the intercrystallite space ΔL_k:

$$P_{\mathrm{inter},k} = \frac{\varepsilon_{\mathrm{inter},k}}{(1-\varepsilon_{\mathrm{inter},k})K}, \quad k = \overline{1, n+1}$$

If $\tau_{m,k} \gg \tau_{M,k}$, $\Gamma_k \ll 1$, the process in the layer ΔL_k is controlled by intracrystallite diffusion. It is the opposite if $\tau_{M,k} \gg \tau_{m,k}$, $\Gamma_k \gg 1$. If $\Gamma_k \approx 1$, inter- and intracrystallite diffusions should control the overall diffusion in such a layer [9].

Putting $Q_k = N_k/X$, $k = \overline{1, n+1}$, into Eqs. (7)–(12), the system becomes

$$\tau_{M,k} \frac{\partial C_k}{\partial t} = \frac{\partial^2 C_k}{\partial Z^2} - \Gamma_k \left(\frac{1}{X}\frac{\partial N_k}{\partial X} - \frac{1}{X^2} N_k\right)_{X=1} \equiv \frac{\partial^2 C_k}{\partial Z^2} - \left[\frac{\partial N_k}{\partial X} - N\right]_{X=1} \tag{13}$$

$$\tau_{m,k} \frac{\partial N_k}{\partial t} = \frac{\partial^2 N_k}{\partial X^2} \tag{14}$$

in the domain:

$$D_n = \left\{ t > 0,\ X \in (0,1),\ Z \in \bigcup_{k=1}^{n+1} (L_{k-1}, L_k);\ L_0 = 0;\ L_{n+1} \equiv 1 \right\}$$

with the initial conditions:

$$C_k(t=0, Z) = 0; \qquad N_k(t=0, X, Z) = 0 \tag{15}$$

the boundary conditions:

$$C_{n+1}(t, Z=1) = 1; \qquad N_k(t, X=1, Z) = C_k(t, Z) \tag{16}$$

$$\frac{\partial C_1}{\partial Z}(t, Z=0) = 0; \qquad N_k(t, X=0, Z) = 0 \tag{17}$$

and the interface conditions:

$$[C_k(t,Z) - C_{k+1}(t,Z)]_{Z=L_k} = 0; \qquad \left[\frac{\partial}{\partial Z} C_k(t,Z) - \frac{\partial}{\partial Z} C_{k+1}(t,Z)\right]_{Z=L_k} = 0, \quad k = \overline{1,n} \tag{18}$$

4. Analytical solution: concentration profiles

The analytical solutions of the problem described by Eqs. (13)–(18) can be obtained using the Laplace integral transformation and the Cauchy function methods. The calculations are too complex and long to be reported here. Moreover, it would be useless, since they are detailed in [23]. We mention here only how the inter- and intracrystallite diffusion coefficients are first calculated at each moment and in each slice of the bed, which allows us then to calculate the corresponding concentrations in each layer.

The intercrystallite concentration $C_{k,t}$, which is *a* function f_C of the layer l_k and the moment t can be written in the form:

$$C_{k,t} = f_C(t, l_k, D_{\mathrm{inter},k}, D_{\mathrm{intra},k}) \tag{19}$$

Similarly, the concentration $Q_{k,t,X}$ in a crystallite is a function f_Q of k, t and the abscissa X:

$$Q_{k,t,X} = f_Q(t, l_k, X, D_{\mathrm{inter},k}, D_{\mathrm{intra},k}) \tag{20}$$

Whence the expression for the total intracrystallite concentration in layer k:

$$Q_{k,t} = \int_0^R f_Q(t, l_k, X, D_{\mathrm{inter},k}, D_{\mathrm{intra},k})\,\mathrm{d}X \tag{21}$$

The measured quantity of gas adsorbed in layer k at the moment t is

$$M_{k,t} = C_{k,t} + Q_{k,t} \tag{22}$$

We have the same for layer $k+1$,

$$M_{k+1,t} = C_{k+1,t} + Q_{k+1,t} \tag{23}$$

If we choose two layers l_k and l_{k+1} very close to each other, which is possible with the apparatus used, it can be assumed that in this case:

$$D_{\mathrm{inter},k,t} \approx D_{\mathrm{inter},k+1,t} \quad \text{and} \quad D_{\mathrm{intra},k,t} \approx D_{\mathrm{intra},k+1,t}$$

which allows us to determine these coefficients by means of Eqs. (22) and (23), then the corresponding concentrations.

