Adsorption and diffusion in zeolites: A computational study
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Chapter 5

Adsorption of mixtures of alkanes in Silicalite*

5.1 Introduction

In the previous chapter we have shown that our model gives a satisfactory description of the adsorption isotherms of pure n-alkanes and 2-methylalkanes for C_4-C_9 on Silicalite. In this chapter, we investigate the mixture isotherms of various alkane isomers. Experimentally, the measurement of an isotherm is more complicated for mixtures than for pure components. One not only has to measure the weight increase of the zeolite as a function of pressure, but also the change in composition of the gas mixture. To the best of our knowledge, only adsorption isotherms of mixtures of short alkanes have been measured [149,205]. In ref. [148] we have shown that for mixtures of ethane and methane our model gives a reasonable prediction of the mixture isotherms. Here we concentrate on the mixtures of C_4 through C_7 isomers.

Using the Maxwell-Stefan theory, we will closer investigate the influence of isotherm inflection on the diffusivity. When we assume that the Maxwell-Stefan diffusion coefficient (sometimes also called the corrected diffusion coefficient) is independent of the loading, the loading dependence of the conventional Fick diffusion coefficient will be completely determined by the adsorption isotherm. We will demonstrate that on the basis of mixture isotherms we can predict the membrane permeation efficiency without having to know the diffusion coefficients exactly.

5.2 Mixture Isotherms

In the previous chapter, we have focussed on adsorption of pure linear and branched alkanes on Silicalite and found that our model is able to reproduce experimental data very well. Here, we will use the same model and simulation technique to study mixtures. In figures 5.1–5.4, the mixture isotherms of C_4, C_5, C_6, and C_7 isomers are presented. We focus on a mixture of a linear alkane and the 2-methyl isomer with a 50%-50% mixture in the gas phase. Details about these simulations can be found in chapter 4. For all mixtures we see the following trends. At low pressure the linear and branched alkanes adsorb independently. The adsorption of the two components is proportional to the Henry coefficients of the pure components. At a total mixture loading of 4 molecules per unit cell the adsorption of the branched alkanes reaches a maximum and decreases with increasing pressure. For C_5, C_6 and C_7 mixtures, the branched alkane is completely removed from the zeolite. The adsorption of the linear alkanes however increases with increasing pressure till saturation is reached.

*This chapter is based on refs. [36,203,204].
It is interesting to investigate the reasons why the branched alkanes are squeezed out by the linear alkanes at high pressures. For the C₆ and C₇ isomers the Henry coefficient of the branched alkanes is slightly larger. One would therefore expect that these branched alkanes would adsorb better. This is indeed observed at low pressures; at high pressures, however, other considerations have to be taken into account. We will explain this on the basis of the mixture behavior for C₆ isomers. As can been seen from figure 5.3 the total loading exhibits inflection behavior at θ₁ + θ₂ = 4. Until this loading there is no competition between C₆ and 2-methylpentane (2MP) and both are almost equally easily adsorbed. Examination of the probability distributions of the linear and branched isomers 100 Pa reveals that all the 2MP molecules are located at the intersections between the straight channels and the zigzag channels whereas C₆ are located everywhere (see ref. [203]). A further important aspect to note is orientation of the 2MP molecules; these have their heads (i.e. the branched end) at the intersections and their tails sticking out into the zigzag or straight channels. The C₆ molecules fit nicely into both straight and zigzag channels [20]; these molecules have a higher “packing efficiency” than 2MP. As the pressure is increased beyond 100 Pa, it is more efficient to obtain higher loadings by “replacing” the 2MP with C₆; this entropic effect is the reason behind the curious maximum in the 2MP isotherm. A similar explanation holds for the C₅ and C₇ isomers. To further test our hypothesis that because of entropic reasons the branched alkanes are squeezed out the zeolite, we have performed a simulation in which we have removed the attractive part of the Lennard-Jones potential interacting between the hydrocarbon atoms and hydrocarbon-zeolite atoms. In such a system with only “hard-sphere” interactions there is no energy scale involved and the only driving force is entropy. Also in this system we have observed that the branched alkane is squeezed out at high pressures, which proves that this squeezing out of the branched alkanes by the linear isomer is an entropic effect.

