Int. J. Heat Mass Transfer. Vol. 26, No. 7, pp. 1063-1067, 1983
Printed in Great Britain

0017-9310/83 $3.00+0.00

FALSE DIFFUSION IN CONVECTION AND DIFFUSION WITH CHEMICAL REACTION

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(*Received* 5 *April* 1982 *and in revised form* 23 *November* 1982)

Abstract—The method of moments is used to obtain the false diffusion coefficient as

$$D_{\text{false}} = \frac{u\Delta x}{2}\left(1 - u\frac{\Delta t}{\Delta x}\frac{1}{1-k\Delta t}\right)$$

for the unsteady state 'reactor-and-tube' model with a first-order chemical reaction. A comparison is made between the upwind finite difference solution (i.e. the continuous stirred chemical reactor in series) and the exact solution with a false diffusion coefficient.

NOMENCLATURE

C,	mass concentration;
C_0,	the initial mass concentration at the entering point of the tubular reactor;
D,	effective axial diffusion coefficient;
D_{false},	false diffusion coefficient;
f,	a dummy function;
i,	index of the reactor number;
j,	index of the time step;
k,	first-order chemical reaction constant;
k_L,	kL/u;
L,	length of tubular reactor;
M,	moment for discrete system;
$\tilde{M}$,	moment about the mean;
N,	the number of cells in a tubular reactor;
P,	$uL/4D$;
p,	moment index;
q,	integer variable;
R,	moment for continuous system;
$\tilde{R}$,	moment about the mean;
s,	Laplace transform parameter;
t,	time variable;
u,	constant axial fluid velocity;
$\bar{u}$,	dimensionless fluid velocity, defined in equation (5);
x,	reactor length variable.

Greek symbols

τ,	ut/L;
ξ,	x/L.

1. INTRODUCTION

THE OBJECTIVE of this paper is to study the false diffusion effect in problems involving convection and diffusion with chemical reaction. The false diffusion effect has caused considerable controversy and confusion among the practitioners of numerical analysis. There is something called 'false diffusion', which is quite commonly misinterpreted, but which, in its proper meaning, represents a major weak point of most convection–diffusion formulations. Recently, false diffusion has been extensively discussed by Patankar [1] and Gosman *et al.* [2] but no one has discussed and shown the false diffusion effect in convection and diffusion with chemical reaction, which is important in heat and mass transfer problems.

The generic transport equation for 1-dim., unsteady state convection with diffusion and a source term is

$$\rho\frac{\partial\phi}{\partial t} + \rho u\frac{\partial\phi}{\partial x} = \Gamma\frac{\partial^2\phi}{\partial x^2} + S_\phi. \tag{1}$$

This is the unsteady state partial differential equation involving the first, second and zero derivatives. If ϕ is the concentration of reactant, and $S_\phi = -k\phi$, the above equation is the mass conservation equation used to model the unsteady state 1-dim. plug flow tubular reactor with a first-order chemical reaction. If ϕ is the temperature, T, the above transport equation would describe the 1-dim. unsteady state temperature distribution in the presence of convection, diffusion and heat transfer from the wall, or internal heat sinks.

In chemical reaction engineering, the governing transport equation for a 1-dim. unsteady plug flow chemical reactor is usually presented in the following form:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} - kC \tag{2}$$

where t is the time from the commencement of the reaction, x is the distance from the point of introduction of the reactive fluid, $C = C(t, x)$ is the concentration of reactant, D is the effective diffusion coefficient, u is the constant axial fluid velocity, and k is the first-order chemical reaction constant. If the diffusion coefficient D is non-zero, a dispersion layer will form in which the concentration gradually changes from the higher value to the lower one by diffusion. On the other hand, if the diffusion coefficient is zero, a dispersion layer will not form, and the concentration will be changed due to convection transfer only. The best way to observe false diffusion is by setting the real diffusion coefficient to zero and comparing the numerical solution with $D = 0$ to the exact solution of equation (2) in which D is equal to the coefficient of false diffusion.

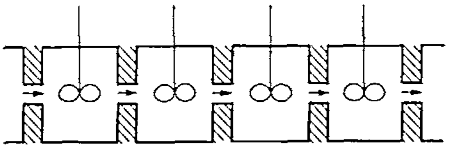

FIG. 1. Reactor-and-tube model.

