APPROXIMATE SOLUTION OF A DIFFUSION MIXING MODEL FOR STATIONARY SYSTEMS

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The possibility of approximate modeling of a stationary reactor with mixing by a system of differential equations is examined.

A system of conjugate second-order differential equations whose autonomy is due to the member-sources must often be solved in applied chemistry. High-order reactions occurring in a reactor of continuous operation, some absorbing and extraction processes, etc., characterize such systems, for example.

Differential equations of the kind mentioned can usually be integrated numerically only, which results in significant difficulty in both conjugation of the parameters and in optimization of the processes. This is namely why three models, which just approximately describe the process but are convenient for processing the results obtained in the following cases, are used extensively:

1. Weak Mixing. The terms with the second derivative, which takes account of mixing, is discarded, i.e., pure convection is assumed whereby the equation becomes a first-order equation.
2. Medium Intensity Mixing. The source is linearized and the equation becomes linear.
3. Strong Mixing. Ideal mixing is assumed, and the diffusion equation therefore goes over into an algebraic equation.

An estimate of the error in the final result due to use of the hypotheses taken is hence given quite rarely.

Among the other type are models in which the mixing is taken into account by the introduction of recirculation, a cascade of total mixing reactors, etc. However, even in these models it is complicated to take account of the effect of a change in the mixing coefficient, and it is almost completely unknown how much the solutions differ for the different models.

It is hence expedient to develop an approximate method within whose framework only first-order differential equations must be solved; it is simple to take account of the influence exerted by a change in the magnitude of the mixing coefficient, and there is the possibility of estimating the error of the approximation.

Henceforth, we consider the case of just one variable to be more explicit, however, we note that this method can easily be applied also to the case of the usual conjugate systems of differential equations containing several dependent variables.

A stationary reaction proceeding in a constant operation mixing reactor whose length is L can be simulated by using the following differential equation:

$$Ax'' + Bx' + f(x) = 0. \tag{1}$$

Here A plays the part of the mixing coefficient, B is the linear velocity, x is the concentration dependent on the coordinate z ($0 \le z \le L$), and f(x) is a source function whose form depends on the order of the reaction.

In applied chemistry this equation is usually solved for Danckwerts boundary conditions

$$\lim_{z \to 0}(Ax' + Bx) = I_0, \quad Ax'(L) = 0. \tag{2}$$

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The crux of the approximation proposed here is that we find the solution of a first-order differential equation with the initial condition

$$\beta y' + f(y) = 0, \quad y(0) = y_0 \tag{3}$$

instead of solving a second-order differential equation satisfying the boundary conditions (2).

An estimate is given below of the deviation of the function x from y and the parameters y_0 and β in (3) are selected in such a way that it would be minimal.

The solution of (3) can be taken as approximate. Moreover, a specific physical meaning can be ascribed to it: it simulates the reaction proceeding in a reactor without mixing. Therefore, we not only obtain a certain approximate computational method but also the dependence which can effectively be used to determine to what extent the initial condition and the reaction flow rate can be altered so as to diminish the influence of the fact that mixing has not been taken into account.

Let us first examine the inhomogeneous linear equation similar to the differential equation (1):

$$Ax'' = Bx' + Cx = -f^*(z). \tag{4}$$

This differential equation can be solved in quadratures and to satisfy the conditions (2)

$$x(z) = \frac{1}{A}\left\{\frac{\lambda_2 e^{\lambda_2 L} e^{\lambda_1 z} - \lambda_1 e^{\lambda_1 L} e^{\lambda_2 z}}{\lambda_1^2 e^{\lambda_1 L} - \lambda_2^2 e^{\lambda_2 L}} I_0 + \frac{\dfrac{\lambda_1 e^{\lambda_1 z} - \lambda_2 e^{\lambda_2 z}}{\lambda_1 - \lambda_2} \displaystyle\int_0^L [\lambda_1 e^{\lambda_1 (L-\xi)} - \lambda_2 e^{\lambda_2 (L-\xi)}] f^*(\xi)\, d\xi}{\lambda_1^2 e^{\lambda_1 L} - \lambda_2^2 e^{\lambda_2 L}} \right.$$
$$\left. - \frac{1}{\lambda_1 - \lambda_2} \int_0^z [e^{\lambda_1 (z-\xi)} - e^{\lambda_2 (z-\xi)}] f^*(\xi)\, d\xi \right\}, \tag{5}$$

where λ_1 and λ_2 are the roots of the algebraic equation

$$A\lambda^2 + B\lambda + C = 0. \tag{6}$$

It should be noted that solution (5) permits determination of the error caused by linearizing the source term in (1).

