MODEL OF RESIDENCE TIME DISTRIBUTION FUNCTION IN THE REACTOR WITH DISPERSION FLOW AND IDEAL MIXING

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Received March 19th, 1979

A function of residence time distribution is derived by the method of generalized Heaviside series and an approximative procedure for the dispersion model coupled with ideal mixing boundary conditions, for "closed–closed" reactor, were used. Model is characterized by two parameters: Peclet number and volume fraction of the region of dispersion flow. The solution is studied numerically and the advantages of the approximative solution are discussed in detail.

Dispersion models describing deviations of liquid flow from plug flow in the reactor are very frequent in literature[1-5]. Solutions of equations describing the modelled reactor depend on used boundary conditions[1]. Danckwerts[2] has for the first time specified the boundary conditions and has given solution of the dispersion model reactor in which the first order reaction takes place in steady state. Later Bischoff[3] has extended the conclusions for solution of equations describing the dispersion model for the boundary conditions according to Danckwerts to the reaction of an arbitrary order. Solutions of these equations (Danckwert's boundary conditions) describing the unsteady state of the model reactor have been studied in detail by Van Cauwenbergh[4]. The dispersion models are usually one-parameter[1-4]. At present are used for the mathematical description of the reactor also multiparameter models whose advantages as compared to those one-parameter lie in greater flexibility which requires more theoretically founded approach to the solution of these mathematical models. The problems are also met in investigation of convergence of infinite series which are used as the solutions.

One of the possible two-parameter models is described in this paper.

DISPERSION MODEL COUPLED WITH IDEAL MIXING

Let us consider the reactor of finite length where the liquid successively flows through the region of dispersion flow and ideal mixing, see Fig. 1.

The material balance of the tracer in the considered model in the dimensionless form can be written as

$$\mathrm{Pe}\left[\varphi \frac{\partial C_1(Z,\Theta)}{\partial \Theta} + \frac{\partial C_1(Z,\Theta)}{\partial Z}\right] = \frac{\partial^2 C_1(Z,\Theta)}{\partial Z^2} \quad \text{for} \quad Z \in \langle 0, \varphi \rangle,\ \Theta \geqq 0 \qquad (1)$$

$$(1-\varphi)\frac{\mathrm{d}C_2(\Theta)}{\mathrm{d}\Theta} + C_2(\Theta) = C_1(\varphi, \Theta) = 0 \quad \text{for} \quad \Theta \geqq 0,$$

$$\varphi \in \langle 0, 1 \rangle, \ \mathrm{Pe} \geqq 0 \,. \tag{2}$$

In case the input signal has the form of the δ-function and concentration of the tracer in time $t = 0$, is zero the initial and boundary conditions, for "closed-closed" reactor in the dimensionless form are

$$C_1(Z, 0) = C_2(0) = 0 \quad \text{for} \quad 0 \leqq Z \leqq \varphi \tag{3}$$

$$\mathrm{Pe}\ \delta(\Theta) = \mathrm{Pe}\ C_1(0^+, \Theta) - \left.\frac{\partial C_1(Z, \Theta)}{\partial Z}\right|_{Z=0^+} \tag{4}$$

$$\left.\frac{\partial C_1(Z, \Theta)}{\partial Z}\right|_{Z=\varphi} = 0 \,. \tag{5}$$

Equations (*1*) and (*2*) for the initial and boundary conditions (*3*)–(*5*) can be solved by the method of Laplace transformation. The Laplace transformation of concentration at the outlet from the reactor then has the form

$$\bar{C}_2(s) = \frac{4a \exp(\mathrm{Pe}\ \varphi/2)}{[1 + s(1-\varphi)]\ \{(1+a)^2 \exp(\mathrm{Pe}\ a\varphi/2) - (1-a)^2 \exp(-\ \mathrm{Pe}\ a\varphi/2\}}\,, \tag{6}$$

