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Modelling of a coiled tubular chemical reactor

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Abstract

First order reactions in laminar Newtonion and non-Newtonion fluids in coiled tubes have been analyzed for high range of Dean numbers ($N_{De} \leq 250$). Process parameters which govern the secondary flow and the reaction parameter on the performance of coiled tube chemical reactor are systematically examined. It is interesting to observe that the phenomenon of covective diffusion with reaction in coiled tube can be simulated. Numerical calculations show the effect of process parameter modelling the rection parameter (α), dimensionless axial distance and power law index (n). The performance of the coiled tube reactor is compared with plug flow and laminar flow reactors.

Keywords: Power-law fluid; Coiled tube; Secondary flow; Chemical reaction

1. Introduction

Curved configurations of circular tubes such as partial coils (bends), and helical coils are often used in industry. The secondary flow which is characteristic of a curved tube causes (i) a higher axial pressure gradient, (ii) a higher critical Reynolds number for transition to turbulent flow, (iii) a residence time distribution that more closely approximates plug flow and (iv) relatively high average heat and mass transfer rates per unit axial pressure drop especially for fluids with high Prandtl and high Schmidt number. Because of these advantages, curved tube are frequently used as heat exchangers [1], chemical reactors [2–4], reverse osmosis unit [5,6], and coiled membrane blood oxygenators [7,8]. They also serve as conceptual modes of physiological phenomena such as the disease mechanism of atherosclerosis [9], the performance of artificial respiration and the flow of soluble materials through lung and blood vessels [10–14].

The study of isothermal convective diffusion of Newtonian and non-Newtonian fluids flowing through curved tubes with reaction is of both academic interest and industrial relevance. Since most of the industrial chemicals and many fluids in the food, polymer processing and biochemical industries under go mass transfer with chemical reaction process either during preparation or in their applications, the present study focuses on understanding the physics of the chemical reaction in coiled tube systems which will be useful in the design of such systems.

The problem of convective diffusion with reaction in Newtonian and non-Newtonian fluids flowing through a straight tube has been well studied in the literature. Cleland and Wilhelm [15] studied both experimentally and theoretically liquid phase, first order, homogenous chemical reactions in a tubular reactor under isothermal conditions. The Newtonion fluid was assumed to be in laminar flow, and axial diffusion was assumed. The convective diffusion equation was solved numerically. Lauwerier [16] investigated the same problem as Cleland and Wilhelm [15] but adopted a different solution technique an eigen function expansion approach in the region far away from the entrance of the reactor and a Leveque [17] type of approximation close to the entrance. In the former case, the classical Sturm–Liouville type of eigen value problem was obtained and Lauwerier [16] presented an asymptotic solution valid for large eigen values, Hsu [18] obtained the first 12 eigen values and eigen functions by numerically integrating the ordinary differential equations. Power-law and Pradtl–Eying fluids were considered by Homsy and Strohman [19]. The resulting eigen function equation was solved by the Galerkin method. The simple closed form analytical solution using Galerkin technique for convective diffusion with a homogeneous first order reaction in the bulk and a heterogenous reaction at the reactor wall in a Newtonian and non-Newtonian laminar flow tubular reactor was given by Nigam et al. [20] and Nigam and Nigam [21,22]. Recently, Adeniyi [23] developed the analytical solution for the convective diffusion of power law fluids in parallel plates and tubular reactor with first order single

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Nomenclature

a	radius of the tube
b	radius of the curvature of the tube
c	dimensionless concentration
C	concentration
C_B	bulk concentration
C_0	initial concentration
d_t	diameter of the tube
D_m	molecular diffusion coefficient
K	first order homogenous reaction rate constant
n	power law index
N_{De}	Dean number, $N_{Re}/\sqrt{\lambda}$
N_{Re}	Reynolds number $[N_{Re} = (d_t^n\, W_a^{2-n}\rho/\mu_p]$
N_{Sc}	Schmidt numbers as defined in Eq. (4)
r	non-dimensional radial coordinate
R	dimensional radial coordinate
u, v, w	non-dimensional velocities in r, θ, ϕ, respectively
U, V, W	dimensional velocities in R, θ, ϕ, respectively
W_a	dimensional average velocity in curved tube

Greek letters

α	Ka^2/D_m (dimensionless homogeneous reaction parameter)
δ	geometric parameter defined in Eq. (4)
ϕ	axial coordinate
λ	curvature ratio (b/a)
μ_p	consistency index
θ	azimuthal coordinate
ξ	dimensionless axial distance ($\lambda\phi/N_{Re}N_{Sc}$))
ρ	density of the fluid

homogenous reaction in the bulk and a catalytic reaction at the wall.