For a homogeneous linear differential equation

$$\beta y' + cy = -g^*(z), \tag{7}$$

similar to differential equation (3), the solution can be found in the same manner

$$y(z) = y_0 e^{-\frac{c}{\beta} z} - \frac{1}{\beta} \int_0^z e^{\frac{c}{\beta}(\xi - z)} g^*(\xi)\, d\xi. \tag{8}$$

Let the requirements $f^*(z) = f(x(z))$, $g^*(z) = f(y(z))$ be satisfied and let the constant c be zero. It is seen that (5) relates the integral equation (9) to the differential equation (1) for the solution x(z) satisfying conditions (2). For differential equation (3), we obtain an integral equation for the solution y(z) satisfying the initial condition in (3) from (8):

$$x(z) = \frac{1}{B}\left\{I_0 - \int_0^z f(x(\xi))\, d\xi - \int_z^L e^{\frac{B}{A}(\xi - z)} f(x(\xi))\, d\xi \right\}, \tag{9}$$

$$y(z) = y_0 - \frac{1}{\beta} \int_0^z f(y(\xi))\, d\xi, \tag{10}$$

which permit the error estimate

$$\Delta(z) = x(z) - y(z). \tag{11}$$

Let us subtract (10) from (9)

$$[x(z) - y(z)] + \frac{1}{B} \int_0^z [f(x(\xi)) - f(y(\xi))]\, d\xi + \frac{1}{B} \int_0^L e^{\frac{B}{A}(\xi - z)} [f(x(\xi)) - f(y(\xi))]\, d\xi = \frac{I_0}{B} - y_0 +$$

$$+\left(\frac{1}{\beta}-\frac{1}{B}\right)\int\limits_0^z f(y(\xi))\,d\xi-\frac{1}{B}\int\limits_z^L e^{\frac{B}{A}(\xi-z)}f(y(\xi))\,d\xi. \tag{12}$$

Let us assume that the source function has a continuous derivative everywhere. Then according to the Lagrange theorem of the mean we have

$$f(x)-f(y)=f'(\xi)(x-y).$$

Hence, (12) is converted to the form

$$\Delta(z)-\int\limits_0^L K(z,\ \xi)\Delta(\xi)\,d\xi=\theta(z), \tag{13}$$

$$K(z,\ \xi)=\begin{cases}\frac{1}{B}f'(\xi^*),\ L\geqslant z\geqslant\xi\geqslant 0,\\ \frac{1}{B}f'(\xi^{**})e^{\frac{B}{A}(\xi-z)}\ ,\end{cases} \tag{14}$$

where ξ^* and ξ^{**} are numbers between the values of x and y in conformity with (12) and

$$\theta=\frac{I_0}{\beta}-y_0+\left(\frac{1}{\beta}-\frac{1}{B}\right)\int\limits_0^z f(y(\xi))\,d\xi-\frac{1}{B}\int\limits_z^L e^{\frac{B}{A}(\xi-z)}f(y(\xi))\,d\xi. \tag{15}$$