where

$$a = (1 + 4\varphi s/\mathrm{Pe})^{1/2} \,. \tag{7}$$

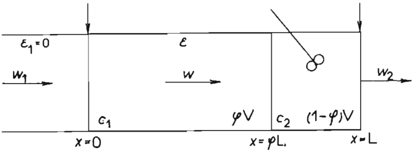

FIG. 1

Dispersion Model Coupled with Ideal Mixing

METHOD OF GENERALISED HEAVISIDE EXPANSION THEOREM

By the inverse transformation of Eq. (*6*), by use of the generalised Heaviside Expansion Theorem for calculation of the residence time distribution function of this model *i.e.* of the so-called **E**-function, which denotes the magnitude or distribution density of "age" of all elements at the outlet from the system, the relation is obtained

$$\mathbf{E}(\Theta) = 4a' \exp\left[\frac{\mathrm{Pe}}{2}\,\varphi - \frac{\Theta}{1-\varphi}\right] \Big/ \left((1-\varphi)\left\{(1+a')^2 \exp\left(\frac{\mathrm{Pe}\,a'\varphi}{2}\right) - (1-a')^2 \exp\left(-\frac{\mathrm{Pe}\,a'\varphi}{2}\right)\right\}\right) + \sum_{k=1}^{\infty} \frac{16\lambda_k \exp\left[\frac{\mathrm{Pe}}{2}\,\varphi + s_k\Theta\right]}{\mathrm{Pe}\,H_1'(s_k)}\,, \qquad (8)$$

where

$$a' = \left(1 - \frac{4\varphi}{\mathrm{Pe}\,(1-\varphi)}\right)^{1/2} \qquad (9)$$

$$s_k = -\frac{4}{\varphi\,\mathrm{Pe}}\left[\lambda_k^2 + \left(\frac{\mathrm{Pe}}{4}\right)^2\right] \qquad (10)$$

$$H_1'(s_k) = (1-\varphi)\left\{\frac{16\lambda_k}{\mathrm{Pe}}\cos 2\lambda_k\varphi + \left[2 - \frac{32\lambda_k^2}{\mathrm{Pe}^2}\right]\sin 2\lambda_k\varphi\right\} + \left\{\left[\frac{8\varphi}{\mathrm{Pe}} + 4\varphi^2\right]\sin 2\lambda_k\varphi - \left[\frac{2\varphi}{\lambda_k} + \frac{\mathrm{Pe}\,\varphi^2}{2\lambda_k} - \frac{8\varphi\lambda_k}{\mathrm{Pe}}\right]\cos 2\lambda_k\varphi\right\}\left[1 + s_k(1-\varphi)\right] \qquad (11)$$

and where λ_k are positive roots of the transcendent equation

$$\left(\operatorname{tg} 2\lambda_k\varphi = \frac{\mathrm{Pe}}{2}\,\lambda_k\right) \Big/ \left[\lambda_k^2 - \left(\frac{\mathrm{Pe}}{4}\right)^2\right] \quad k = 1, 2, 3, \ldots \qquad (12)$$

It is possible to prove that for $\varphi = 1$, Eq. (*8*) is reduced to the form given by Dilman and coworkers[1] for the "closed-closed" dispersion model and for $\varphi = 0$ Eq. (*8*) is reduced to the **E**-function of the ideally mixed reactor.

For the first two moments of **E**-function the relations hold

$$\mu_1 = 1 - \varphi(1-\varphi) \qquad (13)$$

$$\mu_2 = \varphi^4 \left\{1 + \frac{2}{\text{Pe}\,\varphi} - \frac{2}{(\text{Pe}\,\varphi)^2}\left[1 - \exp\left(-\text{Pe}\,\varphi\right)\right]\right\} + \\ + \frac{4\varphi}{\text{Pe}}(1 - \varphi) + \varphi(1 - 2\varphi)(2\varphi - 2)\,. \tag{14}$$

