Supporting Information

Theoretical investigation of thermal effects in an adiabatic chromatographic column using a lumped kinetic model incorporating heat transfer resistances

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Appendix S1: Analytical solutions

The chromatographic model equations along with associated initial and boundary conditions (c.f. Eqs. (17)-(26)) are analytically solved by applying successively the Laplace transformation and eigen-decomposition technique.[2–4] The Laplace transformation is given as[1]

$$\bar{f}(s,x) = \int_0^\infty e^{-s\tau} f(\tau,x)d\tau, \quad f \in \{c_1, c_2\}, \quad \tau \geq 0. \tag{S1-1}$$

On using Eq. (22) in Eq. (19) and then applying the above Laplace transformation, we obtain

$$\bar{q_1} = \frac{Bi}{s+Bi}(R_1\bar{c_1} + R_2\bar{q_2}) + \frac{1}{s+Bi}R_1 c_{1,\text{init}}\,, \tag{S1-2}$$

where Bi, R_1 and R_2 are given by Eqs. (15) and (23). On applying the Laplace transformation on Eq. (20) and then using the Eq. (28) in it, we come up to the following expression

$$\begin{aligned}\bar{q_2} = &\frac{-s\Delta H_A Bi R_1}{C_S(s+Bi)(s+H_S)+s\Delta H_A Bi R_2}\bar{c_1} + \frac{H_S(s+Bi)C_S}{C_S(s+Bi)(s+H_S)+s\Delta H_A Bi R_2}\bar{c_2}\\ &+\frac{\Delta H_A R_1 Bi}{C_S(s+Bi)(s+H_S)+s\Delta H_A Bi R_2}c_{1,\text{init}}\,,\end{aligned} \tag{S1-3}$$

where C_S and H_S are given by Eqs. (3) and (16). On using Eq. (S1-3) in Eq. (S1-2), we get the following expression

$$\begin{aligned}\bar{q_1} = &\left(\frac{BiR_1}{s+Bi} - \frac{s\Delta H_A Bi^2 R_1 R_2}{C_S(s+Bi)^2(s+H_S)+s(u+Bi)\Delta H_A Bi R_2}\right)\bar{c_1}\\ &+\left(\frac{R_1}{s+Bi} + \frac{\Delta H_A R_1 Bi R_2}{C_S(u+Bi)^2(s+H_S)+s(s+Bi)\Delta H_A Bi R_2}\right)c_{1,\text{init}}\\ &+\frac{H_S C_S Bi R_2}{C_S(s+Bi)(s+H_S)+s\Delta H_A Bi R_2}\bar{c_2}.\end{aligned} \tag{S1-4}$$

After applying the Laplace transformation on Eq. (17) and then on putting Eq. (S1-4) in it, we get

$$\begin{aligned}\frac{1}{Pe_c}\frac{\partial^2\bar{c_1}}{\partial x^2} - \frac{\partial\bar{c_1}}{\partial x} = &\left(1+\frac{FBiR_1}{s+Bi} - \frac{F\Delta H_A Bi^2 R_1 R_2 s}{C_S(s+Bi)^2(s+H_S)+s(u+Bi)\Delta H_A Bi R_2}\right)s\bar{c_1}\\ &+\left(1+\frac{FBiR_1}{s+Bi} - \frac{F\Delta H_A Bi^2 R_1 R_2 s}{(s+Bi)^2(s+H_S)+s(s+Bi)\Delta H_A Bi R_2}\right)c_{1,\text{init}}\\ &+\frac{FH_S C_S Bi R_2}{C_S(s+Bi)(s+H_S)+s\Delta H_A Bi R_2}s\bar{c_2},\end{aligned} \tag{S1-5}$$

where Pe_c is given by Eq. (15). After applying the Laplace transformation on Eq. (18) and then on putting Eq. (S1-3) in it, we obtain

$$\begin{aligned}\frac{1}{Pe_T}\frac{\partial^2 \bar{c_2}}{\partial x^2} - \frac{\partial \bar{c_2}}{\partial x} = &\frac{FH_L\Delta H_A BiR_1}{C_S(s+Bi)(s+H_S)+s\Delta H_A BiR_2}s\bar{c_1} \\ &+ \left(1+\frac{FH_LC_S(s+Bi)+\Delta H_A BiFR_2H_L}{C_S(s+Bi)(s+H_S)+s\Delta H_A BiR_2}\right)s\bar{c_2} \\ &- \frac{FH_L\Delta H_A BiR_1}{C_S(s+Bi)(s+H_S)+s\Delta H_A BiR_2}c_{1,\text{init}},\end{aligned} \tag{S1-6}$$