The scheme to be analyzed is based on the 'reactor-and-tube' model, which is referred to in Gosman *et al.* [2] as the 'tank-and-tube' model. As shown in Fig. 1, each control volume can be thought to be a continuously stirred chemical reactor that is connected in series to other reactors by short tubes. The flow through the tubes represents convection. Since the reactors are stirred, each contains a uniform concentration fluid, and the mass conservation equation may be written as

$$C_{j,i} = C_{j-1,i} + \frac{u\Delta t}{\Delta x}(C_{j-1,i-1} - C_{j-1,i}) - kC_{j-1,i}\Delta t \tag{3}$$

where subscripts i and j denote the ith reaction zone and jth time step in which the evaluation is to be made. From a finite difference point of view, equation (3) is also the upwind finite difference scheme for equation (2) with diffusion coefficient $D = 0$. If we compare the coefficients for the central-difference with upwind schemes, it can be shown that the upwind scheme is equivalent to replacing the diffusion coefficient D in the central-difference scheme with D plus false diffusion coefficient [1]. Hence the diffusion coefficient of equation (3) is the false diffusion coefficient.

The method of moments [3] is applied to find the false diffusion of equation (3) by comparing the means and variances of the concentration of equations (2) and (3).

2. MATHEMATICAL ANALYSIS

In order to apply the method of moments, equation (3) is rearranged in the following form:

$$C_{j,i} = (1 - k\Delta t - \bar{u})C_{j-1,i} + \bar{u}C_{j-1,i-1} \tag{4}$$

where

$$\bar{u} = \frac{u\Delta t}{\Delta x}. \tag{5}$$

Let

$$M_{p,j} = \sum_{i=-\infty}^{\infty} i^p C_{j,i} \tag{6}$$

be the pth moment of the distribution of solute at the jth time step in the tubular reactor. The condition to be imposed on $C_{j,i}$ as $i \to \pm\infty$ is such that these moments should exist and be finite, a condition fulfilled if the solute is originally contained in a finite length of the tube reactor.

Substituting equation (4) into equation (6), we get the partial difference equation

$$M_{p,j} = (1 - k\Delta t - \bar{u})M_{p,j-1} + \bar{u}\sum_{q=0}^{p}\binom{p}{q}M_{q,j-1} \tag{7}$$

where

$$\binom{p}{q} = \frac{p!}{q!(p-q)!}, \quad p \geqslant q,$$

and p, q are integers.

The definition of the pth moment about the mean is

$$\tilde{M}_{p,j} = \sum_{i=-\infty}^{\infty}(i - \bar{i})^p C_{j,i} \tag{8}$$

where

$$\bar{i} = \frac{\sum_{i=-\infty}^{\infty} iC_{j,i}}{\sum_{i=-\infty}^{\infty} C_{j,i}} = \frac{M_{1,j}}{M_{0,j}}. \tag{9}$$

$M_{1,j}$ and $M_{0,j}$ can be found from equation (7), hence $\bar{i}$ can be stated as

$$\bar{i} = \frac{j\bar{u}}{1 - k\Delta t}. \tag{10}$$

Setting $p = 0$, 1 and 2 in equation (8), and solving equation (7), one can obtain the solutions of the first three moments about the mean $\tilde{M}_{0,j}$, $\tilde{M}_{1,j}$ and $\tilde{M}_{2,j}$ as given in Table 1.

The method of moments will now be applied to the continuous system as shown in equation (2). The results of the first three moments of the continuous system will correlate to the first three moments of the 'tube-and-reactor' model (i.e. upwind scheme).

Let

$$R_p(t) = \int_{-\infty}^{\infty} x^p C \, \mathrm{d}x \tag{11}$$

be the pth moment of the distribution of solute in the tube at time t. The condition to be imposed on C as $x \to \pm\infty$ is such that these moments should exist and be finite, a condition fulfilled if the solute is originally contained in a finite length of the tube reactor.