In the case that for the expression below the second root in Eq. (*9*) there holds

$$1 - \frac{4\varphi}{\text{Pe}\,(1 - \varphi)} \geqq 0 \tag{15}$$

after arrangement the inequality is obtained

$$\varphi \leqq \text{Pe}/(\text{Pe} + 4) \tag{16}$$

and it is possible for calculation of the **E**-function to use directly Eq. (*8*). If the inequality holds

$$1 - \frac{4\varphi}{\text{Pe}\,(1 - \varphi)} < 0 \tag{17}$$

from which for the volume fraction in the region of dispersion flow results

$$\varphi > \text{Pe}/(\text{Pe} + 4) \tag{18}$$

it is advantageous for calculation of the **E**-function to arrange Eq. (*8*) into the form

$$\mathbf{E}(\Theta) = 2a_1 \exp\left[\frac{\text{Pe}}{2}\,\varphi - \frac{\Theta}{1 - \varphi}\right] \Big/ \\ \Big/ \left((1 - \varphi)\left\{(1 - a_1^2)\sin\frac{\text{Pe}\,a_1\varphi}{2} + 2a_1\cos\frac{\text{Pe}\,a_1\varphi}{2}\right\}\right) + \\ + \sum_{k=1}^{\infty} \frac{16\lambda_k \exp\left[\frac{\text{Pe}}{2}\,\varphi + s_k\Theta\right]}{\text{Pe}\,H_2'(s_k)}\,, \tag{19}$$

where

$$a_1 = \left(\left|1 - \frac{4\varphi}{\text{Pe}\,(1 - \varphi)}\right|\right)^{1/2}. \tag{20}$$

In Eqs (*8*) and (*19*) which were derived for calculation of the **E**-function (when a' is the real or imaginary number) appears the sum of an infinite series. The convergence of this infinite series is slow in the region of small values of Θ for large values of Pe. In the calculation of the sum of the infinite series is the infinite number of terms of the series substituted by a finite number so the made error is negligible. Ten terms of the sum were used here for calculation of the **E**-function. Calculation by use of these relations is very cumbersome and inconvenient.

In Fig. 2 is plotted the dependence of **E**-functions calculated as the sum of ten terms of the sum (*8*) for Pe = 30 and $\varphi = 0{\cdot}4; 0{\cdot}5; 0{\cdot}6; 0{\cdot}7$; and $0{\cdot}8$.

APPROXIMATIVE SOLUTION OF THE MODEL

Analytical solution of the model given by Eq. (*8*) or (*9*) has the form of slowly converging sum, which is not suitable for calculation of the **E**-function. One of the frequently used procedures of derivation of the approximative solution, which is preferably used to those exact solutions is here analysed in detail.

Let us arrange Eq. (*6*) into the form

$$\bar{C}_2(s) = \frac{4 \exp\left(\mathrm{Pe}/2\,\varphi\right)}{(1-\varphi)} \frac{a}{\{s + [1/(1-\varphi)]\}} \,.$$

$$. \left\{(1+a)^2 \exp\left(\frac{\mathrm{Pe}\, a\varphi}{2}\right) - (1-a)^2 \exp\left(\frac{-\mathrm{Pe}\, a\varphi}{2}\right)\right\}^{-1} . \qquad (21)$$

The right-hand side of Eq. (*21*) can be expanded into the sum and written

$$\bar{C}_2(s) = \frac{4 \exp\left(\mathrm{Pe}\,\varphi/2\right)}{(1-\varphi)} \frac{a}{\{s + [1/(1-\varphi)]\}} \sum_{k=0}^{\infty} \frac{(1-a)^{2k}}{(1+a)^{2k+2}} \exp\left[-\frac{\mathrm{Pe}\, a\varphi}{2}(2k+1)\right]. \qquad (22)$$

This infinite series is absolutely convergent, when the real part s is positive and each term of this sum can be inverted to the form corresponding to its original function.

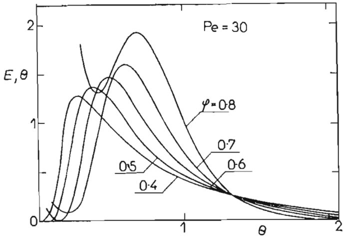

FIG. 2

Exact Solution of **E**-function of Dispersion Model Coupled with Ideal Mixing as the Sum of 10 Terms of the Series (*8*)

When the inverse transformation of the series (*22*) is performed for a greater number of terms ($k = 1, 2, 3, \ldots$) the resulting function of the original should have a complex form and for this reason it should not have any preferences to the relations (*8*) or (*19*) as concerns the simplicity of calculation of residence time distribution function.