There is an important advantage in being able to describe the inflection behavior accurately with the help of the dual-site Langmuir model (DSL); this is because it would then be possible to predict the mixture isotherm from only pure component data. For single components, we have
Figure 5.2: Adsorption isotherm of a 50%-50% mixture of pentane and 2-methylbutane in Silicalite.

shown in section 4.6 that the DSL gives a good description for the adsorption isotherms of linear and branched alkanes on Silicalite. Here, we consider the case that there are two adsorption sites in the zeolite. There are two ways to set up the mixture rule. In the first approach (I) we apply this rule to each of the two sites A and B separately. For each site we apply the multicomponent extension of the Langmuir isotherm [3]; for a mixture of components 1 and 2, therefore, this rule yields:

\[ \theta_A = \frac{\theta_{A1}k_{A1}p_1}{1 + k_{A1}p_1 + k_{A2}p_2} + \frac{\theta_{B1}k_{B1}p_1}{1 + k_{B1}p_1 + k_{B2}p_2} \]

\[ \theta_B = \frac{\theta_{A2}k_{A2}p_2}{1 + k_{A1}p_1 + k_{A2}p_2} + \frac{\theta_{B2}k_{B2}p_2}{1 + k_{B1}p_1 + k_{B2}p_2} \]  

where \( k_{Ai} \) and \( k_{Bi} \) are the Langmuir constants for species \( i \) for sites A and B, \( p_i \) is the partial pressure of the component \( i \) in the gas phase. We expect this mixture scenario to hold when each of the two components 1 and 2 is present in both sites.

The second scenario (II) is to apply the mixture rule to the combination of sites (A+B). This scenario is appropriate to situations in which one of the components is excluded from one particular site (say B); therefore we set up the mixing rule for the total of (A+B), i.e. the entire zeolite. To derive this mixing rule, the most convenient starting point is the right equality of equation 4.1 and the guidelines outlines in the book of Ruthven [3]. This yields for a two-component system the following set of equations:

\[ \theta_A = \frac{(\theta_{A1}k_{A1} + \theta_{B1}k_{B1})p_1 + (\theta_{A1} + \theta_{B1})k_{A1}k_{B1}p_1^2}{1 + (k_{A1} + k_{B1})p_1 + k_{A1}k_{B1}p_1^2 + (k_{A2} + k_{B2})p_2 + k_{A2}k_{B2}p_2^2} \]

\[ \theta_B = \frac{(\theta_{A2}k_{A2} + \theta_{B2}k_{B2})p_2 + (\theta_{A2} + \theta_{B2})k_{A2}k_{B2}p_2^2}{1 + (k_{A1} + k_{B1})p_1 + k_{A1}k_{B1}p_1^2 + (k_{A2} + k_{B2})p_2 + k_{A2}k_{B2}p_2^2} \]  

There are also some qualitative differences between the various alkanes. The maximum in the
isosorption of isobutane in the butane-isobutane mixture is very small and at saturation the ratio of the loadings of butane and isobutane is approximately 5.6:1 (see figure 5.1). For the pentane isomers the maximum is more pronounced and at saturation the concentration of the branched alkane is much lower, about one-sixth that of the linear alkane (see figure 5.2). For the hexane isomers at maximum loading the branched alkane is completely squeezed out of the zeolite. For the heptane isomers a table-mountain maximum is observed (see figure 5.4); here too the branched alkane is completely squeezed out at high pressures.

We see from figures 5.2–5.4 that the simulated isotherms conform very well to the mixture rule II based on the dual-site Langmuir model. For alkanes with carbon atoms in the 5–7 range, we need to set up the mixture rule considering the total Silicalite matrix (including sites A and B) as one entity. This is because the branched alkanes do not easily occupy site B (channel interiors) and for some pressure range the channel interiors are completely devoid of the branched isomers. The simulated isotherm for the 50%-50% mixture of butane-isobutane behaves differently, however. Neither mixture rule, I or II, is completely successful. An average of the two mixture rules, on the other hand, is very successful.

Figure 5.3: Adsorption isotherm of a 50%-50% mixture of hexane and 2-methylpentane in Silicalite.
Figure 5.4: Adsorption isotherm of a 50%-50% mixture of heptane and 2-methylhexane in Silicalite.

