SUPPORTING INFORMATION

Competitive Diffusion of Gases in a Zeolite Bed: NMR and Slice Selection Procedure, Modelling and Parameter Identification

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Appendix A. Supplementary data

The mathematical methodology of parameter identification and modelling competitive diffusion in a microporous crystallite bed

The methodology for solving the direct boundary problem (eqs 1- 6), which describes the diffusion process in a heterogeneous nanoporous bed is developed in ref.1. According to ref.2 the procedure for determining the diffusion coefficients (eqs 8) requires a special technique for calculating the gradients $\nabla J^{n}_{D_{\mathrm{intra}_{sk}}}(t)$, $\nabla J^{n}_{D_{\mathrm{inter}_{sk}}}(t)$ of the residual functional (eq 9), which is a major component of formulas (eq 8). This leads to the problem of optimizing the extended Lagrange functional[2,3].

$$\Phi\left(D_{\mathrm{inter}_{sk}}, D_{\mathrm{intra}_{sk}}\right) = J_s + I_{s_1} + I_{s_2}, \tag{A.1}$$

where I_{s_1}, I_{s_2} are the components given by equations A2 and A3, corresponding to the micro (index 1)-and meso-(index 2) porosity, respectively:

$$I_{s_1} = \int_0^T \int_{L_{k-1}}^{L_k} \phi_{s_k}(t,Z) \left(\frac{\partial C_{s_k}}{\partial t} - \frac{D_{\mathrm{inter}_{sk}}}{l^2} \frac{\partial^2 C_{s_k}}{\partial Z^2} + e_{\mathrm{inter}_k} K_{s_k} \frac{D_{\mathrm{intra}_{s_k}}}{R^2} \left(\frac{\partial Q(t,X,Z)_{s_k}}{\partial X} \right)_{X=1} \right) dZdt, \quad \text{(A.2)}$$

$$I_{s_2} = \int_0^T \int_0^1 \int_{L_{k-1}}^{L_k} \psi_{s_k}(t,X,Z) \left(\frac{\partial Q_{s_k}(t,X,Z)}{\partial t} - \frac{D_{\mathrm{intra}_{sk}}}{R^2} \left(\frac{\partial^2 Q_{s_k}}{\partial X^2} + \frac{2}{X} \frac{\partial Q_{s_k}}{\partial X} \right) \right) XdXdZdt, \quad \text{(A.3)}$$

where J_s is the residual functional (eq 9), ϕ_{s_k}, ψ_{s_k}, $s, = \overline{1,2}$ – unknown factors of Lagrange, to be determined from the stationary condition of the functional $\Phi\left(D_{\mathrm{inter}_{\mathrm{sk}}}, D_{\mathrm{intra}_{\mathrm{sk}}}\right)^{4,5}$:

$$\Delta\Phi\left(D_{\mathrm{inter}_{\mathrm{sk}}}, D_{\mathrm{intra}_{\mathrm{sk}}}\right) \equiv \Delta J_s + \Delta I_{s_1} + \Delta I_{s_2} = 0 \ . \quad \text{(A.4)}$$

The calculation of the components in eq. (A.4) is carried out by assuming that the values $D_{\mathrm{inter}_{\mathrm{sk}}}, D_{\mathrm{intra}_{\mathrm{sk}}}$ are incremented by $\Delta D_{\mathrm{inter}_{\mathrm{sk}}}$, $\Delta D_{\mathrm{intra}_{\mathrm{sk}}}$. As a result, concentration $C_{s_k}(t,Z)$ changes by increment $\Delta C_{sk}(t,Z)$ and concentration $Q_{s_k}(t,X,Z)$ by increment $\Delta Q_{s_k}(t,X,Z)$, $s = \overline{1,2}$.