When only the first term of the sum (*22*) is considered (*i.e.* $k = 0$) the relation holds

$$\bar{C}_2(s) \sim \frac{4 \exp(\mathrm{Pe}\,\varphi/2)}{(1-\varphi)} \frac{a}{\{s + [1/(1-\varphi)]\}} \frac{\exp(-\mathrm{Pe}\,a\varphi/2)}{(1+a)^2} . \qquad (23)$$

When instead of the infinite series (*22*) only the first term of this series is considered, after application of relations *c*) to *f*) the solution of residence time distribution function is obtained. This solution is called "approximative" and has the form

$$\mathbf{E}(\Theta) = \frac{2}{1-\varphi} \sqrt{\frac{\mathrm{Pe}}{\varphi}} \exp\left[\frac{\mathrm{Pe}\,\varphi}{2}\left(1 - \frac{\Theta}{2}\right)\right] h(\Theta) - \frac{2}{1-\varphi} \sqrt{\frac{\mathrm{Pe}}{\varphi}} \left[\frac{1}{1-\varphi} - \frac{\mathrm{Pe}}{4\varphi}\right] .$$
$$. \exp\left[\frac{\mathrm{Pe}\,\varphi}{2} - \frac{\Theta}{1-\varphi}\right] \int_0^\Theta h(p) \exp\left[p\left(\frac{1}{1-\varphi} - \frac{\mathrm{Pe}}{4\varphi}\right)\right] \mathrm{d}p , \qquad (24)$$

where

$$h(p) = 2\sqrt{\frac{p}{\pi}} \exp\left(-\frac{\mathrm{Pe}\,\varphi^3}{4p}\right) - \left(\sqrt{\frac{\mathrm{Pe}}{\varphi}}\, p + \varphi\sqrt{\mathrm{Pe}\,\varphi}\right) \exp\left[\frac{\mathrm{Pe}\,\varphi}{2}\left(1 - \frac{p}{2}\right)\right] .$$
$$. \operatorname{erfc}\left\{\frac{\varphi\sqrt{\mathrm{Pe}\,\varphi}}{2\sqrt{p}} + \sqrt{\frac{\mathrm{Pe}\,p}{4\varphi}}\right\} . \qquad (25)$$

For the numerical calculation of the function erfc (y), when $y \in \langle 0; 1\rangle$ or $y \in (1; \infty)$ the series given in study[9] were used.

The approximative solution of the **E**-function of the model, Eq. (*24*) is plotted in Fig. 3.

It is obvious that the approximative solution of the model, Eq. (*24*) will not give satisfactory results for arbitrary values of parameters Pe and φ. The conditions for which the results are calculated from Eq. (*24*) with sufficient accuracy, can be determined as follows: The simplified form of the series on the right hand side of Eq. (*22*) is denoted $\bar{R}((s/\psi_1^2 + 1)^2)$, so the relation if obtained

$$\bar{R}\left(\frac{s}{\psi_1^2} + 1\right)^{1/2} = \sum_{k=0}^{\infty} \bar{f}_k \left(\frac{s}{\psi_1^2} + 1\right)^{1/2} \exp\left\{-\psi_2\left(\frac{s}{\psi_1^2} + 1\right)^{1/2}(2k+1)\right\} , \qquad (26)$$

where

$$\bar{f}_k\left(\frac{s}{\psi_1^2}+1\right)^{1/2}=\frac{\left[1-\left(\dfrac{s}{\psi_1^2}+1\right)^{1/2}\right]^{2k}}{\left[1+\left(\dfrac{s}{\psi_1^2}+1\right)^{1/2}\right]^{2k+2}}$$

$$\psi_1=(\mathrm{Pe}/4\varphi)^{1/2}\,,\quad \psi_2=\mathrm{Pe}\,\varphi/2\,.$$

The inverse transformation of the series (*26*) has been performed so that at first the property of the Laplace transformation given in Table I point *a*) has been used and then have been successively applied the properties *b*) and *c*). The original form of series (*26*) then has the form

$$R(\Theta)=\frac{\exp(-\Theta)}{2\sqrt{\pi\Theta^3}}\int_0^\infty p\exp\left(-\frac{p^2}{4\Theta}\right)\left[f_0(\psi_1p-\psi_2)+f_1(\psi_1p-3\psi_2)+\right.$$
$$\left.+f_2(\psi_1p-5\psi_2)+\ldots\right]\mathrm{d}p\,. \qquad (27)$$