where Pe_T and H_L are given by Eqs. (15) and (16). The following parameters are introduced to simplify the expressions in Eqs. (S1-5) and (S1-6):

$$\begin{aligned}\alpha_1(s) &= 1+\frac{FBiR_1}{s+Bi} - \frac{F\Delta H_A Bi^2R_1R_2s}{C_S(s+Bi)^2(s+H_S)+s(s+Bi)\Delta H_A BiR_2}, \\ \alpha_2(s) &= \frac{FH_SC_SBiR_2}{C_S(s+Bi)(s+H_S)+s\Delta H_A BiR_2}, \\ \beta_1(s) &= \frac{FH_L\Delta H_A BiR_1}{C_S(s+Bi)(s+H_S)+s\Delta H_A BiR_2}, \\ \beta_2(s) &= 1+\frac{FH_LC_S(s+Bi)+\Delta H_A BiFR_2H_L}{C_S(s+Bi)(s+H_S)+s\Delta H_A BiR_2}.\end{aligned} \tag{S1-7}$$

On using these parameters in Eqs. (S1-5) and (S1-6), they turn out to be

$$\frac{1}{Pe_c}\frac{\partial^2 \bar{c_1}}{\partial x^2} - \frac{\partial \bar{c_1}}{\partial x} = \alpha_1(s)s\bar{c_1} - \alpha_1(s)c_{1,\text{init}} + \alpha_2(s)s\bar{c_2}, \tag{S1-8}$$

$$\frac{1}{Pe_T}\frac{\partial^2 c_2}{\partial x^2} - \frac{\partial c_2}{\partial x} = \beta_1(s)s\bar{c_1} - \beta_1(s)c_{1,\text{init}} + \beta_2(s)s\bar{c_2}. \tag{S1-9}$$

In matrix form, the above two equations can be written as

$$\begin{bmatrix} \frac{1}{Pe_c} \\ \frac{1}{Pe_T} \end{bmatrix} \frac{\partial^2}{\partial x^2} \begin{bmatrix} \bar{c_1} \\ \bar{c_2} \end{bmatrix} - \frac{\partial}{\partial x} \begin{bmatrix} \bar{c_1} \\ \bar{c_2} \end{bmatrix} = \begin{pmatrix} \alpha_1(s) & \alpha_2(s) \\ \beta_1(s) & \beta_2(s) \end{pmatrix} \begin{bmatrix} s\bar{c_1} - c_{1,\text{init}} \\ s\bar{c_2} \end{bmatrix}. \tag{S1-10}$$

Our prime goal is to decouple this system of coupled equations. The eigen-decomposition method serves this purpose quite efficiently.[2–4] The matrix A of the coefficients of the above system is written as

$$A = \begin{pmatrix} \alpha_1(s) & \alpha_2(s) \\ \beta_1(s) & \beta_2(s) \end{pmatrix}. \tag{S1-11}$$

As the above matrix has two distinct eigenvalues, it is diagonalizable. The eigenvalues are given as

$$\lambda_{1,2} = \frac{1}{2}\left[(\alpha_1(s) + \beta_2(s)) \pm \sqrt{(\alpha_1(s) - \beta_2(s))^2 + 4\alpha_2(s)\beta_1(s)}\right] \tag{S1-12}$$

and two associated eigenvectors are expressed as

$$x_1 = \begin{bmatrix} \lambda_1 - \beta_2(s) \\ \beta_1(s) \end{bmatrix}, \quad x_2 = \begin{bmatrix} \lambda_2 - \beta_2(s) \\ \beta_1(s) \end{bmatrix}. \tag{S1-13}$$

On the basis of above eigenvalues, the transformation matrix B can be written as

$$B = \begin{pmatrix} \lambda_1 - \beta_2(s) & \lambda_2 - \beta_2(s) \\ \beta_1(s) & \beta_1(s) \end{pmatrix}. \tag{S1-14}$$

Thus, the following linear transformations can be obtained:

$$\begin{bmatrix} \bar{c}_1 \\ \bar{c}_2 \end{bmatrix} = \begin{pmatrix} \lambda_1 - \beta_2(s) & \lambda_2 - \beta_2(s) \\ \beta_1(s) & \beta_1(s) \end{pmatrix} \begin{bmatrix} \bar{b}_1 \\ \bar{b}_2 \end{bmatrix}. \tag{S1-15}$$