Equation (13) permits an error estimate. Let us assume that

$$\sup_{z\in(0,L]}\int\limits_0^L|K(z,\ \xi)|\,d\xi=\frac{L}{B}\sup_{z\in(0,L]}f'(\xi(z))<1, \tag{16}$$

then

$$\sup_{z\in(0,L]}|\theta(z)|=\sup_{z\in(0,L]}\left|\Delta(z)+\int\limits_0^L K(z,\ \xi)\Delta(\xi)\,d\xi\right|\geqslant\sup_{z\in(0,L]}|\Delta(z)|-\sup_{z\in(0,L)}\int\limits_0^L|K(z,\ \xi)|\,d\xi\sup_{z\in(0,L]}|\Delta(z)|, \tag{17}$$

from which

$$\sup_{z\in(0,L]}|\Delta(z)|\leqslant\frac{\sup_{z\in(0,L]}|\theta(z)|}{1-\frac{L}{B}\sup_{z\in(0,L]}f'(\xi(z))}. \tag{18}$$

There is a possibility for a direct computation of the values of the parameters β and y_0 by finding the absolute (not local) maximum of the function $\theta(z)$ determined by (15), for fixed values of y_0 and β and further minimization of these values in β and y_0. However, this method is not applicable in the general case since it is extremely tedious even for the simplest specific functions f (constants, linear). The complexity is that the values of the argument governing the extremal values of the function $\theta(x)$ vary strongly as a function of the parameters y_0 and β.

Therefore, another means should be selected for the conjugation of the parameters. Let us convert (15) as follows:

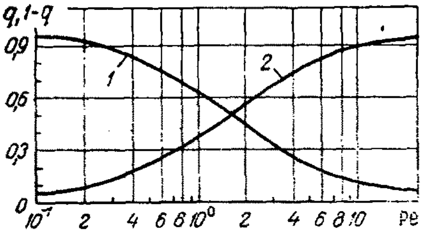
$$\theta(z)=\frac{I_0}{B}-y_0+\left(\frac{1}{\beta}-\frac{1}{B}\right)\int\limits_0^L f(y(\xi))\,d\xi-\int\limits_z^L\left(\frac{1}{\beta}-\frac{1}{B}+\frac{1}{B}e^{\frac{B}{A}(\xi-z)}\right)f(y(\xi))\,d\xi. \tag{19}$$

It is hence seen that the first three members in the right-hand side of the equation are independent of z, while the fourth member vanishes for z = L. We determine the parameters β and y_0 from the assumption that the part of $\theta(z)$ independent of z vanishes while the fourth term can be estimated easily. Let the source function f not change sign and let

$$f_{\max}=\sup_{z\in(0,L]}|f(y(z))|. \tag{20}$$

Then

$$-f_{\max}\int\limits_0^L\left(\frac{1}{\beta}-\frac{1}{B}+\frac{1}{B}e^{-\frac{B}{A}\xi}\right)^- d\xi\leqslant$$



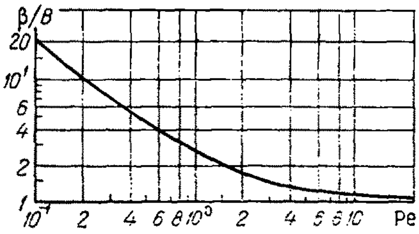


Fig. 1 Fig. 2

Fig. 1. Initial conditions as a function of the number Pe: 1) q(Pe); 2) [1 − q(Pe)].

Fig. 2. Velocity as a function of Pe.

$$\leqslant\int_z^L\left(\frac{1}{\beta}-\frac{1}{B}+\frac{1}{B}e^{-\frac{B}{A}(\xi-z)}\right)f(y(\xi))\,d\xi\leqslant f_{\max}\int_0^L\left(\frac{1}{\beta}-\frac{1}{B}+\frac{1}{B}e^{-\frac{B}{A}\xi}\right)^+d\xi. \tag{21}$$

The plus and minus signs in the exponent in (21) define the positive or negative parts of the functions in the parentheses:

$$g^+(x)=\begin{cases}g(x), & \text{if}\quad g(x)\geqslant 0,\\ 0, & \text{if}\quad g(x)<0;\end{cases}$$
$$g^-(x)=\begin{cases}-g(x), & \text{if}\quad g(x)<0,\\ 0, & \text{if}\quad g(x)\geqslant 0.\end{cases} \tag{22}$$