From the properties of the Laplace transformation point *a*) in Table I results

$$\begin{aligned}
&f_0(\psi_1p-\psi_2)\neq 0 \quad \text{for} \quad p>\psi_2/\psi_1\\
&f_1(\psi_1p-3\psi_2)\neq 0 \quad \text{for} \quad p>3\psi_2/\psi_1\\
&f_2(\psi_1p-5\psi_2)\neq 0 \quad \text{for} \quad p>5\psi_2/\psi_1\\
&\vdots
\end{aligned}$$

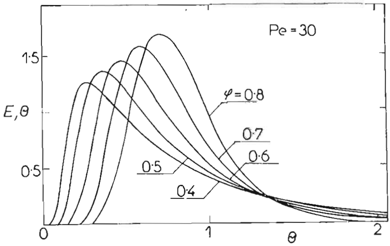

FIG. 3

Approximative Solution of the **E**-function of the Dispersion Model Coupled with Ideal Mixing

As has been already mentioned, in the approximative solution only the first term of the series (*22*) has been taken into consideration. This means that the integral (*27*) must supply sufficiently accurate results for some values of Pe and φ when only the first term of the subintegral function is taken into consideration, *i.e.* the term $f_0(\psi_{1\mathrm{p}} - \psi_2)$. From integral (*27*) is obvious that the accuracy of the calculation of this integral depends on the ratio ψ_2/ψ_1. Thus with increasing ratio ψ_2/ψ_1 decreases the number of terms which must be included into the calculation of Eq. (*27*) at the given accuracy.

In our case the condition has been chosen

$$\psi_2/\psi_1 > 1 \tag{28}$$

i.e. for

$$\varphi \sqrt{(\mathrm{Pe}\, \varphi)} > 1\,. \tag{29}$$

If the condition (*29*) is satisfied, then calculation of the function of residence time distribution by use of Eq. (*24*) gives quite accurate results.

TABLE I
Laplace Transformations

a) $\bar{f}(s/\psi_1) \exp(-\psi_2 s/\psi_1)$	0 $f(\psi_1\Theta - \psi_2)$	$0 \leqq \psi_2/\psi_1$ $\Theta > \psi_2/\psi_1$ $\psi_2, \psi_1 > 0$
b) $\bar{f}(\sqrt{s})$	$\dfrac{1}{2\sqrt{(\pi\Theta^3)}} \displaystyle\int_0^\infty p \exp(-p^2/4\Theta)\, f(p)\, \mathrm{d}p$	
c) $\bar{f}(s + \psi_1)$	$f(\Theta) \exp(-\psi_1\Theta)$	
d) $\dfrac{s^{1/2} \exp(-\psi_1 s^{1/2})}{(s^{1/2} + \psi_2)^2}$	$\dfrac{\mathrm{d}}{\mathrm{d}\Theta}\left[2\sqrt{\dfrac{\Theta}{\pi}} \exp(-\psi_1^2/4\Theta) - (2\psi_2\Theta + \psi_1)\,.\right.$ $\left.\,.\exp(\psi_1\psi_2 + \psi_2^2\Theta)\, \mathrm{erfc}\left(\dfrac{\psi_1}{2\sqrt{\Theta}} + \psi_2\sqrt{\Theta}\right)\right]$	
e) $\dfrac{1}{s + \psi_1}$	$\exp(-\psi_1\Theta)$	
f) $\bar{f}(s) = \bar{f}_1(s)\, \bar{f}_2(s)$	$f(\Theta) = \displaystyle\int_0^\Theta f_1(p)\, f_2(\Theta - p)\, \mathrm{d}p$	

CONCLUSIONS

A two-parameter dispersion model coupled with ideal mixing is proposed and the function of residence time distribution *i.e.* the so-called **E**-function of this model is derived by the method of generalised Heaviside Expansion Theorem and by the approximative procedure.