By implementing the above transformation on Eq. (S1-10), we obtain

$$\frac{1}{Pe_c}\frac{\partial^2 \bar{b}_1}{\partial x^2} - \frac{\partial \bar{b}_1}{\partial x} - s\lambda_1 \bar{b}_1 = -\lambda_1 b_{1,\text{init}}, \tag{S1-16}$$

$$\frac{1}{Pe_T}\frac{\partial^2 \bar{b}_2}{\partial x^2} - \frac{\partial \bar{b}_2}{\partial x} - s\lambda_2 \bar{b}_2 = -\lambda_2 b_{2,\text{init}}\,, \tag{S1-17}$$

where

$$b_{1,\text{init}} = \frac{c_{1,\text{init}}}{\lambda_1 - \lambda_2}\,, \qquad b_{2,\text{init}} = -\frac{c_{1,\text{init}}}{\lambda_1 - \lambda_2}\,. \tag{S1-18}$$

Now, we have two decoupled equations. Our focus is to determine solutions of these two separated equations explicitly. The solution of Eq. (S1-16) is written as

$$\bar{b}_1(s,x) = M_1 e^{m_1 x} + N_1 e^{m_2 x} + \frac{b_{1,\text{init}}}{s}, \tag{S1-19}$$

where

$$m_{1,2} = \frac{Pe_c \pm \sqrt{Pe_c^2 + 4sPe_c\lambda_1}}{2}\,. \tag{S1-20}$$

On the same steps, the solution of Eq. (S1-17) is written as

$$\bar{b}_2(s,x) = M_2 e^{n_1 x} + N_2 e^{n_2 x} + \frac{b_{2,\text{init}}}{s}\,, \tag{S1-21}$$

where

$$n_{1,2} = \frac{Pe_T \pm \sqrt{Pe_T^2 + 4sPe_T\lambda_2}}{2}\,. \tag{S1-22}$$

Here, M_1, M_2, N_1 and N_2 are integration constants which can be evaluated by means of considered BCs at entrance and exit of the column. Now applying the Laplace transformation on BCs in Eqs. (25a) and (25b), we obtain

$$\bar{c_1}(s,0) = \frac{c_{1,\text{inj}}}{s}(1 - e^{-s\tau_{\text{inj}}})\,, \quad \frac{\partial \bar{c_1}(s,\infty)}{\partial x} = 0\,, \tag{S1-23}$$

$$\bar{c_2}(s,0) = \frac{c_{2,\text{inj}}}{s}(1 - e^{-s\tau_{\text{inj}}})\,, \quad \frac{\partial \bar{c_2}(s,\infty)}{\partial x} = 0\,. \tag{S1-24}$$

In $\bar{b}$-domain, the above boundary conditions turn out to be

$$\bar{b}_1(s,0) = \frac{(1 - e^{-s\tau_{\text{inj}}})}{s\beta_1(s)(\lambda_1 - \lambda_2)}\left(\beta_1(s)c_{1,\text{inj}} - (\lambda_2 - \beta_2(s))c_{2,\text{inj}}\right)\,, \quad \frac{\partial \bar{b}_1}{\partial x}(s,\infty) = 0\,, \tag{S1-25}$$

$$\bar{b}_2(s,0) = \frac{(1 - e^{-s\tau_{\text{inj}}})}{s\beta_1(s)(\lambda_2 - \lambda_1)}\left(\beta_1(s)c_{1,\text{inj}} - (\lambda_1 - \beta_2(s))c_{2,\text{inj}}\right)\,, \quad \frac{\partial \bar{b}_2}{\partial x}(s,\infty) = 0\,. \tag{S1-26}$$

Applying the above boundary conditions on Eqs. (S1-19) and (S1-21), we obtain the constants of integration:

$$M_1 = 0, \quad M_2 = 0, \quad N_1 = \bar{b}_1(s,0) - \frac{b_{1,\text{init}}}{s}, \quad N_2 = \bar{b}_2(s,0) - \frac{b_{2,\text{init}}}{s}\,. \tag{S1-27}$$

