An Approach in Modeling the Tubular Polymer Reactor

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Synopsis

An analytical solution for diffusion with a homogeneous first-order reaction in the bulk and a heterogeneous reaction at the reactor wall in a non-Newtonian laminar flow tubular reactor is presented by using the Galerkin technique. The effect of reaction rate constants on dispersion is studied under isothermal conditions. It is found that, for the same mean velocity of the flow, the effective dispersion coefficient decreases with increase in the chemical reaction rate constants.

INTRODUCTION

Diffusion with homogeneous chemical reaction under the condition of laminar flow of Newtonian fluids in tubular reactors has been the subject of a number of papers.[1–8] The analogous problems of non-Newtonian fluids, which are of interest in food processing, biological systems, and polymerization processes, have been discussed in Refs. 9–12. The problem of simultaneous homogeneous and heterogeneous reactions in tubular flow reactors is of importance in several areas.[13] In the case of polymerization reactions, the initiation may often be catalyzed at the tube wall. The problem is also of importance in the case of removal of solutes such as urea from the blood in a tubular haemodialyzer under conditions when significant solute concentration differences exist between red cells and plasma. In spite of the diversity of fields in which the problem may be of interest, surprisingly little work has been done in this specific area. Most theoretical studies concerning the simultaneous homogeneous and heterogeneous reactions in tubular reactors have been confined to Newtonian fluids.[13–17] It is believed that practically no suitable model is available in the literature, which discusses the simultaneous homogeneous and heterogeneous reaction in the non-Newtonian laminar flow tubular reactor.

In the present work, a simple closed form analytical solution within the framework of Taylor's dispersion theory[18] is obtained. The novelty about the work is that Galerkin technique[19,20] has been used for the first time to obtain such a solution which enables one to obtain fairly accurate predictions for the reactor exit conversion without resorting to numerical techniques. The effect of reaction rate constants on the effective dispersion coefficient is also discussed.

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DISTRIBUTED PARAMETER MODEL

The two-dimensional diffusion equation for a laminar flow of a non-Newtonian fluid with a fully developed velocity profile is as follows[21]:

$$\tau\left(\frac{\partial^2 C}{\partial Y^2}+\frac{1}{Y}\frac{\partial C}{\partial Y}\right)-\beta C-\frac{1}{(n+1)}[2-(n+3)Y^{n+1}]\frac{\partial C}{\partial X}=0 \tag{1}$$

where the dimensionless quantities are defined as

$$\tau=\bar{t}D_m/R^2,\quad \beta=K\bar{t},\quad C=c/C_0,\quad Y=r/R \tag{2}$$

The boundary conditions associated with eq. (1) are

$$C=1 \quad \text{at } X=0 \tag{3}$$

$$\frac{\partial C}{\partial Y}=0 \quad \text{at } Y=0 \tag{4}$$

$$\frac{\partial C}{\partial Y}=AC \quad \text{at } Y=1 \tag{5}$$

where A is the heterogeneous reaction rate parameter. Equation (1) with the boundary conditions (3)–(5) was solved numerically by adopting a Crank–Nicolson finite-difference scheme. Herein, we present a closed-form analytical solution for the above problem within the framework of Taylor's dispersion theory by applying the Galerkin method.

GALERKIN'S APPROACH

The Galerkin method[19,20] has been used to solve eq. (1) with boundary conditions given by eqs. (3)–(5). In the present model we have assumed that $\partial C/\partial X$ is independent of Y. This approximation is not valid for low values of X but is useful in practice and has been used by many workers.[4,7,10–13] Under the Galerkin method let C_m be the mth-order solution for C, and

$$C_m=a_0+a_1f_1(Y)+a_2f_2(Y)+\cdots+a_mf_m(Y) \tag{6}$$

where $a_0,a_1,\cdots,a_m$ are constants to be determined. $f_i(Y)$ $(i=1,2,\cdots,m)$ are the first m functions of an infinite sequence $\{f_i(Y)\}$ $(i=1,2,\cdots)$. Each of these functions is twice continuously differentiable on $0\leqslant Y\leqslant 1$ and satisfies the boundary conditions (4) and (5). Further, any finite set of these functions is linearly independent on $0\leqslant Y\leqslant 1$. The constants $a_0,a_1,a_2,\cdots,a_m$ are found out by solving the following system of equations:

$$\int_0^1 L(C_m)Y\,dY=0 \tag{7a}$$

and

$$\int_0^1 YL(C_m)f_i(Y)\,dY=0,\quad i=1,2,3\cdots,m \tag{7b}$$

$$L(C_m)=\tau\left(\frac{\partial^2 C_m}{\partial Y^2}+\frac{1}{Y}\frac{\partial C_m}{\partial Y}\right)-\beta C_m-\frac{1}{(n+1)}[2-(n+3)Y^{n+1}]\frac{\partial C}{\partial X} \tag{8}$$

The above system of equations (7) is a system of linear algebraic equations be-

cause operator L is linear. This system is generated by the application of orthogonality condition of $L(C_m)$ to each of $f_j(Y)$ ($j = 1,2,3,\cdots,m$) over the cross section of the reactor tube.