Conjugate problem. The calculation of the increments $\Delta J_s, \Delta J_{s_1}$, ΔJ_{s_2} in eq A.4 (using integration by parts and the initial and boundary conditions of the direct problem (eqs 1- 6), leads to solving the additional conjugate problem to determine the Lagrange factors ϕ_{s_k}, ψ_{s_k} of the functional (eq A.1):

$$\left. \frac{\partial \phi_{s_k}(t,Z)}{\partial t} + \frac{D_{\mathrm{inter}_{sk}}}{l^2} \frac{\partial^2 \phi_{s_k}}{\partial Z^2} + e_{\mathrm{inter}_k} K_{s_k} \frac{D_{\mathrm{intra}_{s_k}}}{R^2} \frac{\partial \psi_{s_k}(t,X,Z)}{\partial X} \right|_{X=1} = E^n_{s_k}(t) \delta\left(Z - h_k\right) \quad \text{(A.5)}$$

where $E^n_{s_k}(t) = C_{s_k}\left(D^n_{\mathrm{intra}_{sk}}, D^n_{\mathrm{inter}_{sk}}; t, h_k\right) + \bar{Q}_{s_k}\left(D^n_{\mathrm{intra}_{sk}}, D^n_{\mathrm{inter}_{sk}}; t, h_k\right) - M_{sk}(t)$,

$\delta\left(Z - h_k\right)$ - function of Dirac[1].

$$\frac{\partial\psi_{s_k}(t,X,Z)}{\partial t}+\frac{D_{\mathrm{intra}_{sk}}}{R^2}\left(\frac{\partial^2\psi_{s_k}}{\partial X^2}+\frac{2}{X}\frac{\partial\psi_{s_k}}{\partial X}\right)=E^n_{s_k}(t)\delta(Z-h_k). \tag{A.6}$$

$$\phi_{s_k}(t,Z)_{|t=T}=0;\ \psi_{s_k}(t,X,Z)_{|t=T}=0 \text{ (conditions at } t=T\text{)}; \tag{A.7}$$

$$\frac{\partial}{\partial X}\psi_{s_k}(t,X,Z)_{|X=0}=0;\ \psi_{s_k}(t,X,Z)_{|X=1}=\varphi_{s_k}(t,Z); \tag{A.8}$$

$$\phi_{s_k}(t,Z=L_k)=0,\ \phi_{s_{k-1}}(t,Z=L_{k-1})=0;\ s=\overline{1,2},\ k=\overline{N,2}, \tag{A.9}$$

$$\phi_{s_1}(t,L_1)=0,\ \frac{\partial\phi_{s_1}}{\partial Z}(t,Z=0)=0, \tag{A.10}$$

We have obtained the solution ϕ_{sk}, ψ_{sk} of the conjugate problem (eqs A.5 - A.10) by the procedure described in ref.1 using Heaviside's operational method:

$$\phi_{sk}(t,Z)=-\frac{\Delta L^2}{D_{\mathrm{inter}_{sk}}}\int_0^t \mathcal{H}^{inter}_{sk}(t-\tau,Z)E^n_{s_k}(\tau)\,d\tau,\qquad s=\overline{1,2},\ k=\overline{1,N}. \tag{A.11}$$

$$\Psi_{sk}(t,X,Z)=-\frac{\Delta L^2}{D_{\mathrm{inter}_{sk}}}\int_0^t\left(\mathcal{H}^{intra}_{sk}(t-\tau,X,Z)+\mathcal{IE}_{sk}(t-\tau,X)\delta(Z-h_k)\right)E^n_{s_k}(\tau)\,d\tau,\ s=\overline{1,2},\ k=\overline{1,N}, \tag{A.12}$$

$$\mathcal{H}^{inter}_{sk}(t,Z)=\frac{4R^2}{\Delta L^2}\frac{e_{\mathrm{inter}_k}}{3}\frac{D_{\mathrm{inter}_{sk}}}{D_{\mathrm{intra}_{sk}}}\sum_{n=0}^{\infty}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\Phi_{sk_{nij}}(t,Z),$$

$$\mathcal{H}^{intra}_{sk}(t,Z)=\frac{4R^2}{\Delta L^2}\frac{e_{\mathrm{inter}_k}}{3}\frac{D_{\mathrm{inter}_{sk}}}{D_{\mathrm{intra}_{sk}}}\sum_{n=0}^{\infty}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\Phi_{sk_{nij}}(t,Z)\frac{\sin\left(\beta_{sk_{jn}}X\right)}{\sin\left(\beta_{sk_{jn}}\right)}, \tag{A.13}$$

where β_{sk_i} are the roots of the transcendental equation, $\frac{e_{\mathrm{inter}_1}}{3}\beta^2-\beta ctg\beta+1=0$,