The best estimate of the absolute value is obtained when the lower and upper bounds presented above differ only in sign. Hence

$$\int_0^L\left(\frac{1}{\beta}-\frac{1}{B}+\frac{1}{B}e^{-\frac{B}{A}\xi}\right)d\xi=0,\quad \beta=B\frac{1}{1-\frac{A}{BL}\left(e^{-\frac{B}{A}L}-1\right)}. \tag{23}$$

The following estimate is obtained for such a value of β

$$\left|\int_z^L\left(\frac{1}{\beta}-\frac{1}{B}+\frac{1}{B}e^{-\frac{B}{A}(\xi-z)}\right)f(y(\xi))\,d\xi\right|\leq$$

$$\leqslant\frac{L}{B}\left\{\frac{A}{BL}\left\{\frac{A}{BL}\left(e^{-\frac{B}{A}L}-1\right)\left[1-\ln\frac{A}{BL}\left(e^{\frac{BL}{A}}-1\right)\right]\right\}\right\}f_{\max}=\frac{Lf_{\max}}{B}\Phi\left(\frac{BL}{A}\right). \tag{24}$$

If the sum of the first three terms, independent of z, in the expression for θ equals zero, then (24) is the upper bound of |θ|, i.e., yields sup |θ|. This is assured by the algebraic equation

$$y_0=\frac{I_0}{B}\left[1-\frac{A}{BL}\left(e^{-\frac{BL}{A}}-1\right)\right]+\frac{A}{BL}\left(e^{-\frac{BL}{A}}-1\right)y_L. \tag{25}$$

Let us introduce the following notation

$$-\frac{BL}{A}=\mathrm{Pe}\,(>0),\qquad \frac{1-e^{-\mathrm{Pe}}}{\mathrm{Pe}}=q\,(\mathrm{Pe}),$$

$$\frac{1}{\mathrm{Pe}}\left[1+\frac{1-e^{-\mathrm{Pe}}}{\mathrm{Pe}}\left(\ln\frac{1-e^{-\mathrm{Pe}}}{\mathrm{Pe}}-1\right)\right]=\Phi(\mathrm{Pe}). \tag{26}$$

The results are extended as follows in this notation. The solution of differential equation (1) satisfying the boundary conditions (2) can best approximate one of the solutions of the differential equation (3) to its initial condition for which

$$\beta=B\frac{1}{1-q},\quad y_0=(1-q)\frac{I_0}{B}+qy_L. \tag{27}$$

The difference between the approximate and exact solutions can be given if (16) is satisfied,

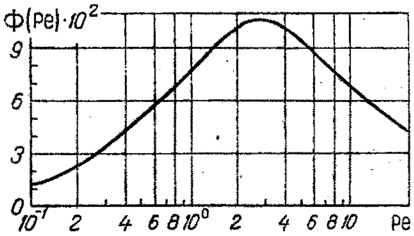


Fig. 3. Error coefficient of the approximation as a function of the number Pe.

and then

$$\sup_{z\in(0,L]} |x(z)-y(z)| \leqslant \frac{1}{\frac{B}{L}-\sup\limits_{z\in(0,L]} |f'(\xi(z))|}\,\Phi(\mathrm{Pe}). \tag{28}$$

It is seen that the differential equation and initial condition in (3) correspond again to the recirculation model when the parameters are selected according to (27). It is shown in Figs. 1 and 2 in what manner the parameters of the approximate recirculation model depend on the characteristic mixing parameter of the initial diffusion model, the number Pe. A relative approximation error is given in Fig. 3 as a function of Pe. For the Pe encountered in practice, this quantity is ordinarily sufficiently small, hence the error estimate is determined by another factor dependent on the remaining parameters.

It is perfectly evident that both the solution (9) of the differential equation (1) and the error estimate (28) diverge in the case $A \to 0$, and conversely, the solution (10) of the differential equation (1), obtained as an approximation, exists even in the case $A = 0$, where the other solutions converge to it as $A \to 0$. Hence, differential equation (3) should be considered the best mathematical model of the process in this sense.

In many cases condition (16) imposes too strong a constraint. However, weakening it need not be considered here since uniqueness of the solution is not assured in this case.

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