On putting the values of M_1 and N_1 in Eq. (S1-19) and values of M_2 and N_2 in Eq. (S1-21), we have

$$\bar{b}_1(s,x) = \left\{\frac{(1 - e^{-s\tau_{\text{inj}}})}{s\beta_1(s)(\lambda_1 - \lambda_2)}\left(\beta_1(s)c_{1,\text{inj}} - (\lambda_2 - \beta_2(s))c_{2,\text{inj}}\right)\right\} e^{m_2 x} + \frac{b_{1,\text{init}}}{s}\left(1 - e^{m_2 x}\right)\,, \tag{S1-28}$$

$$\bar{b}_2(s,x) = \left\{\frac{(1 - e^{-s\tau_{\text{inj}}})}{s\beta_1(s)(\lambda_2 - \lambda_1)}\left(\beta_1(s)c_{1,\text{inj}} - (\lambda_1 - \beta_2(s))c_{2,\text{inj}}\right)\right\} e^{n_2 x} + \frac{b_{2,\text{init}}}{s}\left(1 - e^{n_2 x}\right)\,. \tag{S1-29}$$

To get solutions in the Laplace domain, we implement the transformation in Eq. (S1-15) and the solutions come out to be:

$$\begin{aligned}
\bar{c_1}(s,x) =& \frac{c_{1,\text{inj}}(1-e^{-s\tau_{\text{inj}}})}{s(\lambda_1-\lambda_2)}\left[(\lambda_1-\beta_2(s))e^{m_2x}-(\lambda_2-\beta_2(s))e^{n_2x}\right] \\
&- \frac{\lambda_2-\beta_2(s)}{s}\left[\frac{c_{2,\text{inj}}(\lambda_1-\beta_2(s))(1-e^{-s\tau_{\text{inj}}})}{\beta_1(s)(\lambda_1-\lambda_2)}\left(e^{m_2x}-e^{n_2x}\right)-b_{2,\text{init}}(1-e^{n_2x})\right] \\
&+ \frac{b_{1,\text{init}}(\lambda_1-\beta_2(s))}{s}(1-e^{m_2x})\,, \qquad \text{(S1-30)}\\
\bar{c_2}(s,x) =& \frac{c_{1,\text{inj}}(1-e^{-s\tau_{\text{inj}}})\beta_1(s)}{s(\lambda_1-\lambda_2)}\left(e^{m_2x}-e^{n_2x}\right)+\frac{\beta_1(s)b_{1,\text{init}}}{s}(1-e^{m_2x}) \\
&- \frac{c_{2,\text{inj}}(1-e^{-s\tau_{\text{inj}}})}{s(\lambda_1-\lambda_2)}\left[(\lambda_2-\beta_2(s))e^{m_2x}-(\lambda_1-\beta_2(s))e^{n_2x}\right] \\
&+ \frac{\beta_1(s)b_{2,\text{init}}}{s}(1-e^{n_2x})\,. \qquad \text{(S1-31)}
\end{aligned}$$

To obtain time domain solutions $c_j(\tau,x)$ $(j=1,2)$, the analytical inverse Laplace transforms of Eqs. (S1-30) and (S1-31) are not possible. Therefore, to obtain solutions in the original time domain, we use the numerical Laplace inversion of Durbin[1,5] which is based on a Fourier series expansion as explained below.

Solutions in the time domain $c_j(\tau,x)$ can be obtained by using the exact formula for the back transformation, viz.,

$$c_j(\tau,x) = L^{-1}[\bar{c}_j(s,x)] = \frac{1}{2\pi i}\int_{v-i\infty}^{v+i\infty} e^{-\tau s}\bar{c}_j(s,x)ds\,, \quad j=1,2, \qquad \text{(S1-32)}$$

with $s=v+iw$; $v,w\in\mathbb{R}$. Integration is along the Bromwich contour. Thus, the real constant v exceeds the real part of all the singularities of $\bar{c}_j(s,x)$. The integrals in Eqs. (S1-1) and (S1-32) exist for $\text{Re}(s)>\alpha\in\mathbb{R}$ if

(a) c_j is locally integrable,

(b) there exists a $\tau_0\geq 0$ and $p,\alpha\in\mathbb{R}$, such that $c_j(\tau,x)\leq pe^{\alpha\tau}$ for all $\tau\geq\tau_0$,

(c) for all $\tau \in (0, \infty)$, there is a neighborhood in which c_j is of bounded variation.