Substituting equation (2) into equation (11), one can arrive at

$$\frac{\mathrm{d}R_p}{\mathrm{d}t} + kR_p = upR_{p-1} + Dp(p-1)R_{p-2}. \tag{12}$$

Table 1. Moments about the mean

pth order	$\tilde{M}_{p,j}$	$\tilde{R}_p(t)$
0th	$M_0(1-k\Delta t)^j$	$R_0(0)\,\mathrm{e}^{-kt}$
1st	0	0
2nd	$-j\bar{u}^2M_0(1-k\Delta t)^{j-2}$ $+j\bar{u}M_0(1-k\Delta t)^{j-1}$ $+M_{2,0}(1-k\Delta t)^j$	$[2DR_0(0)+R_2(0)]\,\mathrm{e}^{-kt}$

The mean moment about the mean is now defined as

$$\tilde{R}_p = \int_{-\infty}^{\infty} (x-\bar{x})^p C \, \mathrm{d}x, \tag{13}$$

where

$$\bar{x} = \frac{\int_{-\infty}^{\infty} xC \, \mathrm{d}x}{\int_{-\infty}^{\infty} C \, \mathrm{d}x} = \frac{R_1(t)}{R_0(t)}. \tag{14}$$

$R_1(t)$ and $R_0(t)$ can be found from equation (12), and the solution of $\bar{x}$ can be stated as

$$\bar{x} = ut. \tag{15}$$

Setting $p = 0$, 1 and 2 in equation (13) and solving equation (12), one can obtain the solutions of the first three moments about the mean $\tilde{R}_0(t)$, $\tilde{R}_1(t)$ and $\tilde{R}_2(t)$ as given in Table 1.

In Table 1,

$$M_0 = \sum_{i=-\infty}^{\infty} C_{0,i} \quad \text{and} \quad R_0(0) = \int_{-\infty}^{\infty} C(0,x) \, \mathrm{d}x.$$

The zeroth moments in Table 1 are automatically satisfied in the limit since:

$$\lim_{\Delta t \to 0} (1-k\Delta t)^j = \lim_{\Delta t \to 0} (1-k\Delta t)^{t/\Delta t} = \mathrm{e}^{-kt}.$$

The second moments can be equated by the following identity:

$$D_{\text{false}} = \frac{u\Delta x}{2}\left(1 - u\frac{\Delta t}{\Delta x}\frac{1}{1-k\Delta t}\right). \tag{16}$$

This is the false diffusion coefficient of a 'tube and reactor' model. For the steady state, i.e. $\Delta t = 0$, $D_{\text{false}} = u\Delta x/2$, which is consistent with ref. [1]. It is interesting to note that the chemical reaction does not affect the false diffusion coefficient in steady state diffusion and convection problems.

For the case of no chemical reaction, i.e. $k = 0$,

$$D_{\text{false}} = \frac{u\Delta x}{2}\left(1 - \frac{u\Delta t}{\Delta x}\right). \tag{17}$$

It can be seen from equation (17) that when the distance step and time step are related by $\Delta x = u\Delta t$, the false diffusion of equation (3) will be zero. We can show this phenomenon by setting $\Delta x = u\Delta t$ and $k = 0$ in equation (3).

For the finite tubular reactor, we know

$$\Delta x = \frac{L}{N} \tag{18}$$

where L is the length of the tubular reactor and N is the number of finite difference control volumes. From equations (18) and (16) we have the following dimensionless false diffusion coefficients:

$$\frac{D_{\text{false}}}{uL} = \frac{1}{2N}\left[1 - \frac{\Delta\left(\frac{ut}{L}\right)}{\Delta\left(\frac{x}{L}\right)} \frac{1}{1-\left(\frac{kL}{u}\right)\Delta\left(\frac{ut}{L}\right)}\right]. \tag{19}$$

3. RESULTS AND DISCUSSION

The exact analytical solution of equation (2), where D is equal to the false coefficient given in equation (16), can be compared with the numerical solution of equation (3) using an upwind difference scheme. An example is stated as follows:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} - kC, \tag{2}$$

initial condition at

$$t = 0, \quad C = 0,$$

boundary condition at

$$x = 0, \quad C = C_0 \frac{L}{u}\delta(t),$$

$$x = L, \quad \frac{\partial C}{\partial x} = 0.$$

An exact solution of the above equation at exit $x = L$, i.e. $\xi = 1$, when uL/D is large is

$$c_e(\tau) = 2\left(\frac{P}{\pi\tau}\right)^{1/2}\left(\frac{1}{\tau} - 1\right)\mathrm{e}^{2P-(P+k_L)\tau-(P/\tau)} + 2P\,\mathrm{e}^{4P-k_L\tau}\operatorname{erfc}\left[\left(\frac{P}{\tau}\right)^{1/2} + (P\tau)^{1/2}\right] \tag{20}$$

where

$$c = \frac{C}{C_0}, \quad \tau = \frac{ut}{L}, \quad \xi = \frac{x}{L}, \qquad P = \frac{uL}{4D}, \quad k_L = \frac{kL}{u} \tag{21}$$

and

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) = 1 - \frac{2}{(\sqrt{\pi})}\int_0^x \mathrm{e}^{-x^2} \, \mathrm{d}x.$$

(The detailed solution of equation (20) is given in the Appendix.)

