A CORRECT DERIVATION OF EXACT SOLUTION OF DISPERSION MODEL FOR TRACER PULSE IN A BATCH LOOP REACTOR

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Dear Sir:

The exact form of Eq. (5)¹⁾ has been recently found to be correctly derived by a Laplace transform method. In addition, there is an incorrect expression in the initial condition of Eq. (2).¹⁾

We propose a correct expression of the initial condition and briefly a process of solving directly the dispersion model under the boundary conditions of Eqs. (3) and (4)¹⁾ together with the initial condition corrected.

The initial condition was expressed as

$$C(x, 0) = \bar{C}\delta(x) \quad (1)$$

in the paper.¹⁾ It is incorrect in dimension. The mean concentration of $\bar{C}$ [mol·m⁻³] in Eq. (1) should be replaced with moles per unit area $E = \bar{C} \cdot L$ [mol·m⁻²],²⁾ because $\delta(x)$ has the dimension of the reciprocal of length [m⁻¹]. Then Eq. (1) is correctly expressed as

$$C(x, 0) = E\delta(x) = f(x) \quad (2)$$

Equations (1), (3) and (4)¹⁾ together with Eq. (2) are expressed in the form of a Laplace transform as

$$d^2 Y/dx^2 - (\bar{U}/D_a)(dY/dx) - sY/D_a = -f(x)/D_a \quad (3)$$

$$Y(0, s) = Y(L, s) \quad (4)$$

$$dY(0, s)/dx = dY(L, s)/dx \quad (5)$$

Equation (3) is a second-order linear differential equation with constant coefficients. Then the general solution is given as

$$\begin{aligned} Y(x, s) = & \left[C_1(s) - \int_0^x f(\xi) \exp(-r_1 \xi) / \{D_a(r_1 - r_2)\} d\xi \right] \\ & \times \exp(r_1 x) \\ & + \left[C_2(s) + \int_0^x f(\xi) \exp(-r_2 \xi) / \{D_a(r_1 - r_2)\} d\xi \right] \\ & \times \exp(r_2 x) \end{aligned} \quad (6)$$

where

$$r_1 = \bar{U}/2D_a + \sqrt{(\bar{U}/2D_a)^2 + s/D_a},$$

$$r_2 = \bar{U}/2D_a - \sqrt{(\bar{U}/2D_a)^2 + s/D_a}.$$

Integral constants $C_1(s)$ and $C_2(s)$ in Eq. (6) are determined by the use of boundary conditions of Eqs. (4) and (5) as

$$\begin{aligned} C_1(s) = & -B_1(s) \exp(r_1 L) / [1 - \exp(r_1 L)] \\ = & + B_1(s) \sum_{n=0}^{\infty} \exp(-nr_1 L); \end{aligned}$$

$$B_1(s) = \int_0^L f(\xi) \exp(-r_1 \xi) / \{D_a(r_1 - r_2)\} d\xi \quad (7)$$

$$\begin{aligned} C_2(s) = & +B_2(s) \exp(r_2 L) / [1 - \exp(r_2 L)] \\ = & +B_2(s) \sum_{n=1}^{\infty} \exp(+nr_2 L); \end{aligned}$$

$$B_2(s) = \int_0^L f(\xi) \exp(-r_2 \xi) / \{D_a(r_1 - r_2)\} d\xi \quad (8)$$

When one determines $C_1(s)$ and $C_2(s)$, he must skillfully expand them in power series so as to make the signs of root terms in r_1 and r_2 negative, as shown by the underlines in Eqs. (7) and (8). In this way, the inverse Laplace transform of Eq. (6) is performable.

Substituting Eqs. (7) and (8) and $f(\xi) = E\delta(\xi)$ into Eq. (6), it is rearranged to

$$\begin{aligned} Y(x, s) = & E \left[\sum_{n=1}^{\infty} \exp\{-r_1(nL - x)\} \right. \\ & \left. + \sum_{n=0}^{\infty} \exp\{+r_2(nL + x)\} \right] / \{D_a(r_1 - r_2)\} \end{aligned} \quad (9)$$

Substitute r_1 and r_2 into Eq. (9) and move the image-space by $-(\bar{U}^2/4D_a)$ through multiplying the original function $C(x, t)$ by $\exp(\bar{U}^2/4D_a)$. Then perform the inverse Laplace transform by use of the well-known formula $\exp(-k\sqrt{s})/\sqrt{s} \rightarrow \exp(-k^2/4t)/$

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$\sqrt{\pi t}$; $k > 0$. Thus is derived the exact form of Eq. (5) in the paper.¹⁾

At that time $C_1(s)$ was expanded in power series as

$$C_1(s) = -B_1(s) \exp(r_1 L) / [1 - \exp(r_1 L)]$$

$$= -B_1(s) \sum_{n=1}^{\infty} \exp(+nr_1 L) \quad (10)$$

in the same form as $C_2(s)$. Then the inverse Laplace transform was not successfully performed and the exact solution could not be derived in a complete form.

Care is necessary not to fall in "a trap" of expansion in power series.

Nomenclature

$C(x, t)$	= concentration	$[\text{mol} \cdot \text{m}^{-3}]$
D_a	= longitudinal dispersion coefficient	$[\text{m}^2 \cdot \text{s}^{-1}]$

E	= moles of tracer pulse per unit area	$[\text{mol} \cdot \text{m}^{-2}]$
k	= constant greater than zero	$[-]$
L	= total length of loop reactor	$[\text{m}]$
n	= integer variable number	$[-]$
s	= Laplace parameter	$[-]$
t	= time	$[\text{s}]$
$\bar{U}$	= average circulating velocity	$[\text{m} \cdot \text{s}^{-1}]$
$Y(x, s)$	= Laplace transform of concentration	$[\text{mol} \cdot \text{m}^{-3}]$
x	= axial position of loop reactor	$[\text{m}]$
$\delta(x)$	= delta function	$[\text{m}^{-1}]$

<Superscript>

— = mean

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