$p_{sk_i}=\frac{D_{\mathrm{intra}_{sk}}}{R^2}\beta^2_{sk_i}$; and $\beta_{sk_{ij}}$, $\beta_{s\,l_{ij}}$ the roots of transcendental equations, respectively:

$$\frac{e_{\mathrm{inter}_k}}{3}\beta^2-\beta ctg\beta+\left(1-\frac{e_{\mathrm{inter}_k}}{3}\frac{3}{R^2}\frac{\Delta L^2}{D_{\mathrm{inter}_{sk}}}\frac{D_{\mathrm{intra}_{sk}}}{\Delta L}\frac{n}{\Delta L}\pi\right)=0,\ n=\overline{0,\infty},\ k=\overline{2,N},$$

$$\frac{e_{\mathrm{inter}_1}}{3}\beta^2-\beta ctg\beta+\left(1-\frac{e_{\mathrm{inter}_1}}{3}\frac{3}{R^2}\frac{\Delta L^2}{D_{\mathrm{inter}_{s1}}}\frac{D_{\mathrm{intra}_{s1}}}{2\Delta L}\frac{2n-1}{2\Delta L}\pi\right)=0,\ n=\overline{1,\infty}; \tag{A.14}$$

$$\Phi_{sk_{nij}}(t,Z)=\omega\left(\beta_{sk_i}\right)\omega\left(\beta_{sk_{ij}}\right)\frac{B_{sk}\left(Z,\beta_{sk_{ij}}\right)}{\Delta L(-1)^j}\frac{e^{\frac{\mathrm{D}_{\mathrm{intra}_{sk}}}{R^2}\beta^2_{sk_{ij}}t}-e^{\frac{\mathrm{D}_{\mathrm{intra}_{sk}}}{R^2}\beta^2_{sk_i}t}}{\frac{\mathrm{D}_{\mathrm{intra}_{sk}}}{R^2}\left(\beta^2_{sk_i}-\beta^2_{sk_{ij}}\right)},$$

$$\omega(\beta)=\frac{\sqrt{\frac{e_{\mathrm{inter}_k}}{3}+\frac{cot\beta}{\beta}-\frac{1}{\beta^2}}}{\left[\frac{cot\beta}{\beta}-\frac{1}{sin^2\beta}+\frac{2e_{\mathrm{inter}_k}}{3}\right]},$$

$$\begin{aligned}B_{sk}(Z,\beta)=&\ sin\left(\gamma_{sk}(\beta)(Z-L_{k-1})\right)sin\left(\gamma_{sk}(\beta)(L_k-h_k)\right)+\\&+sin\left(\gamma_{sk}(\beta)(h_k-L_{k-1})\right)sin\left(\gamma_{sk}(\beta)(L_k-Z)\right)\end{aligned},$$

$$\gamma_{sk}(\beta)=\left(\frac{3}{e_{\mathrm{inter}_k}}\frac{\mathrm{D}_{\mathrm{intra}_{sk}}}{\mathrm{D}_{\mathrm{inter}_{sk}}}\frac{\Delta L^2}{\mathrm{R}^2}\left[\frac{e_{\mathrm{inter}_k}}{3}\beta^2+\beta cot\beta-1\right]\right)^{\frac{1}{2}},$$

$$\mathcal{IE}_{sk}(t,X)=-\frac{D_{\mathrm{intra}_k}}{R^2}\left[1+\sum_{i=1}^{\infty}(-1)^i\begin{pmatrix}\sin\bar\beta_{sk_i}X\left[1-\cos\bar\beta_{sk_i}(1-X)\right]-\\-\sin\bar\beta_{sk_i}(1-X)\left[1-\cos\bar\beta_{sk_i}X\right]\end{pmatrix}e^{\bar\beta^2_{sk_i}}\right]. \tag{A.15}$$