If we assume the dimensionless time step $\Delta\tau = 0.005$, the dimensionless step length $\Delta\xi = 0.01$, and the dimensionless first-order chemical reaction constant, $k_L = 2$, then we have

$$\frac{D_{\text{false}}}{uL} = 2.4747 \times 10^{-3}. \tag{22}$$

A comparison of equation (3) with equations (20) and (22) is shown in Fig. 2. The points (○) are calculated from equation (3), and the solid line is calculated from equations (20) and (22).

The initial boundary condition of this example is the inplus tracer $C = C_0(L/u)\delta(t)$. In the plug flow tubular reactor without diffusion, if we input the inplus tracer at the entering point of the tube, we should get the inplus tracer output at the exit of the tube [4]. Without diffusion, the inplus tracer output at the exit of the tube is

$$C = 0.1354\, C_0 \frac{L}{u}\delta(t - L/u). \tag{23}$$

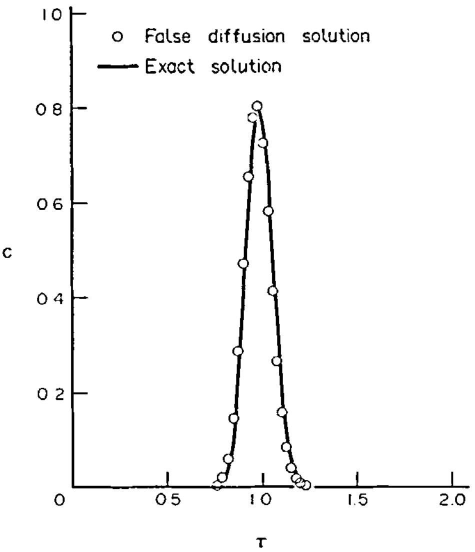

FIG. 2. Comparison of false diffusion with exact solution.

Equation (23) can be obtained from the first-order chemical reaction equation or the partial differential equation for the unsteady state plug flow reactor.

If we take

$$\delta(t-L/u) \simeq \frac{1}{\Delta t} \quad \text{at} \quad t = \frac{L}{u},$$

equation (23) can be written as

$$c = \frac{C}{C_0} \simeq 0.1354\frac{1}{\Delta\tau} = 27.07 \quad \text{at} \quad \tau = 1. \qquad (24)$$

We see that the exact solution for the unsteady state plug flow reactor in equation (24) is much different than the upwind solution in Fig. 2. The upwind solution in Fig. 2 is a bell type curve due to the false diffusion and convection. The solution of equation (24) is single valued as this is due to convection transfer only.

4. CONCLUSION

This study has shown that:

(1) The false diffusion coefficient can be obtained from the method of moments.

(2) The chemical reaction in mass transfer or internal heat source or sink in heat transfer can affect the false diffusion coefficient in unsteady state problems.

REFERENCES

1. S. V. Patankar, *Numerical Heat Transfer and Fluid Flow*, pp. 105–109. Hemisphere, Washington, D.C. (1980).
2. A. D. Gosman, W. M. Pun, A. K. Runchal, D. B. Spalding and M. Wolfshtein, *Heat and Mass Transfer in Recirculating Flows*, pp. 132, 158. Academic Press, London (1968).
3. R. Aris, On the dispersion of a solute in a fluid flowing through a tube, *Proc. R. Soc.* A235, 67–77 (1956).
4. O. Levenspiel, *Chemical Reaction Engineering* (2nd edn.) p. 260. John Wiley, New York (1972).