Although coiled tubes have been used rather commonly as chemical reactors in industries, there have been very few prior studies where the complete problem of convective diffusion with reaction in coiled tube has been examined. Most of the studies appearing in the literature on coiled tubes confine to the residence time distribution and axial dispersion [24–26,39,40] and [27,28]. The state-of-the-art review on the RTD and axial dispersion in straight and coiled tubes was reported by Nigam and Saxena [29]. Such studies have been helpful in describing the performance of a coiled tube reactor in terms of a lumped parameter dispersion number but this does not provide information on the detailed spatial concentration distribution. Southwick and Seader [3] provide an elegant experimental demonstration of the advantage of secondary flow in enhancing the rate of reaction. To the best of our knowledge, only one theoretical study of Mashelkar and Venkatasubramanian [30] has been reported in the literature to understand the influence of secondary flow on convective diffusion with reaction. They analyzed the influence of secondary flow on the spatial concentration distribution as well as the bulk average concentration for first order reaction in Newtonian and non-Newtonian fluids flowing through curved circular tubes. Mashelkar and Venkatasubramanian [30] have examined the phenomenon under low Dean number ($N_{De} < 20$) conditions where the influence of secondary flow is not expected to have significant contribution. To overcome the limitation of small Dean numbers, the influence of secondary flow in convective diffusion with reaction in Newtonian and non-Newtonian fluids flowing through coiled tubes is analyzed numerically for higher values of Dean number ($N_{De} \approx 250$). The present analysis illustrates the interaction between the shear thinning property of the fluid, the process parameters governing the secondary flow and the reaction parameter itself.

2. Hydrodynamics in coiled tubes

In order to obtain the solution of convective diffusion with reaction in a coiled tube, the details of the hydrodynamics need to be understood. Dean [31,32] showed that a single dynamic similarity parameter Dean number ($N_{De} = N_{Re}\sqrt{a/b}$, where N_{Re} is Reynolds number and a and b are the radius of the tube and curvature, respectively) can characterize the flow phenomenon of Newtonian fluid in a coiled tube. A comprehensive review of hydrodynamics of Newtonian fluids flowing through coiled tube was published by Berger et al. [33], Ito [41,42] and Berger [34]. Most of the studies are confined to Newtonian fluids, very little attention has been paid to the flow of now-Newtonian fluids in curved circular tubes despite their importance in the area of polymer, biomedical and biochemical processing. A state-of-art review on the flow of power law fluids flowing through circular curved tube has been reported by Agrawal et al. [27,28].

3. Mathematical formulation

In order to obtain an exact solution of the convective diffusion equation with reaction in coiled tubes, the equations of continuity, momentum and mass need to be solved. The equation of continuity and motion for Newtonian and power law fluid flowing through curved circular tube have been solved numerically by Agrawal et al. [27,28]. These results are then used to solve the convective diffusion equation for determining the concentration profiles along the length of the coiled tube as chemical reactor.

A systematic representation of a curved tube and its coordinate system is shown in Fig. 1. The toroidal geometry is a good approximation for helically coiled tubes with a small pitch. As shown in Fig. 1, a is the radius of the tube and b the radius of curvature of the coil. The flow occurs in the increasing ϕ direction. The velocity vector V has components

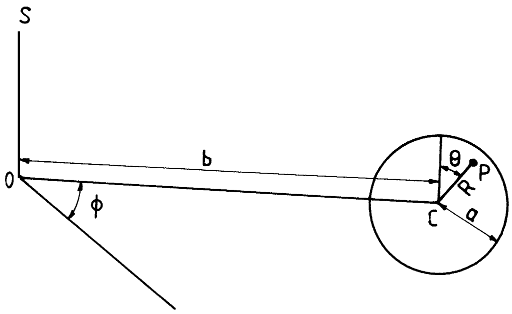

Fig. 1. Toroidal coordinate system.