In the following we always assume that c_j obeys the above conditions and in addition that there are no singularities of $\bar{c}_j(s,x)$ to the right of the origin. Therefore, Eqs. (S1-1) and (S1-32) are defined for all $y > 0$. The possibility to choose $v > 0$ arbitrarily, is the basis of the methods of Durbin.[5] The integral in Eq. (S1-32) is equivalently expressed in the interval $[0, 2T]$ as[5]

$$c_j(\tau, x) = \frac{e^{v\tau}}{\pi} \int_0^\infty [\mathrm{Re}\{\bar{c}_i(s,x)\} \cos(w\tau) - \mathrm{Im}\{\bar{c}_i(s,x)\} \sin(w\tau)] dw. \tag{S1-33}$$

Durbin derived the following approximate expression for Eq. (S1-33):

$$\begin{aligned} c_j(\tau, x) = & \frac{e^{v\tau}}{T} \left[-\frac{1}{2} \mathrm{Re}\{\bar{c}_j(v,x)\} + \sum_{p=0}^{\infty} \mathrm{Re}\left\{ \bar{c}_j\left(v + i\frac{p\pi}{T}, x\right)\right\} \cos\left(\frac{p\pi\tau}{T}\right) \right. \\ & \left. - \sum_{p=0}^{\infty} \mathrm{Im}\left\{ \bar{c}_j\left(v + i\frac{p\pi}{T}, x\right)\right\} \sin\left(\frac{p\pi\tau}{T}\right) \right], \quad j = 1, 2. \end{aligned} \tag{S1-34}$$

In the numerical computations, the infinite series in Eq. (S1-34) can be summed up to a finite number N_p of terms only. Thus, a truncation error occurs in the numerical computations. In this work, the numerical Laplace inversion formula in Eq. (S1-34) is applied to obtain the time domain solution $c_j(\tau, x)$ by considering $N_p = 10^3$.

Appendix S2: Analytical moments

Analytical expression of the first two temporal moments could be derived from the Laplace-transformed solutions of the concentration and heat balances taking advantage of the simplification of assuming a linearized equilibrium condition (Eq. (22)).

In order to calculate analytical moments for rectangular concentration pulses of finite width, the following moment generating property of the Laplace transform is exploited for $j = 1, 2$:[4]

$$M_{0,c_j} = \frac{L}{u} \lim_{s\to 0}(\bar{c}_j(x=1,s)), \quad M_{n,c_j} = \left(-\frac{L}{u}\right)^n \lim_{s\to 0} \frac{d^n(\bar{c}_j(x=1,s))}{ds^n}, \quad n = 1, 2, \cdots . \tag{S2-1}$$

Furthermore, it is considered that column is regenerated initially and has a reference temperature, i.e.

$$c_{j,\text{init}} = 0, \quad j = 1, 2. \tag{S2-2}$$

The first two moments are evaluated by means of Laplace-transformed solutions in Eqs. (S1-30) and (S1-31). The zeroth, first and second moments of concentration and temperature are provided below.

Zeroth moments: The zeroth moments of c_1 (concentration) and c_2 (temperature) are expressed as

$$\mathbf{M}_0 = \begin{bmatrix} M_{0,c_1} \\ M_{0,c_2} \end{bmatrix} = \begin{bmatrix} c_{1,\text{inj}} t_{\text{inj}} \\ c_{2,\text{inj}} t_{\text{inj}} \end{bmatrix} \tag{S2-3}$$

First moments: The first temporal moments are given as

$$\mathbf{M}_1 = \begin{bmatrix} M_{1,c_1} \\ M_{1,c_2} \end{bmatrix} = \begin{pmatrix} \mu_{11} & \mu_{12} \\ \mu_{21} & \mu_{22} \end{pmatrix} \begin{bmatrix} M_{0,c_1} \\ M_{0,c_2} \end{bmatrix}, \tag{S2-4}$$

where

$$\mu_{11} = \frac{t_{\text{inj}}}{2} + \frac{L}{u}\nu_1, \quad \mu_{12} = \frac{L}{u}\nu_2, \quad \mu_{21} = \frac{L}{u}\nu_3 \quad \mu_{22} = \frac{t_{\text{inj}}}{2} + \frac{L}{u}\nu_4 \tag{S2-5}$$

and

$$\nu_1 = 1 + FR_1, \quad \nu_2 = FR_2, \quad \nu_3 = F\frac{R_1\Delta H_A}{C_L}, \quad \nu_4 = 1 + F\frac{C_S}{C_L} + F\frac{R_2\Delta H_A}{C_L}. \tag{S2-6}$$

Here, C_L and C_S are given by Eq. (3). Here, μ_{ij} represents the mean retention time of component i due to input variation of component j.

