ESTIMATION METHOD OF THE AXIAL DISPERSION COEFFICIENT UTILIZING THE LAPLACE TRANSFORM

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The imperfect pulse method has proven to be a powerful technique for estimating parameters in describing mixing in chemical engineering processes. Bischoff¹⁾ has shown that an imperfect pulse can be used for any model that is represented by a transfer function. Ostergaard and Michelson⁵⁾ have developed a method for estimating the dispersion coefficient using the transfer function of the theoretical relationship.

In this paper, the authors present a method based on the Laplace transform method²⁻⁴⁾ for estimating the axial dispersion coefficient under arbitrary inlet and outlet boundary conditions. This method utilizes the Laplace transform of the axially dispersed piston flow model equation and the Laplace integral of the concentration responses. It will be shown that the present method is the general theory of the transfer function method⁵⁾.

1. Principle

The axially dispersed piston flow model is expressed by:

$$\frac{\partial C}{\partial t} = E \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} \quad (1)$$

The Laplace transform of Eq. (1) is

$$\frac{d^2 \bar{C}}{dx^2} - \frac{u}{E} \frac{d\bar{C}}{dx} - \frac{s}{E} \bar{C} = 0 \quad (2)$$

with the initial condition

$$C=0 \text{ at } t=0 \quad (3)$$

The general solution of Eq. (2) is

$$\bar{C} = Ae^{\alpha x} + Be^{\beta x} \quad (4)$$

where

$$\alpha = \left(\frac{u}{E} + \sqrt{\frac{u^2}{E^2} + \frac{4s}{E}} \right) / 2$$

$$\beta = \left(\frac{u}{E} - \sqrt{\frac{u^2}{E^2} + \frac{4s}{E}} \right) / 2$$

The Laplace integral $\bar{C}_i$ of the concentration response C_i at each of three positions x_i ($i=1, 2, 3$) indicated in Fig. 1 is obtained in accordance with Eq. (5):

$$\bar{C}_i = \int_0^\infty e^{-st} C_i dt \quad (5)$$

Equation (6) is easily obtained by substituting $\bar{C}_1$, $\bar{C}_2$ and $\bar{C}_3$ into Eq. (4) respectively for x_1 , x_2 and x_3 . Thus

$$(e^{\alpha x_2 + \beta x_3} - e^{\alpha x_3 + \beta x_2}) \bar{C}_1 + (e^{\alpha x_3 + \beta x_1} - e^{\alpha x_1 + \beta x_3}) \bar{C}_2 + (e^{\alpha x_1 + \beta x_2} - e^{\alpha x_2 + \beta x_1}) \bar{C}_3 = G(E, s) = 0 \quad (6)$$

In Eq. (6), the unknown values are E and s . Owing to the nature of the Laplace transform, s may be assumed as being an arbitrary, finite and positive value to the extent Eq. (5) is capable of convergence. Thus, E can be determined.

It is understood that the above theory holds good regardless of the boundary conditions. This means that the theory can be used under arbitrary tracer conditions of both inlet and outlet. On the basis of this general theory, several measuring systems are proposed. For example, where one boundary condition is fixed, the number of measuring positions decreases and the equation becomes simple. Table 1 shows four examples of derived practical measuring systems. Let us consider the semi-infinite model ($C=0$ at $x=\infty$) illustrated by (a) in Table 1. It is understood that A becomes 0 in Eq. (4) and two measuring positions are enough. The equation for determining E becomes Eq. (7) or a positive function of Eq. (7'). In the cases of (a), (b) and (c), one boundary condition is fixed, and two measuring