5. Results

5.1. Benzene adsorption curves

Fig. 4 represents the variation with time of the concentration of benzene adsorbed at 25 °C in the bed of ZSM5 zeolite, 15 mm high and internal diameter 4 mm. To simplify the figure we have chosen only eight layers at 2 mm intervals of height. It must be noted that the z coordinate is determined relative to the bottom of the tube. For example, z = 15 mm (dimensionless Z = 1) corresponds to the surface of the bed directly in contact with the gas phase.

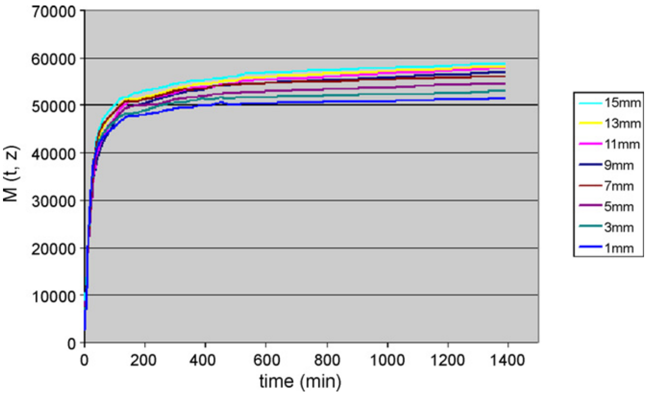


Fig. 4. Amount (arbitrary units) of adsorbed benzene against time in each layer k of the bed, from z = 15 mm (layer in contact with the gas phase) to z = 1 mm (layer near the bottom of the bed) (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.).

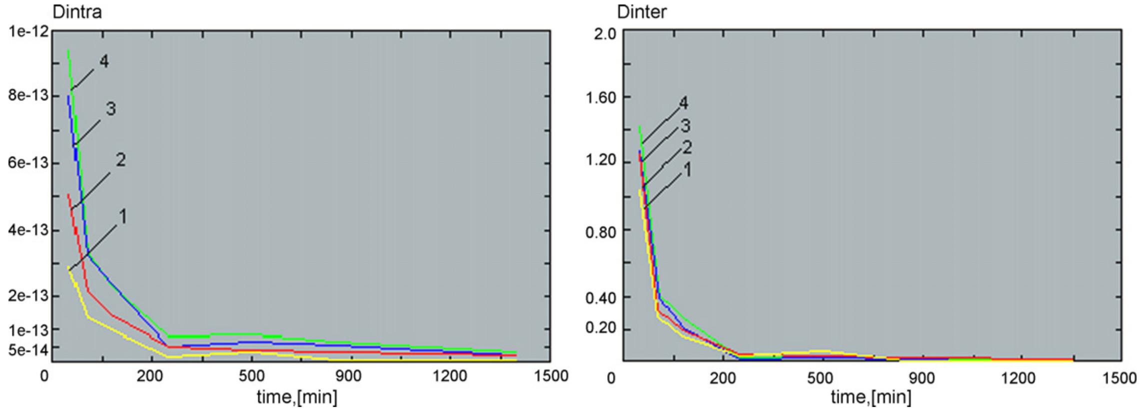


Fig. 5. Benzene diffusion coefficient profiles D_{intra} and D_{inter} ($m^2\ s^1$) against time t (min) curves: (1) $z = 14$ mm; (2) $z = 10$ mm; (3) $z = 7$ mm; (4) $z = 3$ mm.

The amount of adsorbed benzene at the equilibrium of adsorption is 1.25 mmol g^{-1}, in agreement with the references.