Thus once the sequence of functions $\{f_i(Y)\}$ ($i = 1,2,\cdots$) is known, any order solution for C may be found out by calculating $a_0,a_1,\cdots,a_m$, etc. from eq. (7). We choose the following sequence of the functions:

$$f_i(Y) = Y^{2i}\left[1 - \frac{A}{A+2i}\frac{n+1}{n+3} - \frac{2}{n+3}Y^{i(n+1)}\right] \qquad i = 1,2,3,\cdots. \tag{9}$$

These functions are algebraic polynomials which are easier to tackle mathematically. Substitution of these functions in eq. (7) gives a nonhomogeneous, nonsingular linear system of $(m + 1)$ algebraic equations. We have $(m + 1)$ unknowns $(a_0,a_1,\cdots,a_m)$, which can be obtained by solving the system of equations. In the present analysis we obtain a second-order solution by considering only the first two functions of eq. (9). Putting $m = 2$ in eq. (6) and solving eqs. (7), we get the second-order solution for C as

$$C_2 = a_0 + a_1Y^2\left(1 - \frac{A}{A+2}\frac{n+1}{n+3} - \frac{2}{n+3}Y^{n+1}\right) + a_2Y^4\left(1 - \frac{A}{A+4}\frac{n+1}{n+3} - \frac{2Y^{2n+2}}{n+3}\right) \tag{10}$$

where

$$a_0 = -\frac{n+1}{n+3}\left[\frac{a_1}{A+2}\left(\frac{A+n+7}{n+5} + \frac{4A}{\alpha}\right) + \frac{a_2}{A+4}\left(\frac{2A+4n+24}{3n+12} + \frac{8A}{\alpha}\right)\right] \tag{11}$$

$$a_1 = \frac{12}{\tau}\frac{n+1}{n+3}\frac{(A+2)\phi_1}{F}\left[\phi_2(16\eta_0 + 32\eta_1A + 2\eta_2A^2 + 4\eta_3A^3) - \frac{\phi_3}{\alpha}(8\eta_4 + 2\eta_5A + \eta_6A^2 + 5\eta_7A^3)\right]\frac{\partial C}{\partial X} \tag{12}$$

$$a_2 = \frac{30}{\alpha\tau}\frac{n+1}{n+3}\frac{(A+4)(n+6)(2n+7)\phi_1}{F} \times [2\eta_8 + A\eta_9 + A^2\eta_{10} + 2A^3\eta_{11}]\frac{\partial C}{\partial X} \tag{13}$$

$$\phi_1 = (n+4)(n+5)(n+9)(3n+11) \tag{14}$$

$$\phi_2 = 10(n+6)(n+9)(2n+7)(3n+11) \tag{15}$$

$$\phi_3 = (n+5)(n+7) \tag{16}$$

$$\phi_4 = 24(n+4)(n+7)(n+9)(3n+11) \tag{17}$$

$$F = 48\phi_1\phi_2[16(n+3)\eta_0 + \psi_1A + \psi_2A^2 + \psi_3A^3 + \psi_4A^4] + \frac{\phi_4}{\alpha}[\psi_5 + \psi_6A + \psi_7A^2 + \psi_8A^3 + \psi_9A^4] + \frac{\phi_3}{\alpha^2}[\psi_{10} + \psi_{11}A + \psi_{12}A^2 + \psi_{13}A^3 + \psi_{14}A^4] \tag{18}$$

$\eta_0,\eta_1,\cdots,\eta_{11}$ and $\psi_0,\psi_1,\cdots,\psi_{14}$ are polynomials of n and can be easily derived using Table I.

The volumetric flow rate defined by

$$Q = \frac{2\pi R^2}{n+1}\overline{V}_x \int_0^1 C_2 Y[2-(n+3)Y^{n+1}]\,dY \tag{19}$$

and based upon the present solution is

$$Q = -\frac{2\pi R^2}{\tau}\overline{V}_x \frac{\partial C}{\partial X} P(n,A,\alpha) \tag{20}$$

where

$$P(n,A,\alpha) = \frac{1}{F}\left\{\frac{24\phi_1,\phi_2}{n+5}(8\eta_0 + 16\eta_1 A + \eta_2 A^2 + 2\eta_3 A^3) + \frac{4\phi_1}{\alpha(n+4)(n+7)}[16\lambda_0 + 2\lambda_1 A + 2\lambda_2 A^2 + 10\lambda_3 A^3 + \phi_2(n^2+7n+16)A^4]\right\} \tag{21}$$

λ_0, λ_1, λ_2, and λ_3 are polynomials of n and are given in Table I. Calculation of any polynomial of n, say p_m, appearing in the solution can be done as

$$p_m = M(b_0 + b_1 n + b_2 n^2 + \cdots + b_8 n^3)$$

where $M,b_0,b_1,\cdots,b_8$ are given in Table I for every polynomial.