U, V, W in the R, θ and ϕ directions, respectively. The study of the phenomenon of convective diffusion with reaction in a coiled tube for steady, fully developed flow of incompressible Newtonian and non-Newtonian fluids has been carried out under the assumption axial diffusion is neglected [35].

The convective diffusion equation for first order reaction in the toroidal coordinate system is

$$U\frac{\partial C}{\partial R}+\frac{V}{R}\frac{\partial C}{\partial \theta}+\frac{W}{b+R\sin\theta}\frac{\partial C}{\partial \phi} = D_{\mathrm{m}}\left\{\frac{1}{R}\frac{\partial}{\partial R}\left[R\frac{\partial C}{\partial R}\right]+\frac{\sin\theta}{b+R\sin\theta}\frac{\partial C}{\partial R}+\frac{1}{R^2}\frac{\partial^2 C}{\partial \theta^2} +\frac{\cos\theta}{R(b+R\sin\theta)}\frac{\partial C}{\partial \theta}\right\}-KC \tag{1}$$

Eq. (1) in nondimensionalized using the following groups:

$$c=\frac{C}{C_0},\quad r=\frac{R}{a},\quad u,v,w=\frac{U,V,W}{(\rho a^n/\mu_{\mathrm{p}})^{1/(n-2)}} \tag{2}$$

The dimensionless form of the governing equation is

$$u\frac{\partial c}{\partial r}+\frac{v}{r}\frac{\partial c}{\partial \theta}+\frac{\lambda^{-1}}{\delta}\frac{\partial c}{\partial \phi} = \frac{1}{N_{Sc}}\left[\frac{\partial^2 c}{\partial r^2}+\frac{1}{r^2}\frac{\partial^2 c}{\partial \theta^2}+\frac{1}{r}\frac{\partial c}{\partial r}+\delta_1\frac{\partial c}{\partial r}+\frac{\delta_2}{r}\frac{\partial c}{\partial \theta}\right] -\frac{\alpha}{N_{Sc}}c \tag{3}$$

where $\lambda=b/a$ (curvature ratio)

$$\delta=\lambda^{-1}r\sin\theta+1$$
$$\delta_1=\frac{\lambda^{-1}\sin\theta}{\delta}$$
$$\delta_2=\lambda^{-1}\cos\theta+\delta \tag{4}$$
$$N_{Sc}=\frac{a}{D_{\mathrm{m}}}\left[\frac{\rho a^n}{\mu_{\mathrm{p}}}\right]^{1/(n-2)}$$
$$\alpha=\frac{Ka^2}{D_{\mathrm{m}}}$$

Eq. (3) is subject to the following boundary and initial conditions:

$$\Phi=0,\qquad c=1$$
$$\frac{\partial c}{\partial \theta}\left(r,\pm\frac{\pi}{2}\right)=0$$
$$\frac{\partial c}{\partial r}(1,\theta)=0 \tag{5}$$
$$\frac{\partial c}{\partial r}(0,0)=0$$

4. Method of solution

Eq. (3) together with then associated boundary and initial conditions (Eq. (5)) represented a complete mathematical description of the problem. The Eq. (3) is somewhat analogous to the two-dimensional unsteady state heat conduction equation and an alternating direction implicit (ADI) method has been applied. Details of ADI method are available in the original paper of Douglas and Gunn [36] and Peaceman and Rachford [37]. This technique retains the accuracy of the well known Crank Nicolson method [38] but simplifies the computation using a two-step procedure, each step involving concentration implicitly in a single direction. In the partial differential equation, the standard second order central difference operators were used for the first and second derivatives of c in both the radial and angular directions. The steady state values of u, v and w for given values of Reynolds number and curvature ratio as reported by Agarwal et al. [28] were used in Eq. (3) to calculate the concentration profile as a function of ϕ.