5.2. Numerical simulation and analysis

A program in the Microsoft Visual C++ environment was especially developed to provide the solutions of the previous equations:

- Using the experimental curves of Fig. 4, the intercrystallite D_{inter} (macropores) and the intracrystallite D_{intra} (micropores of the crystallites) diffusion coefficients;
- Using these diffusion coefficients, the concentration distribution in the intercrystallite space $C(t, Z)$, in the intracrystallite space $Q(t, X, Z)$ and the integral mass $M(t, Z)$.

We have used about 10 curves going from $z = 14$ to $z = 3$ mm. For the sake of clarity Fig. 5 shows the computed variations of D_{inter} and D_{intra} versus time at four only different distances z (in mm) from the bottom of the bed: $z = 14$; $z = 10$; $z = 7$; $z = 3$. However, the curves corresponding to other values of z fit homogeneously between these ones. D_{inter} and D_{intra} decrease approximately exponentially with time increase, which is normal since the crowding increases in parallel with the concentration of adsorbed

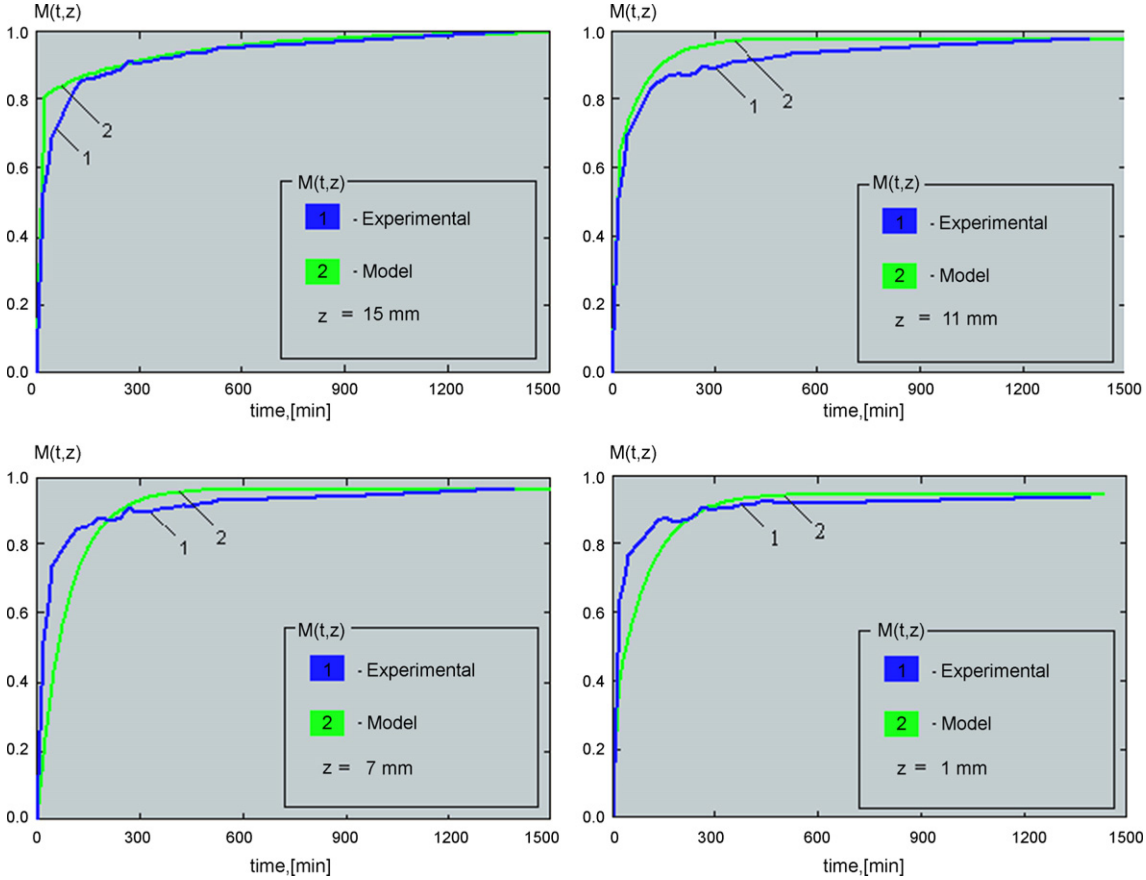


Fig. 6. Model and experimental kinetic curves of dimensionless total adsorbed mass versus time t (min) for different values of distance (mm) from the bottom of the zeolite bed z.