EFFECTIVE DISPERSION COEFFICIENT

The effective dispersion coefficient for steady state laminar dispersion in power law fluids undergoing first-order homogeneous reaction in the bulk and heterogeneous reaction at the reactor wall is derived in the present analysis as

$$\mathrm{Pe} = \overline{V}_x L/D = \tau/2P(n,A,\alpha) \tag{22}$$

where Pe is the Peclet number, which can be rewritten as

$$K_c = DD_m/\overline{V}_x^2 d_t^2 = \tfrac{1}{2}P(n,A,\alpha) \tag{23}$$

where K_c is the measure of dispersion.

The expression for the effective dispersion coefficient for the first-order homogeneous reaction taking place in the laminar flow tubular reactor can be derived from the present analysis as a limiting case by putting $A = 0$ in eq. (23). Thus the effective dispersion coefficient for this case becomes

$$K_c = \frac{DD_m}{\overline{V}_x^2 d_t^2} = \tfrac{1}{2}P(n,0,\alpha) = 32\phi_1\left[\frac{3\phi_2\eta_0}{n+5} + \frac{\lambda_0}{\alpha(n+4)(n+7)}\right]\Big/\left[768\phi_1\phi_2(n+3)\eta_0 + \frac{\phi_4\psi_4}{\alpha} + \frac{\phi_3\psi_8}{\alpha^2}\right] \tag{24}$$

The expression for the effective dispersion coefficient in the case of heterogeneous

TABLE I
The Value of Coefficients of Different Polynomials

P_m	M	b_8	b_7	b_6	b_5	b_4	b_3	b_2	b_1	b_0
η_0	$(n+3)$	0	0	0	0	1	38	393	1544	2056
η_1	$(n+3)(n+5)$	0	0	0	0	0	0	5	53	134
η_2	1	0	0	0	0	5	142	1305	4864	6356
η_3	$(n+5)$	0	0	0	0	0	0	1	13	34
η_4	$(n+3)^2$	0	0	0	6	181	1630	4649	−3022	−22,344
η_5	$(n+3)$	0	0	0	114	2179	14,620	37,221	9202	−63,336
η_6	1	0	0	0	162	2937	19,900	62,123	87,246	41,832
η_7	$(n+6)(2n+7)$	0	0	0	0	0	0	3	17	30
η_8	$(n+3)^2$	0	0	0	3	101	1221	6315	12,664	4656
η_9	$(n+3)$	0	0	0	27	717	7069	32,323	68,584	54,480
η_{10}	1	0	0	0	27	651	5927	26,093	56.990	50,472
η_{11}	$(n+9)(3n+11)$	0	0	0	0	0	0	1	7	16
ψ_1	$8(n+3)^2(n+4)$	0	0	0	0	0	1	54	489	1184
ψ_2	$2(n+3)$	0	0	0	0	45	886	6369	19,800	22,436
ψ_3	$(n+3)$	0	0	0	0	5	146	1377	5260	7036
ψ_4	$2(n+3)^3(n+5)$	0	0	0	0	0	0	1	13	34
ψ_5	$8(n+3)^3$	0	18	933	19,895	220,577	1,376,199	4,870,858	9,133,840	7,057,680
ψ_6	$2(n+3)^2$	6	841	30,330	486,374	4,213,578	21,214,161	62,305,270	99,284,480	66,480,960
ψ_7	$(n+3)$	72	6024	149,382	1,813,428	12,599,424	52,831,908	132,681,402	184,296,480	109,138,680
ψ_8	$(n+3)$	0	138	5933	98,080	842,272	4,144,084	11,833,283	18,317,750	11,933,040
ψ_9	$5(n+6)(2n+7)$	0	0	0	3	80	748	3310	7121	6018
ψ_{10}	$4(n+3)^4$	18	1077	30,095	486,105	4,727,847	47,684,034	94,696,680	173,343,072	130,707,072
ψ_{11}	$4(n+3)^3$	54	4419	135,663	2,073,057	17,784,015	89,781,996	264,996,156	423,551,712	283,508,928
ψ_{12}	$(n+3)^2$	234	29,229	835,907	11,117,397	82,623,171	365,103,982	956,550,912	1,376,684,544	841,146,624
ψ_{13}	$6(n+3)$	18	2481	65,843	800,661	5,452,755	22,243,402	54,284,184	73,441,632	42,537,024
ψ_{14}	1	18	2481	62,495	722,361	4,713,423	18,576,790	44,098,512	58,289,328	33,050,592
λ_0	$(n+3)^2$	6	289	6178	75,010	561,446	2,649,005	7,702,802	12,650,928	9,013,536
λ_1	$(n+3)$	228	10,862	215,184	2,348,560	15,595,528	65,003,010	167,102,276	243,487,104	154,582,848
λ_2	1	432	17,343	296,496	2,837,960	16,726,482	62,462,865	144,934,894	191,674,536	110,853,792
λ_3	1	0	42	1429	20,305	157,473	725,333	1,997,546	3,061,200	2,020,032