Fig. 1 Experimentation for axial dispersion and coordinates

Table 1 Some practical measuring systems

	Meas. System	Boundary C.	Relation	Equation
(a)	any input x_1 x_2 any	$C=0$ at $x=\infty$	$e^{\beta x_2} \bar{C}_1 - e^{\beta x_1} \bar{C}_2 = 0$	(7)
			$E = \frac{s(x_2 - x_1)^2 + u(x_2 - x_1) \ln(\bar{C}_1 / \bar{C}_2)}{(\ln(\bar{C}_1 / \bar{C}_2))^2}$	(7')
(b)	any x_1 x_2	$-E \frac{\partial C}{\partial x} = 0$ at $x=L$	$(\alpha e^{\beta x_2} - \beta e^{\alpha x_2 + (\beta - \alpha)L}) \bar{C}_1 - (\alpha e^{\beta x_1} - \beta e^{\alpha x_1 + (\beta - \alpha)L}) \bar{C}_2 = 0$	(8)
(c)	any x_1 x_2	$C=0$ at $x=L$	$(e^{\beta x_2} - e^{\alpha x_2 + (\beta - \alpha)L}) \bar{C}_1 - (e^{\beta x_1} - e^{\alpha x_1 + (\beta - \alpha)L}) \bar{C}_2 = 0$	(9)
(d)	delta x_1	$C=d(t)$ at $x=0$ $C=0$ at $x=\infty$	$E = \frac{s x_1 + u x_1 \ln(\bar{C}_1)}{(\ln(\bar{C}_1))^2}$	(10)

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Fig. 2 Numerical test and the model

positions are needed. But with (d), two boundary conditions are fixed, and one measuring position is sufficient.

Ostergaard and Michelson⁵⁾ have derived Eq. (11) for determining $Pe=u(x_2-x_1)/E$ and $\tau=(x_2-x_1)/u$.

$$\left\{ \ln \left(\frac{1}{F(s)} \right) \right\}^{-1} = \tau s \left\{ \ln \left(\frac{1}{F(s)} \right) \right\}^{-2} - \frac{1}{Pe} \quad (11)$$

However, Eq. (11) is easily shown to be simply identical with Eq. (7'). This fact shows that the present theory, which is not based on the concept of transfer function, is the general theory of the transfer function method.

2. Numerical Test

To confirm the nature of the method and clarify its uses, a numerical test is shown.

The analytical solution of concentration responses when a step-wise input is added at $x=0$ and the concentration gradient is assumed zero at $x=L$ is presented by Yagi and Miyauchi⁶⁾. The three solid lines in Fig. 2 (A) are the responses calculated by the solution under the predetermined values of L , u , E , and x_i , which are indicated in the figure. Let us apply the present theory to these responses assuming that they were obtained by experiment. In Fig. 2 (A), e^{-st} ($s=0.4/\text{min}$), $e^{-st}C'_1$ and $\bar{C}'_1$, which correspond to the hatched area, are illustrated by way of example. The Laplace integral calculation was performed by the Simpson numerical method. The three dotted lines in Fig. 2 (B) are the Laplace integral values illustrated as a function of sT , and the solid line is the resultant dispersion coefficient. In the range of a large sT , the results agree well with the predetermined value.

3. Selection of s Value

The disagreement between the results and the pre-

determined value as observed for a smaller range of sT in Fig. 2 (B) is ascribable to the fact that the Laplace integration was not performed to infinity, but only to T . Principally, the integration should be performed to infinity as defined by Eq. (5). However, the value of $e^{-st}C'_i$ is a function which converges to 0 as the value of t increases. Therefore, there exists the period T at which Eq. (12), shown below, is approximately satisfied.

$$\int_0^\infty e^{-st}C'_i dt = \int_0^T e^{-st}C'_i dt \quad (12)$$

It is recognized that the accuracy of this approximation depends on the magnitude of sT . The authors have carried out many numerical tests for various response curves and have recognized that the approximation was generally satisfied in the range of $sT \geq 8$. When the value of sT is too large, however, the results should be evaluated using data obtained with a short span of initial time. Thus the authors recommend a selection of sT in accordance with Eq. (13) in the case of a finite value of C'_i at $t \geq T$. Within the range of Eq. (13), the value of s can be freely selected.

$$8 \leq sT \leq 12 \quad (13)$$

On the other hand, where measurements are performed by pulse-like responses, the period T_0 when the concentration responses revert to zero initial conditions may be determined. In this case, Eq. (12) holds true as long as the measuring period T is selected to be larger than T_0 . Thus, there exists no lower limit of s value.

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Nomenclature

C	= concentration	[mol/m ³]
$\bar{C}$	= Laplace integral	[mol·min/m ³]
E	= axial dispersion coefficient	[cm ² /min]
$F(s)$	= transfer function	[—]
N	= sampling number	[—]
s	= Laplace parameter	[1/min]
T	= measuring period	[min]
t	= time	[min]
u	= velocity of flow	[cm/min]
x	= length coordinate	[cm]

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