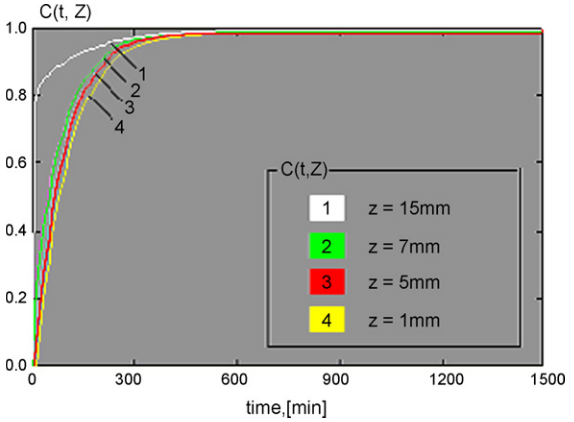


Fig. 7. Intercrystallite concentration profiles versus time *t* (min) for different values of the distance *z* (mm) from the bottom of the bed.

molecules. D_{inter} decreases from 1.4 $\mathrm{m^2\,s^{-1}}$ at the beginning of adsorption to 0.001 $\mathrm{m^2\,s^{-1}}$ near the equilibrium state. In the same way, D_{intra} decreases from 10^{-12} to 5×10^{-14} $\mathrm{m^2\,s^{-1}}$. These results are in good agreement with the references data [24,25].

It may appear surprising that the beginning of the curve corresponding to $z = 14$ mm presents a lower diffusion coefficient than the others for the same time. This is due to the fact that there is not a perfect concordance between the moment the solid comes into contact with the benzene and the acquisition of the first NMR signals. The first signals correspond then to the upper layers which have already adsorbed a significant amount of gas making thus diffusion more difficult.

Using the values of D_{inter} and D_{intra}, we can determine the concentration distributions in the intercrystallite space $C(t, z)$, in the intracrystallite space $Q(t, X, z)$ and the total adsorbed mass $M(t, z)$, for each time and position in the bed (z) and in the crystallites (z, r). For example, Fig. 6 shows the calculated and experimental kinetic curves of dimensionless total adsorbed mass $M(t, z)$ versus time t for four positions z (mm) from the bottom of the bed: $z = 15$; $z = 11$; $z = 7$; $z = 1$. The calculated variations agree satisfactory with the experimental ones.

Fig. 7 shows the concentration profiles of C_6H_6 in intercrystalline space $C(t, z)$ for four values of z. Fig. 8 presents the calculated profiles of C_6H_6 concentrations in crystallites, $Q(t, X, z)$, as a function of dimensionless distance from the crystallite center X for different times t (min) and four distances from the bottom of the crystallite bed z (mm).

6. Conclusion

The analytical solution of the equations of gas diffusion in a zeolite bed has been shown, assuming it to consist of a large number of very thin layers of solid, perpendicular to the direction