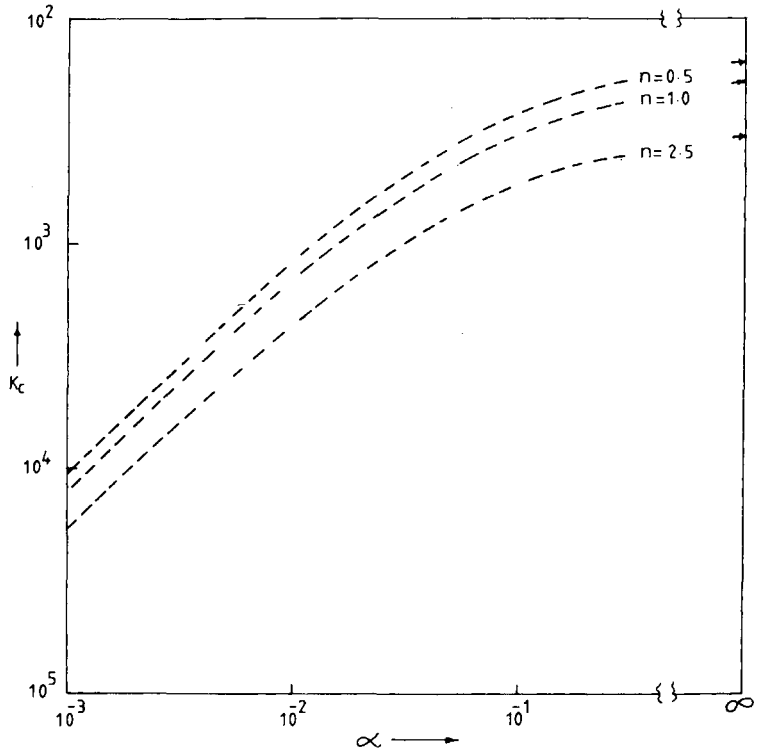

Fig. 1. Effect of reaction rate on dispersion: $A = 0$.

reaction can be deduced from the present model by taking the limit $\alpha \to \infty$ in eq. (23) as

$$K_c = \frac{DD_m}{\overline{V}_x^2 d_t^2} = \tfrac{1}{2}P(n,A,\infty)$$

$$= \frac{1}{2(n+5)}[4\eta_0 + 8\eta_1 A + 0.5\eta_2 A^2 + \eta_3 A^3]/[16(n+3)\eta_0 + \psi_1 A + \psi_2 A^2 + \psi_3 A^3 + \psi_4 A^4] \quad (25)$$

Similarly, the effective dispersion coefficient derived by Fan and Hwang[21] for unsteady laminar dispersion in power law fluids under nonreacting conditions can be derived from the present analysis as a limiting case by putting A = 0 in eq. (25). Thus for this case

$$K_c = DD_m/\overline{V}_x^2 d_t^2 = 1/8(n+3)(n+5) \quad (26)$$

It is interesting to mention that such a simple expression for the effective dispersion coefficient for the case of heterogeneous reaction in a laminar flow tubular reactor has not been reported in the literature. Thus, the present model is the most general case from which individual cases reported in the literature[12,21] for different situations can be derived as limiting cases.