Second central moments: The second central moments are calculated from the first and second temporal moments. They are given as

$$\mathbf{M}_2' = \begin{bmatrix} M'_{2,c_1} \\ M'_{2,c_2} \end{bmatrix} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \begin{bmatrix} M_{0,c_1} \\ M_{0,c_2} \end{bmatrix}, \tag{S2-7}$$

where

$$\sigma_{11} = \frac{t_{\text{inj}}^2}{12} + \frac{L^2}{u^2}\Bigg[\nu_2\nu_3 + \left(\nu_1^2 + \nu_2\nu_3\right)\left(\frac{1}{Pe_c} + \frac{1}{Pe_T}\right) + \frac{\nu_1^3 + \nu_2\nu_3\nu_4 - \nu_1^2\nu_4 + 3\nu_1\nu_2\nu_3}{2\phi - (\nu_1 + \nu_4)}$$
$$\left(\frac{1}{Pe_c} - \frac{1}{Pe_T}\right) + \left(\frac{2FR_1}{Bi} + \frac{2FR_1R_2\Delta H_A}{C_LH_L}\right)\Bigg], \tag{S2-8}$$

$$\sigma_{12} = t_{\text{inj}}\frac{L}{u}\nu_2 + \frac{L^2}{u^2}\Bigg[\nu_2(\nu_1 + \nu_4)\left(1 + \frac{1}{Pe_c} + \frac{1}{Pe_T}\right) + \nu_2\frac{\nu_1^2 + \nu_4^2 + 2\nu_2\nu_3}{2\phi - (\nu_1 + \nu_4)}\left(\frac{1}{Pe_c} - \frac{1}{Pe_T}\right)$$
$$-\nu_2^2 + \left(\frac{2FR_2}{Bi} + \frac{2FR_2(\Delta H_AR_2 + C_S)}{C_LH_L}\right)\Bigg], \tag{S2-9}$$

$$\sigma_{21} = t_{\text{inj}}\frac{L}{u}\nu_3 + \frac{L^2}{u^2}\Bigg[\nu_3(\nu_1 + \nu_4)\left(1 + \frac{1}{Pe_c} + \frac{1}{Pe_T}\right) + \nu_3\frac{\nu_1^2 + \nu_4^2 + 2\nu_2\nu_3}{2\phi - (\nu_1 + \nu_4)}\left(\frac{1}{Pe_c} - \frac{1}{Pe_T}\right)$$
$$-\nu_3^2 + \left(\frac{2FR_1\Delta H_A}{C_LBi} + \frac{2FR_1\Delta H_A(C_S + \Delta H_AR_2)}{C_L^2H_L}\right)\Bigg], \tag{S2-10}$$

$$\sigma_{22} = \frac{t_{\text{inj}}^2}{12} + \frac{L^2}{u^2}\Bigg[\nu_2\nu_3 + (\nu_4^2 + \nu_2\nu_3)\left(\frac{1}{Pe_c} + \frac{1}{Pe_T}\right) + \frac{\nu_4^3 + \nu_1\nu_2\nu_3 - \nu_4^2\nu_1 + 3\nu_2\nu_3\nu_4}{2\phi - (\nu_1 + \nu_4)}$$
$$\left(\frac{1}{Pe_c} - \frac{1}{Pe_T}\right) + \left(\frac{2FR_2\Delta H_A}{C_LBi} + \frac{2F(\Delta H_AR_2 + C_S)^2}{C_L^2H_L}\right)\Bigg]. \tag{S2-11}$$

Here,

$$\phi = \frac{1}{2}\Big[(\nu_1 + \nu_4) + \sqrt{(\nu_1 - \nu_4)^2 + 4\nu_2\nu_3}\Big]. \tag{S2-12}$$

Moreover, all the dimensionless parameters are given by Eqs. (14)-(16) and σ_{ij} indicates the mean variance of component i due to input variation of component j. For large mass and heat transfer rates, i.e. for $k \to \infty$ and $h \to \infty$, the above moments reduces to the moments of non-isothermal EDM presented in our previous article.[4]

The moments derived above are very useful to analyze peaks areas (masses), mean retention times, and broadenings of both the concentration and temperature profiles.

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