Figure 5.5: Pictorial representation of the Maxwell-Stefan diffusivities.
5.3 Consequences for Diffusion

5.3.1 The Maxwell-Stefan theory for zeolite diffusion

Using the Maxwell-Stefan theory for microporous diffusion, the following expression can be derived for diffusion of species i in a zeolite [206,207]:

\[- \frac{1}{RT} \frac{d\mu_i}{dz} = \sum_{j=1}^{n} \frac{\theta_i}{\theta_{\text{max}}} \frac{u_i - u_j}{D_{ij}} + \frac{u_i}{D_{iZ}}, \quad i = 1, 2, \ldots, n (5.3)\]

where \(-d\mu_i/dz\) is the force acting on species i tending to move it within the zeolite at a velocity \(u_i\), \(D_{iZ}\) is the Maxwell-Stefan diffusivity describing the interaction between component i and the zeolite (Z), and \(D_{ij}\) is the Maxwell-Stefan describing the interchange between components i and j within the zeolite structure. The \(D_{iZ}\) are also called the corrected diffusivity in the literature [3]. Figure 5.5 is a pictorial representation of the three Maxwell-Stefan diffusivities describing diffusion of a binary mixture consisting of species 1 and 2. Procedures for estimation of the \(D_{iZ}\) and the interchange diffusivity \(D_{ij}\) are discussed by Krishna in refs. [206,207]. If there is no possibility of interchange between species 1 and 2, the first term on the right side of equation 5.3 can be ignored. Writing equation 5.3 in terms of the diffusion fluxes \(N_i\)

\[N_i = \rho \theta_i u_i (5.4)\]

we get

\[- \frac{\theta_i}{RT} \frac{d\mu_i}{dz} = \sum_{j=1}^{n} \frac{\theta_i N_i - \theta_i N_j}{\rho \theta_{\text{max}} D_{ij}} + \frac{N_i}{\rho D_{iZ}}, \quad i = 1, 2, \ldots, n (5.5)\]

where \(\theta_i\) is the molecular loading within the zeolite, expressed in molecules per unit cell, \(\theta_{\text{max}}\) is the maximum molecular loading, \(\theta_{\text{max}} = (\theta_A + \theta_B)\), and \(\rho\) represents the number of unit cells per \(m^3\) of Silicalite.

The chemical potential gradients are related to the gradients in the component loadings by

\[\frac{\theta_i}{RT} \frac{d\mu_i}{dz} = \sum_{j=1}^{n} \Gamma_{ij} \frac{d\theta_j}{dz}; \quad \Gamma_{ij} = \frac{\theta_i}{\rho_i} \frac{\partial p_i}{\partial \theta_j}; \quad i, j = 1, 2, \ldots, n (5.6)\]

where we have defined a matrix of thermodynamic correction factors \([\Gamma]\). The elements \(\Gamma_{ij}\) of this matrix can be determined from a knowledge of the sorption isotherms. Combining these equations we can write down an explicit expression for the fluxes \(N_i\) using n-dimensional matrix notation

\[(N) = -\rho [B]^{-1} [\Gamma] \frac{d(\theta)}{dz} (5.7)\]

where the elements of the matrix \([B]\) are

\[B_{ii} = \frac{1}{D_{iZ}} + \sum_{j \neq i} \frac{\theta_i}{\theta_{\text{max}}} \frac{1}{D_{ij}}; \quad B_{ij} = -\frac{\theta_i}{\theta_{\text{max}}} \frac{1}{D_{ij}} (i \neq j) (5.8)\]

The more commonly used Fick diffusivity matrix is defined as

\[(N) = -\rho [D] \frac{d(\theta)}{dz} (5.9)\]
Comparing these equations we obtain the following inter-relation between the Fick and the Maxwell-Stefan diffusivities

\[ [D] = [B]^{-1} \Gamma \]  \hspace{1cm} (5.10)

Since the thermodynamic correction factor matrix \([\Gamma]\) is generally non-diagonal, the matrix of Fick diffusivities is also generally non-diagonal. Generally speaking the Maxwell-Stefan diffusivities \(D_{12}\) are better behaved than the elements of Fick diffusivity matrix \([D]\). The latter diffusivities are strongly influenced by the thermodynamic non-idealities in the system. In this work we examine, in turn, the influence of \([\Gamma]\) on the diffusion behavior of single components and binary mixtures in Silicalite for which the isotherms are described by the dual-site Langmuir model.