APPENDIX

From equations (2) and (21) we have

$$\frac{\partial c}{\partial \tau} + \frac{\partial c}{\partial \xi} = \frac{1}{4P}\frac{\partial^2 c}{\partial \xi^2} - k_L c, \qquad \text{(A1)}$$

initial condition at

$$\tau = 0, \qquad c = 0,$$

boundary condition at

$$\xi = 0, \qquad c = \delta(\tau),$$

$$\xi = 1, \qquad \frac{\partial c}{\partial \xi} = 0.$$

Set

$$c(\tau, \xi) = f\,e^{2P\xi - (P + k_L)\tau}. \qquad \text{(A2)}$$

Putting equation (A2) into equation (A1), we get

$$\frac{\partial f}{\partial \tau} = \frac{1}{4P}\frac{\partial^2 f}{\partial \xi^2}, \qquad \text{(A3)}$$

initial condition at

$$\tau = 0, \qquad f = 0,$$

boundary condition at

$$\xi = 0, \qquad f = \delta(\tau)\,e^{(P + k_L)\tau},$$

$$\xi = 1, \qquad \frac{\partial f}{\partial \xi} + 2Pf = 0.$$

Applying the Laplace transformation into equation (A3) we have

$$\bar{f}(s, \xi) = \frac{(\sqrt{Ps} - P)\,e^{-2\sqrt{Ps}(1-\xi)} + (\sqrt{Ps} + P)\,e^{2\sqrt{Ps}(1-\xi)}}{(\sqrt{Ps} + P)\,e^{2\sqrt{Ps}} + (\sqrt{Ps} - P)\,e^{-2\sqrt{Ps}}}. \qquad \text{(A4)}$$

At the end of the tubular reactor, where $\xi = 1$,

$$\bar{f}(s, 1) = \frac{2\sqrt{Ps}}{(\sqrt{Ps} + P)\,e^{2\sqrt{Ps}} + (\sqrt{Ps} - P)\,e^{-2\sqrt{Ps}}}. \qquad \text{(A5)}$$

For large P, we can simplify equation (A5) to

$$\bar{f}(s, 1) \simeq \frac{2\sqrt{Ps}}{(\sqrt{Ps} + P)\,e^{2\sqrt{Ps}}}. \qquad \text{(A6)}$$

The inversion of the Laplace transformation of equation (A6) is

$$f(\tau, 1) = 2\left(\frac{P}{\pi\tau^3}\right)^{1/2} e^{-P/\tau} - 2\left(\frac{P}{\pi\tau}\right)^{1/2} e^{-P/\tau} + 2P\,e^{2P + P\tau}\,\mathrm{erfc}\left[\left(\frac{P}{\tau}\right)^{1/2} + (P\tau)^{1/2}\right]. \qquad \text{(A7)}$$

From equations (A2) with $\xi = 1$ and (A7) we get equation (20).

FAUSSE DIFFUSION EN CONVECTION ET DIFFUSION AVEC REACTION CHIMIQUE

Résumé—La méthode des moments est utilisée pour obtenir le coefficient de fausse diffusion

$$D_{\text{false}} = \frac{u\Delta x}{2}\left[1 - u\frac{\Delta t}{\Delta x}\frac{1}{1-k\Delta t}\right]$$

pour le modèle instationnaire "réacteur et tube" avec un réacteur chimique de premier ordre. Un comparaison est faite entre la solution récurrente par volumes finis (par exemple, la série de réacteurs chimiques continuellement agités) et la solution exacte avec un coefficient de fausse diffusion.

SCHEINDIFFUSION BEI KONVEKTION UND DIFFUSION MIT CHEMISCHER REAKTION

Zusammenfassung—Die Momentenmethode wird angewandt, um den Scheindiffusions-Koeffizienten als

$$D_{\text{false}} = \frac{u\Delta x}{2}\left[1 - u\frac{\Delta t}{\Delta x}\frac{1}{1-k\Delta t}\right]$$

für ein instationäres Rohrreaktor-Modell mit einer chemischen Reaktion erster Ordnung zu bestimmen. Ein Vergleich zwischen einer Lösung mittels finiter Differenzen (z. B. für den kontinuierlich gerührten Reaktor in Reihenschaltung) und der exakten Lösung mit Hilfe des Scheindiffusions-Koeffizienten wird durchgeführt.

ЭФФЕКТИВНАЯ ДИФФУЗИЯ ПРИ КОНВЕКЦИИ И ДИФФУЗИИ В ПРИСУТСТВИИ ХИМИЧЕСКОЙ РЕАКЦИИ

Аннотация—Методом моментов рассчитывается коэффициент эффективной диффузии

$$D_{\text{эфф}} = \frac{u\Delta x}{2}\left[1 - u\frac{\Delta t}{\Delta x}\frac{1}{1 - k\Delta t}\right]$$

для нестационарной модели проточного реактора при протекании химической реакции первого порядка. Проведено сравнение между решением методом конечных разностей (химический реактор с непрерывным перемешиванием) и точным решением, в котором учитывается эффективный коэффициент диффузии.