It can be seen from eq. (23) that, in a non-Newtonian laminar flow tubular reactor, the effective dispersion coefficient is a function of reaction rate constants

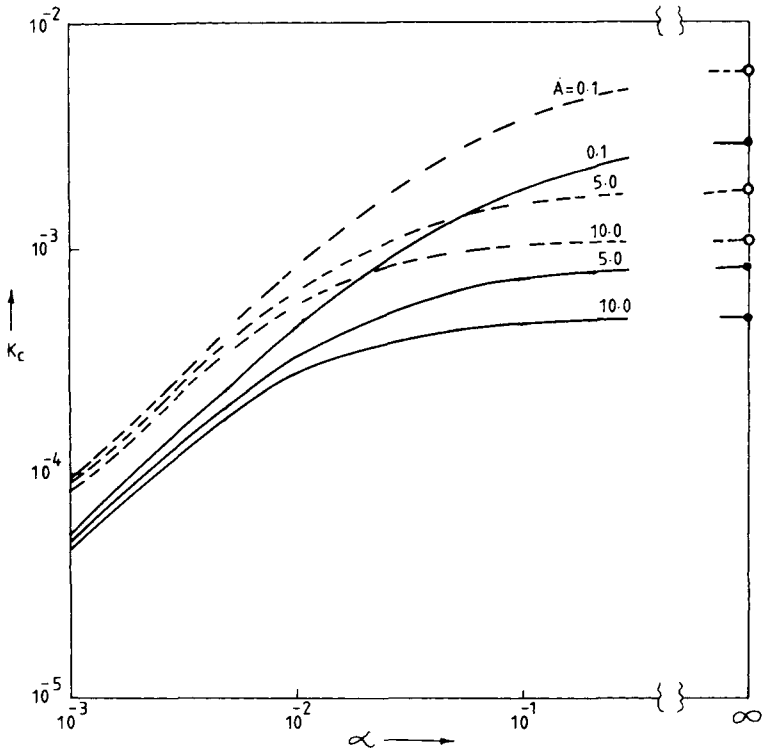

Fig. 2. Effect of reaction rate on dispersion for $n = 0.5$ (- - -) and $n = 2.5$ (—).

(A,α) and power law index (n) when first-order homogeneous chemical reaction is taking place in the bulk and heterogeneous reaction at the reactor wall.

Figures 1 and 2 show the effect of homogeneous reaction rate parameter (α) on effective dispersion coefficient for different values of power law index (n) and heterogeneous reaction rate parameter (A). It can be concluded from these figures that, for the same mean velocity of the flow, the effective dispersion coefficient decreases as the chemical reaction rate constants (A,k) increase. The value of the effective dispersion coefficient for different values of power law index under the condition of very slow homogeneous reaction (i.e., $\alpha \rightarrow \infty$) using eq. (25) is also shown in the figures. It can be seen that the curves obtained by the present model approach these values for large values of α. At large values of α about a fivefold reduction in the value of effective dispersion coefficients can be obtained for a given fluid (i.e., for a fixed value of n) by increasing the heterogeneous reaction rate parameter (A) from 0.1 to 10. These figures also depict that the effective dispersion coefficient decreases as the power law index (n) increases for the same mean velocity. About a twofold reduction in the value of the effective dispersion coefficient can be obtained by increasing the value of n from 0.5 to 2.5 for fixed values of the reaction rate constants.

SIMPLE SOLUTION

The concept of axial dispersion has been widely used for predicting the effect of backmixing on the performance of chemical reactors.[22,23] The concept has

TABLE II
Peclet Number Calculation $\beta = 1.0$ and $n = 0.5$

	$A = 0.0$		$A = 1.0$		$A = 5.0$		$A = 10.0$	
α	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)
10^{-4}	2.522	3.85×10^{-3}	2.544	5.77×10^{-3}	2.659	1.35×10^{-2}	2.800	2.31×10^{-2}
10^{-3}	2.560	3.85×10^{-2}	2.599	5.77×10^{-2}	2.763	1.35×10^{-1}	2.942	2.31×10^{-1}
10^{-2}	2.930	3.85×10^{-1}	3.138	5.77×10^{-1}	3.853	1.35	4.528	2.31
10^{-1}	6.432	3.85	8.370	5.77	15.735	13.50	24.157	23.10
3×10^{-1}	14.139	11.55	19.927	17.33	42.630	40.43	70.052	69.31

TABLE III
Peclet Number Calculation for $\beta = 5.0$ and $n = 0.5$

	$A = 0.0$		$A = 1.0$		$A = 5.0$		$A = 10.0$	
α	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)
10^{-4}	12.610	1.925×10^{-2}	12.721	2.888×10^{-2}	13.293	6.738×10^{-2}	14.000	1.155×10^{-1}
10^{-3}	12.8000	1.925×10^{-1}	12.995	2.888×10^{-1}	13.813	6.738×10^{-1}	14.711	1.155
10^{-2}	14.646	1.925	15.692	2.888	19.265	6.738	22.639	11.55
10^{-1}	32.159	19.25	41.849	28.88	78.675	67.38	120.784	115.50
3×10^{-1}	70.696	57.75	99.634	86.625	213.15	202.14	350.262	346.55