### 5.3.2 Diffusion of a single component in Silicalite

For single component diffusion equations 5.5 and 5.8 degenerate to their scalar forms

\[ \Gamma = \frac{\theta \partial p}{p \partial \theta} \]  \hspace{1cm} (5.11)

and

\[ D = \Gamma \Theta \]  \hspace{1cm} (5.12)

For the DSL model isotherm, the thermodynamic factor can be determined by analytic differentiation of equation 4.1; the result is

\[ \Gamma = \frac{\left[1 + (k_A + k_B)\partial p + k_A k_B p^2\right]^2}{\left[(\theta_A k_A + \theta_B k_B) + 2\theta_{\text{max}} k_A k_B \left[1 + (k_A + k_B)\partial p + k_A k_B p^2\right]\right] \partial p} - \left[(\theta_A k_A + \theta_B k_B)\partial p + \theta_{\text{max}} k_A k_B p^2\right] \left[(k_A + k_B) + 2k_A k_B p\right] \frac{\theta}{p} \]  \hspace{1cm} (5.13)

This correction factor shows two extrema: a maximum at the inflection point \(\theta_A = 4\) and a minimum at a loading \(\theta_A < \theta < \theta_B\). This behavior is illustrated for adsorption of benzene on Silicalite at temperatures of 303K and 323K; see figure 5.6. Since the Fick diffusivity is proportional to the thermodynamic factor, it can be expected to also exhibit two extrema. This is indeed verified by the experimental data of Shah et al. [208] for Fick diffusivity at 303K and 323K; see figure 5.6. The Maxwell-Stefan diffusivities, calculated from equation 5.12 are seen to be practically constant, emphasizing the importance of thermodynamic correction factors on the diffusion behavior.

### 5.3.3 Diffusion of binary mixtures

For diffusion of a binary mixture in Silicalite equations 5.5 and 5.8 reduce to

\[ (N) = -\rho [D] \frac{d(\theta)}{dz} ; \quad [D] = \begin{bmatrix} \frac{1}{\Theta_{11Z}} & \frac{1}{\Theta_{12Z}} & -\frac{1}{\Theta_{12\theta_{\text{max}}}} \\ -\frac{1}{\Theta_{12\theta_{\text{max}}}} & \frac{1}{\Theta_{22Z}} & \frac{1}{\Theta_{22\theta_{\text{max}}}} \end{bmatrix}^{-1} \begin{bmatrix} \Gamma_{11} & \Gamma_{12} \\ \Gamma_{21} & \Gamma_{22} \end{bmatrix} \]  \hspace{1cm} (5.14)

The interchange mechanism is often ignored and the following formulation used

\[ (N) = -\rho [D] \frac{d(\theta)}{dz} ; \quad [D] = \begin{bmatrix} \Theta_{11Z} & 0 \\ 0 & \Theta_{22Z} \end{bmatrix} \begin{bmatrix} \Gamma_{11} & \Gamma_{12} \\ \Gamma_{21} & \Gamma_{22} \end{bmatrix} \]  \hspace{1cm} (5.15)
Adsorption of mixtures of alkanes in Silicalite

Figure 5.6: Thermodynamic correction factors (top) and diffusivities (bottom) for diffusion of benzene in Silicalite at (left) 303K and (right) 323K. The experimental diffusivity data are from Shah et al. [208].

Recent work of Van de Graaf et al. [209] and Kapteijn et al. [210] has shown that for diffusion of binary mixtures in Silicalite, the complete Maxwell-Stefan formulation, equation 5.14, taking interchange into account provides a much better description of binary permeation experimental results across a Silicalite membrane than with a model ignoring the interchange mechanism (portrayed by $\mathcal{D}_{12}$).