Relationship between the direct (eqs 1 - 6) and the conjugate (eqs A.5 - A.10) problems

Substituting in the direct problem (1) - (6) $D_{\mathrm{inter_{sk}}}, D_{\mathrm{intra_{sk}}}$, $C_{s_k}(t,Z)$ and $Q_{s_k}(t,X,Z)$ by the corresponding values with increments $D_{\mathrm{inter_{sk}}}+\Delta D_{\mathrm{inter_{sk}}}$, $D_{\mathrm{intra_{sk}}}+\Delta D_{\mathrm{intra_{sk}}}$, $C_{s_k}(t,Z)+\Delta C_{s_k}(t,z)$

and $Q_{s_k}(t,X,Z)+\Delta Q_{s_k}(t,X,Z)$, and subtracting the first equations from the transformed ones and neglecting second-order terms of smallness, we obtain basic equations of the problem (eqs 1 - 6) in terms of increments $\Delta C_{s_k}(t,Z)$ and $\Delta Q_{s_k}(t,X,Z)$, $s=\overline{1,2}$ in the operator:

$$\mathcal{L}w_{s_k}(t,X,Z)=\mathrm{X}_{s_k},\ w_{s_k}\in(0,1)\quad \Omega_{kT},\ k=\overline{1,N}, \tag{A.16}$$

Similarly, we write the system of the basic equations of conjugate boundary problem (A.5-A.10) in the operator:

$$\mathcal{L}^*\Psi_{s_k}(t,X,Z)=E_{s_k}(t)\delta\left(Z-h_k\right),\ \Psi_{s_k}\in(0,1)\quad \Omega_{kT},\ k=\overline{1,N}, \tag{A.17}$$

where $$\mathcal{L}=\begin{bmatrix} \dfrac{\partial}{\partial t}-\dfrac{\partial}{\partial Z}\left(D_{\text{inter}_{sk}}\dfrac{\partial}{\partial Z}\right) & e_{\text{int}\,er_k}\dfrac{D_{\text{intra}_{sk}}}{R}\dfrac{\partial}{\partial X}\Big|_{X=1} \\ 0 & \dfrac{\partial}{\partial t}-\dfrac{D_{\text{intra}_{sk}}}{R^2}\left(\dfrac{\partial^2}{\partial X^2}+\dfrac{2}{X}\dfrac{\partial}{\partial X}\right) \end{bmatrix},$$

$$\mathcal{L}^*=\begin{bmatrix} \dfrac{\partial}{\partial t}+\dfrac{\partial}{\partial Z}\left(D_{\text{inter}_{sk}}\dfrac{\partial}{\partial Z}\right) & e_{\text{int}\,er_k}\dfrac{D_{\text{intra}_{sk}}}{R^2}\dfrac{\partial}{\partial X}\Big|_{X=1} \\ 0 & \dfrac{\partial}{\partial t}+\dfrac{D_{\text{intra}_{sk}}}{R^2}\left(\dfrac{\partial^2}{\partial X^2}+\dfrac{2}{X}\dfrac{\partial}{\partial X}\right) \end{bmatrix},$$

$$w_{s_k}(t,X,Z)=\begin{bmatrix} \Delta C_{s_k}(t,Z) \\ \Delta Q_{s_k}(t,X,Z) \end{bmatrix},\ \Psi_{s_k}(t,X,Z)=\begin{bmatrix} \phi_{s_k}(t,Z) \\ \psi_{s_k}(t,X,Z) \end{bmatrix}.$$