TABLE IV
Peclet Number Calculation for $\beta = 1.0$ and $n = 2.5$

	$A = 0.0$		$A = 1.0$		$A = 5.0$		$A = 10.0$	
α	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)
10^{-4}	4.563	8.25×10^{-3}	4.594	1.239×10^{-2}	4.726	2.931×10^{-2}	4.889	5.074×10^{-2}
10^{-3}	4.672	8.25×10^{-2}	4.736	1.239×10^{-1}	4.977	2.931×10^{-1}	5.233	5.07×10^{-1}
10^{-2}	5.639	8.25×10^{-1}	6.057	1.239	7.525	2.931	8.993	5.074
10^{-1}	13.431	8.25	17.550	12.39	33.743	29.31	52.993	50.74
3×10^{-1}	30.004	24.75	42.395	37.163	92.337	87.94	154.078	152.22

TABLE V
Peclet Number Calculation for $\beta = 5.0$ and $n = 2.5$

	$A = 0.0$		$A = 1.0$		$A = 5.0$		$A = 10.0$	
α	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)	Pe model, eq. (22)	Pe simple, eq. (25)
10^{-4}	22.817	4.125×10^{-2}	22.968	6.194×10^{-2}	23.633	1.466×10^{-1}	24.445	2.537×10^{-1}
10^{-3}	23.361	4.125×10^{-1}	23.682	6.194×10^{-1}	24.886	1.466	26.165	2.537
10^{-2}	28.196	4.125	30.284	6.194	37.628	14.66	44.965	25.37
10^{-1}	67.156	41.25	87.751	61.94	168.715	146.60	264.963	253.70
3×10^{-1}	150.020	123.75	211.975	185.82	461.686	439.73	770.391	761.12

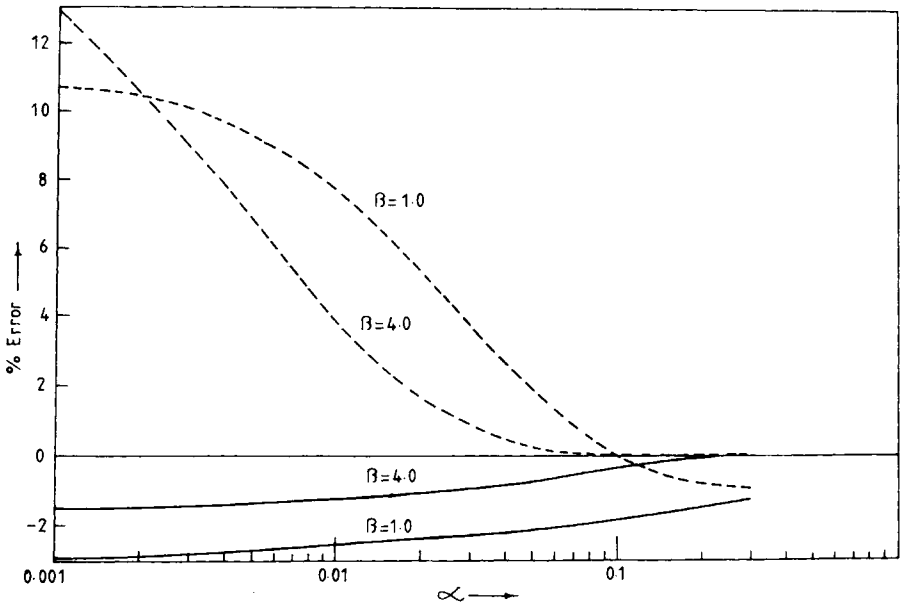

Fig. 3. Percent error in conversion using the present model (—) and Fans and Hwang analysis (- - -) with two-dimensional analysis, $n = 2.5$.

also been applied to a homogeneous reaction under non-Newtonian laminar flow conditions.[10,11] The parameter Pe (Peclet number) used in these studies was the Fan and Hwang dispersion coefficient for a nonreacting system. In the present study, the Peclet number was calculated using simple solution, eq. (25), as well as by the present model eq. (22), for different values of α, β, n, and A. These values are given in Tables II–V for different fluids. It is interesting to note that as the values of α and A increase agreement between predictions of the present model, eq. (22), and the simple solution, eq. (25), improves. It can be seen that, for any value of β and n, the two models nearly give the same value of Peclet number, provided $\alpha > 0.1$ and $A > 5$. This suggests that under these conditions the simple solution, eq. (25), may be used for cases where simultaneous homogeneous and heterogeneous reaction occurs.