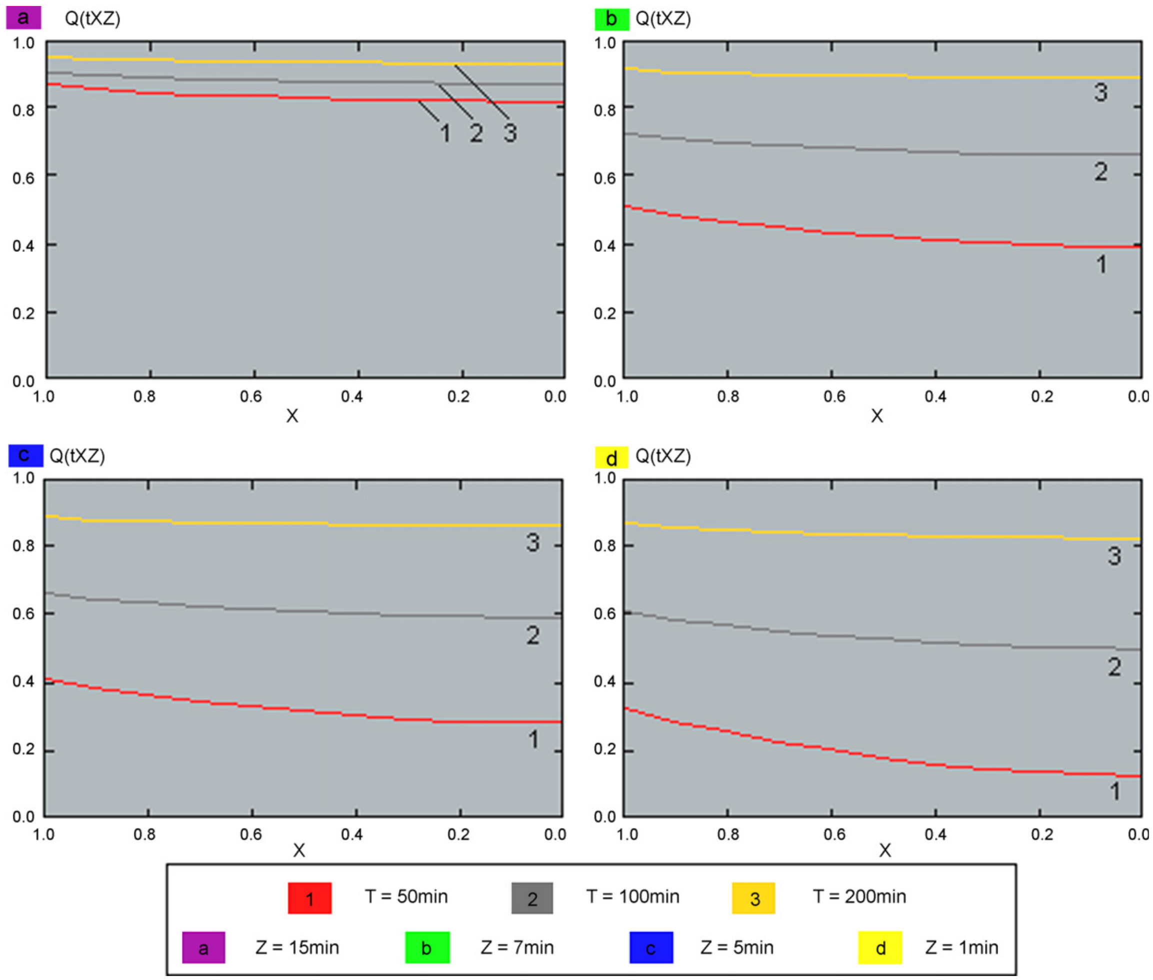


Fig. 8. Concentration profiles, $Q(t, X, z)$, in zeolite crystallites located at different positions *z* (mm) in the bed, and for different times *t* (min): (a) $z = 15$ mm; (b) $z = 7$ mm; (c) $z = 5$ mm; (d) $z = 1$ mm.

of propagation of the gas. The solution is based on the integral Laplace transformation and Cauchy methods. The analytical solution to the study of benzene diffusion in the macropores and micropores of a ZSM5 zeolite bed has been applied.

We managed to calculate the inter- and intracrystallite diffusion coefficients, D_{inter} and D_{intra} of benzene, respectively, as a function of time and the crystallite position in the bed. For each position inside the micro- and macropores of a ZSM5 bed, we have determined the variation of the concentration of this gas against time.

This technique proved to be very interesting for studying the co-diffusion of several gases in a catalytic bed, since it will make it possible to indentify the characteristic spectra of each gas at every moment and position in the bed. The first step of a general study has been presented here.

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