$$\mathrm{X}_{s_k}(t,X,Z)=\begin{bmatrix} \dfrac{\partial}{\partial Z}\left(\Delta D_{\text{inter}_{sk}}\dfrac{\partial}{\partial Z}C_{s_k}\right)-e_{\text{int}\,er_k}\dfrac{\Delta D_{\text{intra}_{sk}}}{R^2}\dfrac{\partial}{\partial X}Q_{s_k}(t,X,Z)_{X=1} \\ \dfrac{\Delta D_{\text{intra}_{sk}}}{R^2}\left(\dfrac{\partial^2}{\partial X^2}+\dfrac{2}{X}\dfrac{\partial}{\partial X}\right)Q_{s_k}(t,X,Z) \end{bmatrix}, \tag{A.18}$$

where $\mathcal{L}^*$ is the conjugate Lagrange operator of operator $\mathcal{L}$.

Obtaining the increment formula of the residual functional. The calculated increment of the residual functional (eq 9), neglecting second-order terms, has the form:

$$\Delta J_s\left(D_{\text{inter}_{sk}}, D_{\text{intra}_{sk}}\right) = \int_0^T E_{s_k}(t)\left(\Delta C_{s_k} + \Delta \bar{Q}_{s_k}\right)dt = \int_0^T \int_{L_{k-1}}^{L_k} E_{s_k}(t)\Delta C_{s_k}\delta\left(Z-h_k\right)dZdt + \int_0^T \int_{L_{k-1}}^{L_k} \int_0^1 E_{s_k}(t)\delta\left(Z-h_k\right)\Delta Q_{s_k} XdXdZdt$$

Using the change of variable $w_{s_k} = \mathcal{L}^{-1}\mathrm{X}_{s_k}$, where $\mathcal{L}^{-1}$ is the inverse operator of operator $\mathcal{L}$, we obtain

$$\begin{aligned}\Delta J_s\left(D_{\text{intra}_{sk}}, D_{\text{inter}_{sk}}\right) &= \int_0^T \int_{L_{k-1}}^{L_k} \mathcal{L}^{-1}\mathrm{X}_{s_{k,1}}(t,Z)\cdot E_{s_k}(t)\delta\left(Z-h_k\right)dZdt + \\ &+ \int_0^T \int_{L_{k-1}}^{L_k} \int_0^1 \mathcal{L}^{-1}\mathrm{X}_{s_{k2}}(t,X,Z)\cdot E_{s_k}(t)\delta\left(Z-h_k\right)XdXdZdt\end{aligned} \tag{A.19}$$

Defining the scalar product:

$$\left(\mathcal{L}w_{s_k}(t,X,Z), \Psi_{s_k}(t,X,Z)\right) = \begin{bmatrix} \iint\limits_{\Omega_{kT}} \mathcal{L}\Delta C_{s_k}(t,Z)\phi_{s_k}(t,Z)dZdt \\ \iiint\limits_{(0,R)\ \Omega_{kT}} \mathcal{L}\Delta Q_{s_k}(t,X,Z)\psi_{s_k}(t,X,Z)XdXdZdt \end{bmatrix}, \tag{A.20}$$

and taking into account (eq A.19) Lagrange's identity[2,3]:

$$\left(\mathcal{L}w_{s_k}(t,X,Z), \Psi_{s_k}(t,X,Z)\right) = \left(w_{s_k}(t,X,Z), \mathcal{L}^{*}\Psi_{s_k}(t,X,Z)\right) \tag{A.21}$$

and the equality: $\mathcal{L}^{-1*}\left[E_{s_k}(t)\delta\left(Z-h_k\right)\right] = \Psi_{s_k}$, we obtain the increment of the residual functional expressed by the solution of conjugate problem (eqs A.6 - A.10) and the vector of the right-hand parts of equations A.18:

$$\Delta J_s\left(D_{\text{inter}_{sk}}, D_{\text{intra}_{sk}}\right) = \left(\Psi_{s_k}(t,X,Z),\ \mathrm{X}_{s_k}(t,X,Z)\right), \tag{A.22}$$

where $\phi_{s_k}(t,Z)$ and $\psi_{s_k}(t,X,Z)$ belong to $\bar{\Omega}_{kT}$ and $[0,1]$ $\bar{\Omega}_{kT}$, respectively; $\mathcal{L}^{-1*}$ - conjugate operator to inverse operator $\mathcal{L}^{-1}$, Ψ_{s_k} - solution of conjugate problem (eqs A.5 - A.10).