REACTOR PERFORMANCE

The axial dispersion model solution with appropriate boundary conditions as discussed in Refs. 8, 24–27 was used to calculate the bulk mean concentration for the parameter values of $0.001 \leqslant \alpha \leqslant 0.3$, $1 \leqslant \beta \leqslant 5$, $0.5 \leqslant n \leqslant 2.5$, and $0 \leqslant A \leqslant 10$. The predictions of the present model were compared with the numerical solution of the exact two-dimensional convective diffusion equation for the case of homogeneous reaction. The results are shown in Figure 3 and 4 for two different values of the power law index. It can be seen that the present model predicts results with a maximum error of 2%. In the literature,[10–12] Fan and Hwang analysis, which is for nonreacting systems, has been used to predict the

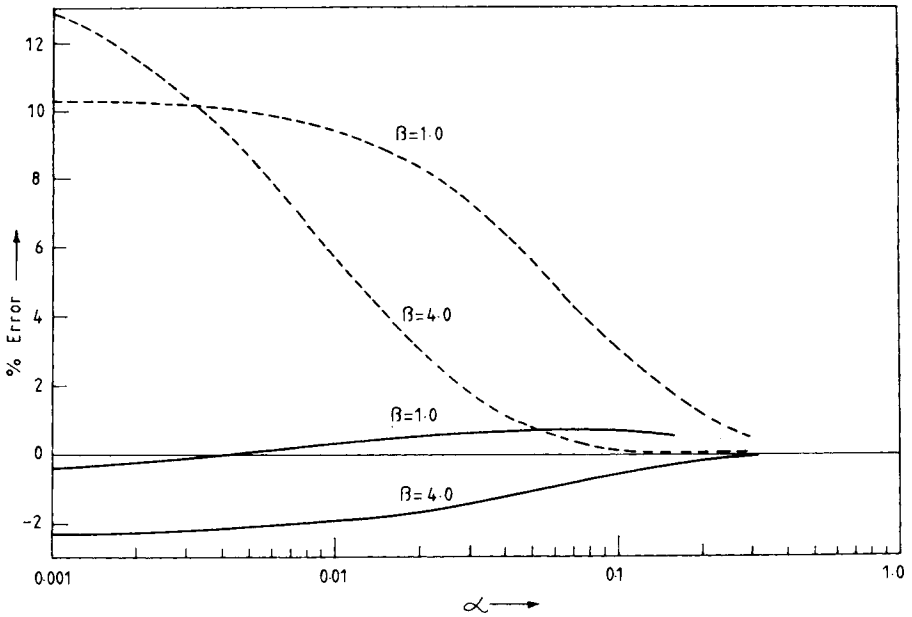

Fig. 4. Percent error in conversion using the present model (—) and Fans and Hwang (- - -) analysis with two-dimensional analysis, $n = 0.5$.

reactor performance of a non-Newtonian laminar flow tubular reactor. The percent error in predicting the conversion by Fan and Hwang analysis is also shown in Figures 3 and 4. It can be seen from these figures that for fast reaction (i.e., $\alpha \leqslant 0.01$) the Fan and Hwang analysis predicts highly inaccurate results.

The present model predictions in case of homogeneous and heterogeneous reactions in a Newtonian laminar flow tubular reactor were compared with the reported values.[13] The agreement between the present model and the numerical solution was very good. Some of the typical results for a non-Newtonian laminary flow tubular reactor are shown in Figures 5 and 6. For a given reaction time (β) and heterogeneous reaction rate parameter (A) the exit concentration decreases with increase in the value of homogeneous reaction rate parameter (α) for all values of power law index (n), as shown in Figure 5. It can also be seen from this figure that as the power law index increases (i.e., the velocity profile becomes more flat) the exit concentration decreases for any given value of α. The maximum difference in the exit concentration for different fluids occurs at low values of α (i.e., for fast homogeneous reaction). At large values of α (i.e., for slow homogeneous reaction) the concentration profile seems to be same for different fluids. Figure 6 shows the variation of exit concentration with α for a fixed value of the power law index at different values of β and A. It can be observed from the figure that, for a given value of β, the concentration decreases with increase in the value of heterogeneous reaction rate parameter (A). However, as the value of β increases, the concentration decreases for fixed value of A. The difference in concentrations corresponding to two different values of heterogeneous rate reaction parameter also decreases at large values of β.