To calculate the $\Gamma_{ij}$ we need the sorption isotherms for mixtures. However, experimental data on sorption isotherms of mixtures are scarce. To illustrate the influence of $\Gamma_{ij}$ on the diffusion we consider a mixture of n-hexane (n-C$_6$) and 3-methylpentane (3MP) and use the Configurational-Bias Monte Carlo (CBMC) simulation technique described earlier (see chapters 2 and 4) to generate the pure component and 50%-50% mixture isotherm data at 362K. The results of these CBMC simulations are shown in figure 5.7. The continuous lines in 5.7 are DSL fits of the pure component isotherms (parameter values are given in the caption). The mixture isotherms are well represented by the DSL mixture model (equation 5.2, mixing rule II) as can be seen in figure 5.7 wherein the mixture isotherms are predicted using only pure component data. The branched alkane 3MP exhibits a maximum with respect to molecular loading within the Silicalite structure, this is similar for a mixture of 2MP and hexane.

The four elements of $\Gamma_{ij}$ can be obtained by analytic differentiation of equation 5.6. The result is

$$\Gamma = \begin{bmatrix} A_3 (B_2 - \theta_2 B_4)/p_1 & A_3 \theta_1 B_4/p_1 \\ B_3 \theta_2 A_4/p_2 & B_3 (A_2 - \theta_1 A_4)/p_2 \end{bmatrix}$$

$$A_2 B_2 - \theta_1 A_4 B_2 - \theta_2 A_2 B_4$$

(5.16)
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where

\[
\begin{align*}
A_2 &= (\theta_{1A} k_{1A} + \theta_{1B} k_{1B}) + 2 (\theta_{1A} + \theta_{1B}) k_{1A} k_{1B} p_1 \\
A_3 &= (\theta_{1A} k_{1A} + \theta_{1B} k_{1B}) p_1 + (\theta_{1A} + \theta_{1B}) k_{1A} k_{1B} p_1^2 \\
A_4 &= (k_{1A} + k_{1B}) + 2 k_{1A} k_{1B} p_1 \\
B_2 &= (\theta_{2A} k_{2A} + \theta_{2B} k_{2B}) + 2 (\theta_{2A} + \theta_{2B}) k_{2A} k_{2B} p_2 \\
B_3 &= (\theta_{2A} k_{2A} + \theta_{2B} k_{2B}) p_2 + (\theta_{2A} + \theta_{2B}) k_{2A} k_{2B} p_2^2 \\
B_4 &= (k_{2A} + k_{2B}) + 2 k_{2A} k_{2B} p_2
\end{align*}
\] (5.17)

To demonstrate the consequences of the influence of \( \Gamma_{ij} \) on diffusion, consider the permeation of hydrocarbon isomers across a Silicalite membrane (figure 5.8). To obtain the values of the permeation fluxes \( N_i \) we need to solve the set of two coupled partial differential equations:

\[
\frac{\partial (\theta)}{\partial t} = - \frac{\partial}{\partial z} \left( \left[ D \right] \frac{\partial (\theta)}{\partial z} \right)
\] (5.18)

subject to the initial and boundary conditions

\[
t = 0; \ 0 \leq z \leq \delta; \ \theta_{iz} = 0
\] (5.19)

\[
t > 0; \ z = 0; \ i = 1, 2
\]

\[
\theta_{i0} = \frac{(\theta_{iA} k_{iA} + \theta_{iB} k_{iB}) p_{i0} + (\theta_{iA} + \theta_{iB}) k_{iA} k_{iB} p_{i0}^2}{1 + (k_{1A} + k_{1B}) p_{10} + k_{1A} k_{1B} p_{10}^2 + (k_{2A} + k_{2B}) p_{20} + k_{2A} k_{2B} p_{20}^2}
\] (5.20)

The set of two coupled partial differential equations (equation 5.18) subject to the initial and boundary conditions (equations 5.19 and 5.20) were solved using the method of lines [211] to determine the fluxes, as described in ref. [212]. In the calculations presented here we assume that the pure component Maxwell-Stefan diffusivities are identical for the isomers, i.e. \( \mathcal{D}_{1z} = \mathcal{D}_{2z} \); this assumption is a conservative one from the viewpoint of separation of the isomers as we expect the branched isomer to have a lower mobility within the Silicalite structure. The simulations were carried out with the complete Maxwell-Stefan model for \( [D] \), i.e. equation 5.14. Since the interchange coefficient \( \mathcal{D}_{12} \) has a value intermediate between \( \mathcal{D}_{1z} \) and \( \mathcal{D}_{2z} \) [213] we must also have \( \mathcal{D}_{1z} = \mathcal{D}_{2z} = \mathcal{D}_{12} \). A further point to note is that in the calculation of the fluxes we have made the assumption that the Maxwell-Stefan diffusivities are independent of the loading. Though this assumption is not always true (see refs. [214, 215]), the values of the ratio of fluxes, i.e. selectivity for separation, is not expected to be influenced by this assumption.