Solution of the **E**-function of this model obtained by the method of generalised Heaviside Expansion Theorem in the form of the convergent series are Eq. (*8*) or (*19*). Convergence of this series is especially slow in the region of small values of Θ for large values of Pe. In such cases the **E**-function calculated as the sum of ten terms of the series (Eq. (*8*)) in the region of small values of Θ is decreasing and the **E**-function starts to have the expected dependence only for larger values of Θ, see Fig. 2.

For φ close to the ratio $\mathrm{Pe}/(\mathrm{Pe} + 4)$ and at the same time for large Pe numbers the solution by the method of generalised Heaviside Expansion Theorem (Eq. (*8*)) (calculated as the sum of ten terms of the series) is affected by a considerable numerical error in a relatively wide range of values Θ, see Fig. 2, curve for $\mathrm{Pe} = 30$; $\varphi = 0{\cdot}8$. It is obvious from these results that the range of applicability of the solution for the **E**-function calculated as the sum of ten terms of the series is relatively limited. Though for small values of Pe number the solution obtained by the method of generalized Heaviside Expansion Theorem (calculated as the sum of ten terms of the series) gives correct results, problems related with its numerical calculation are frequently a great disadvantage in practical application of this solution. As is given in this study, in the calculation of the **E**-function by use of the infinite series (*8*), only ten terms of the series were taken into consideration. The use of ten terms suffices only in case when the product $\mathrm{Pe}\,\varphi < 15$. In this case the solution obtained by the method of generalized Heaviside Expansion Theorem gives accurate results for all values $\Theta \geqq 0$.

The approximative solution given by Eq. (*24*) overcomes the problems related with the numerical calculation of the **E**-function by use of the solution obtained by the method of generalized Heaviside Expansion Theorem (Eqs (*8*) and (*19*)). The approximative solution holds for the whole interval of values $\varphi \in \langle 0; 1 \rangle$ in the region of small values of Θ the **E**-function increases from zero for any values of Pe (Fig. 3) and the numerical calculation of the **E**-function from Eq. (*24*) is considerably simpler than in the last case.

Though the approximative solution of the **E**-function gives sufficiently accurate results (compare Figs 2 and 3) this solution is preferred for its simplicity to the exact solution only when the condition (*29*) is satisfied.

The proposed model of dispersion flow coupled with ideal mixing is another theoretical contribution to mathematical modelling of flow systems. The model includes 2 parameters-volume fraction of the region of dispersion flow and the Pe number-which guarantees a greater flexibility of the model in comparison to single parameter models of similar type in description of hydrodynamic conditions either experimental or industrial units. Similarly, as other published models also the two-parameter dispersion model given in this paper can also be succesfully applied in the description of complex unit operations. From Fig. 1, which gives the dispersion model coupled ideal mixing is obvious that the proposed model can be more frequently used in processes consisting of two different characters of fluid flow: ideal mixing and plug flow. The resulting form of solution obtained by the method of generalised Heaviside Expansion Theorem or approximative solution of the **E**-function of the model is independent of location of the region of perfect mixing *i.e.* if this region is situated in the inlet or outlet part of the equipment. But the order of individual regions is not arbitrary in reaction systems in which nonlinear processes with respect to concentration appear.

LIST OF SYMBOLS

a, a', a_1	quantities defined by Eqs (*7*), (*9*) and (*20*)
c_1, c_2	concentration of tracer kg/m^3
C	dimensionless relative concentration of tracer
$\overline{C}$	Laplace transformation of function C
$\mathbf{E}(\Theta)$	function of residence time distribution
L	length of the system (m)
p	variable
$\mathrm{Pe} = wL/\varepsilon$	Peclet number
s, s_k	Laplace variable
t	residence time (s)
x	spacial variable (m)
V	volume of the system (m^3)
w	fluid velocity (m/s)
$Z = x/L$	dimensionless spacial variable
$\delta(\Theta)$	Dirac's function
ε	longitudinal disperion coefficient (m^2/s)
μ_i	moment of the i-th order
λ_k	k-th root of the transcendent Eq. (*12*)
φ	volume fraction of the dispersion flow region
$\Theta = wt/L$	dimensionless residence time

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Translated by M. Rylek.