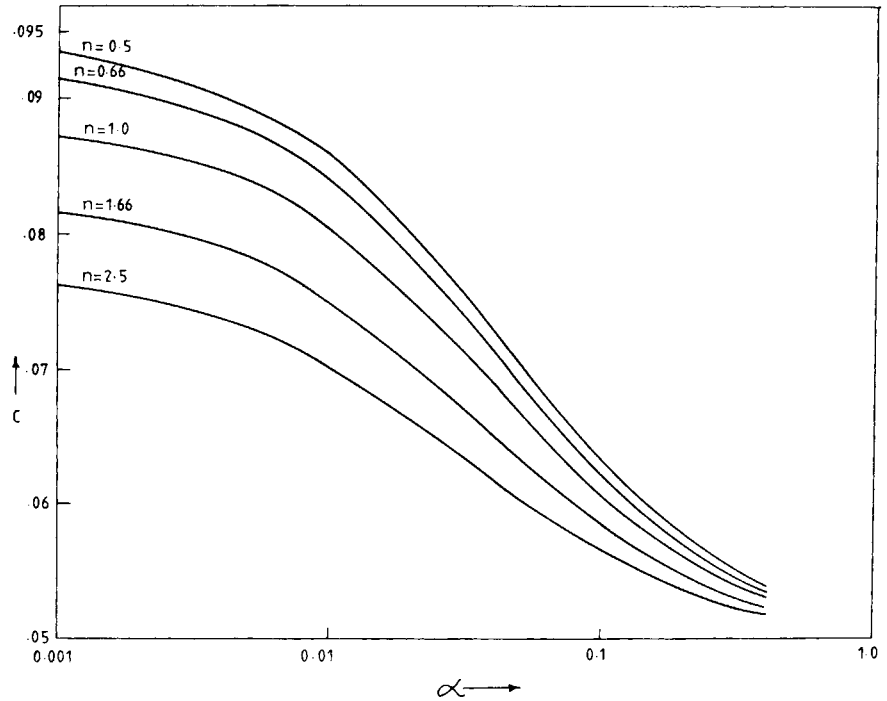

Fig. 5. Variation of bulk mean concentration with homogeneous reaction rate for different values of power law index: $A = 2.0$ and $\beta = 3.0$.

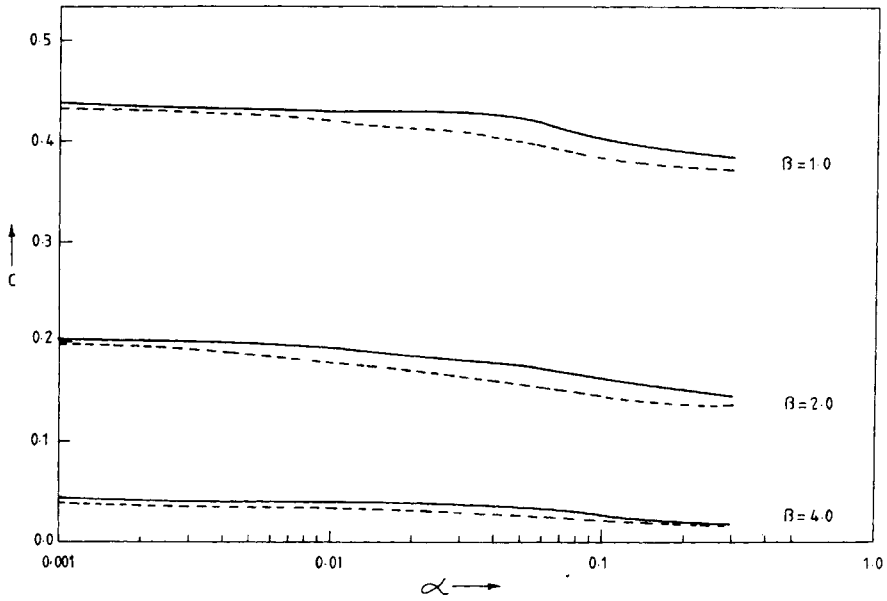

Fig. 6. Variation of bulk mean concentration with homogeneous reaction rate for different values of A and β, $n = 0.5$: (---) $A = 10.0$; (—) $A = 1.0$.

CONCLUSIONS

The present model predicts the reactor performance fairly well and saves a significant numerical effort required to solve each individual problem as a new case. Under certain conditions the use of simple solution has been demonstrated.

NOMENCLATURE

a_i	coefficients in eq. (6)
A	dimensionless heterogeneous reaction rate parameter (= $k'R/D$)
b_i	polynomials of n
c	point concentration
C_0	initial concentration
C	dimensionless concentration (= c/C_0)
C_m	mth-order solution for c
d_t	reactor tube diameter
D	effective diffusion coefficient
D_m	molecular diffusion coefficient
$f_i(Y)$	sequence of functions given by eq. (9)
k	homogeneous reaction rate constant
k'	heterogeneous reaction rate constant
K_c	measure of dispersion (= $DD_m/\overline{V}_x^2 d_t^2$)
L	length of the reactor
n	power law index
Pe	Peclet number (= $\overline{V}_x L/D$)
Q	volumetric flow rate
r	Radial distance
R	reactor radius
$\bar{t}$	mean time
$\overline{V}_x$	Average velocity
X	dimensionless axial distance
Y	dimensionless radial distance
	Greek Letters
α	dimensionless homogeneous reaction rate (= D_m/kR^2)
β	dimensionless reaction time (= $k\bar{t}$)
τ	characteristic time (= $\alpha\beta$).

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