Reporting in equation (A.22) the components $\mathrm{X}_{s_k}(t, X, Z)$ taking into account the equality (eq A.18), we obtain the formula which establishes the relationship between the direct problem (eqs 1 - 6) and the conjugate problem (eqs A.6 - A.10) and which makes it possible to obtain the analytical expressions of components of the residual functional gradient:

$$\Delta J_s\left(D_{\mathrm{intra}_{\mathrm{sk}}}, D_{\mathrm{inter}_{\mathrm{sk}}}\right)=\begin{matrix}\left(\phi_{s_k}(t,Z),\ \frac{\partial}{\partial Z}\left(\Delta D_{\mathrm{inter}_{\mathrm{sk}}}\frac{\partial}{\partial Z}C_{s_k}\right)-e_{\mathrm{int}\,er_k}\frac{\Delta D_{\mathrm{intra}_{\mathrm{sk}}}}{R^2}\frac{\partial}{\partial X}Q_{s_k}\left(t,X,Z\right)_{X=1}\right)+ \\ +\left(\psi_{s_k}(t,X,Z),\ \frac{\Delta D_{\mathrm{intra}_{\mathrm{sk}}}}{R^2}\left(\frac{\partial^2}{\partial X^2}+\frac{2}{X}\frac{\partial}{\partial X}\right)Q_{s_k}\left(t,X,Z\right)\right)\end{matrix} \qquad \text{(A.23)}$$

Analytical expressions of the gradients of the residual functional. Differentiating expression A.23, by $\Delta D_{\mathrm{intra}_{\mathrm{sk}}}$ and $\Delta D_{\mathrm{inter}_{\mathrm{sk}}}$, respectively, and calculating the scalar products according to eq A.20, we obtain the required analytical expressions for the gradient of the residual functional with respect to the components necessary of diffusion coefficients as a function of time in the intra- and intercrystallite spaces, respectively:

$$\nabla J_{D_{\mathrm{intra}_{\mathrm{sk}}}}\left(t\right)=-\frac{e_{\mathrm{int}\,er_k}}{R^2}\int_{L_{k-1}}^{L_k}\frac{\partial}{\partial X}Q_{s_k}\left(t,1,Z\right)\phi_{s_k}(t,Z)dZ+\frac{1}{R^2}\int_{L_{k-1}}^{L_k}\int_0^1\left(\frac{\partial^2}{\partial X^2}+\frac{2}{X}\frac{\partial}{\partial X}\right)Q_{s_k}\left(t,X,Z\right)\psi_{s_k}(t,X,Z)XdXdZ$$

(A.24)

$$\nabla J_{D_{\mathrm{inter}_{\mathrm{sk}}}}\left(t\right)=\int_{L_{k-1}}^{L_k}\frac{\partial^2 C_{s_k}(t,Z)}{\partial Z^2}\phi_{s_k}(t,Z)dZ\ . \qquad \text{(A.25)}$$

The formulas of gradients $\nabla J^n_{D_{\mathrm{int}\,ra_{s_k}}}\left(t\right)$,$\nabla J^n_{D_{\mathrm{int}\,er_{s_k}}}\left(t\right)$ include analytical expressions of the direct problem solutions (eqs 1 - 6). They provide high performance of computing process, avoiding a large number of inner loop iterations by using exact analytical methods.

Another advantage of the formulas (eqs 8) is that they make it possible to determine the unknown kinetic parameters as a function of time ($D_{\mathrm{int}\,ra_{s_k}}\left(t\right)$, $D_{\mathrm{int}\,er_{s_k}}\left(t\right)$) and other coordinates. It makes it possible to specify internal diffusion kinetics in inter- and intracrystallite spaces and to get an overall vision of the whole process.

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