The transient fluxes for the \( C_6 \) isomers are presented in figure 5.9 in dimensionless form. Examination of the transient fluxes reveals a slight maximum in the flux of the branched alkanes; this maximum is a direct consequence of the corresponding maximum in mixture isotherms; see figure 5.7. The ratio of the fluxes of \( n-C_6 \) and 3MP is found to be 32. There is some evidence in the published literature for permeation of a 50%-50% mixture of \( n-C_6 \) and 3MP at 362K across a Silicalite membrane [216] to suggest that this high selectivity values for separation of the \( C_6 \) isomers can be realized in practice. These high selectivities are entirely due to the strong inflection observed for the branched alkane; this is described by a much lower value of the Henry coefficient \( k_B \) for site B than for the linear alkane. If both sites A and B had the same sorption capability, then the selectivity for the separation would be close to unity. Another important point to note is that in the membrane permeation experiment we must ensure that the values of the upstream partial pressures of the hydrocarbon isomers are high enough (say higher than 5 kPa) to ensure that the branched alkane is virtually "excluded". More details about temperature and pressure dependence of the permeation selectivity can be found in ref. [203].
Figure 5.7: Pure component and 50%-50% mixture isotherms at 362K in Silicalite. The open square and circle symbols represent the CBMC simulations for (1) n-C₆ and (2) 3MP respectively. The continuous and dashed lines are the dual-site Langmuir (DSL) fits with the parameter values determined only from pure component CBMC simulation data. The dual-site Langmuir parameter values are for n-C₆: θ₁A = 4, θ₁B = 4, k₁A = 0.07 Pa⁻¹, k₁B = 2 × 10⁻³ Pa⁻¹ and for 3MP: θ₂A = 4, θ₂B = 4, k₂A = 0.045 Pa⁻¹, k₂B = 5 × 10⁻⁶ Pa⁻¹.
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Figure 5.8: Schematic representation of a Silicalite membrane separation process for separation of C₆ isomers.

Figure 5.9: Transient diffusion fluxes for permeation of n-C₆ and 3MP across a Silicalite membrane. The conditions used in the simulations are identical to those used in the experiments of Funke et al. [216]. The upstream and downstream compartments are maintained at a total pressure of 84 kPa (atmospheric pressure at Boulder, Colorado, USA). In the upstream compartment the hydrocarbons account for 18 mole %, the remainder being inert gas helium. The partial pressures of n-C₆ and 3MP in the upstream compartment work out to 0.18 × 42 kPa for each isomer. An excess of sweep gas in the downstream compartment ensures that the partial pressures of the hydrocarbons are virtually zero.
5.4 Conclusions

- CBMC simulations of isotherms of 50%-50% binary mixtures of C₅, C₆ and C₇ hydrocarbon isomers showed some remarkable and hitherto unreported features. The loading of the branched isomer in all three binary mixture reaches a maximum when the total mixture loading corresponds to 4 molecules per unit cell. Higher loadings are obtained by “squeezing out” of the branched alkane from the Silicalite and replacing these with the linear alkane. This “squeezing out” effect is found to be entropic in nature; the linear alkanes have a higher packing efficiency and higher loadings are more easily achieved by replacing the branched alkanes with the linear alkanes.

- The mixture isotherms can be predicted quite accurately by applying the appropriate mixture rule to the dual-site Langmuir model. This model allows the mixture isotherm to be predicted purely on the basis of the parameters describing the isotherms of the pure components, linear and branched alkane.

- The sorption selectivity exhibited by Silicalite for the linear alkane in preference to the branched alkane in mixtures of C₅, C₆ and C₇ hydrocarbon isomers, provides a potential for the development of a novel separation technique based on entropy driven sorption selectivity [203].