The computed values of concentration, $c(r, \theta)$ were used to obtain the bulk average concentration for different axial distance in the following manner.

$$C_{\mathrm{B}}=\frac{\int_0^1\int_{-\pi/2}^{\pi/2}crw\,\mathrm{d}r\,\mathrm{d}\theta}{\int_0^1\int_{-\pi/2}^{\pi/2}rw\,\mathrm{d}r\,\mathrm{d}\theta}$$

The numerical solution was checked by comparing it with the results of Mashelkar and Venkatasubramanian [30]. For $N_{De}=10$, there was very good agreement between the two solutions.

5. Results and discussion

The motivation behind the present theoretical analysis was to understand the influence of secondary flow for high Dean numbers when simultaneous diffusion and reaction take place in a coiled tube. The numerical solutions were computed for the range of $1<N_{De}\le 250$, $1<N_{Sc}<14000$, $10\le\lambda\le 100$ and $10\le\alpha\le 1000$.

5.1. Influence of process variables on bulk mean concentration

The variation of bulk mean concentration (C_{B}) along the dimensionless axial distance [$\xi=\lambda\phi/N_{Re}N_{Sc}$] was

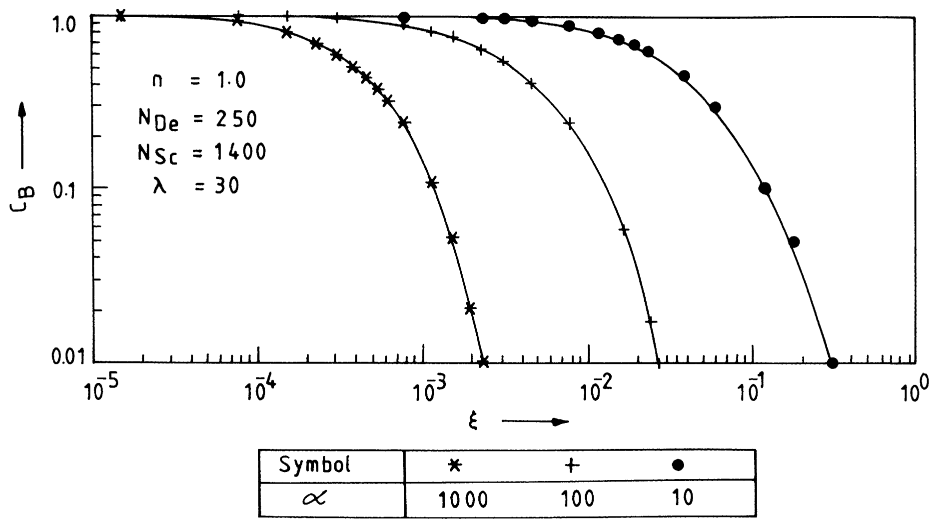

Fig. 2. Variation of bulk concentration along the dimensionless length (ξ) for different values of α.

examined as a function of the process variables α, N_{Sc}, N_{De} and λ.

The effect of reaction parameter α on the variation of bulk mean concentration along the dimensionless axial distance (ξ) is shown in Fig. 2 for $N_{De} = 250$, $N_{Sc} = 1400$ and $\lambda = 30$. For a given value of α, the bulk concentration decreases with increases in axial distance. It is also evident from Fig. 2 that with an increase in α, the bulk mean concentration decreases, i.e. conversion increases at a particular axial distance. Actually, the reaction parameter α is the ratio of molecular diffusion time (a^2/D_m) to the reactive time ($1/k$). The reaction rate increases with increases in α. Therefore, the conversion is faster for higher values of α.

The variation of bulk mean concentration along the dimensionless axial distance for different values of Dean number and curvature ratio for a given fluid ($N_{Sc} = 1400$) and reaction parameter ($\alpha = 100$) is presented in Figs. 3 and 4, respectively. It may be seen from the figures that, for a given value N_{Sc} and α, the variation of concentrations along the dimensionless axial distance [$\xi = \lambda\phi/N_{Re}N_{Sc}$] is independent of the value of N_{De} and λ. This can be explained as follows. The dimensionless axial distance ξ is actually a ratio of convective time (Z/W_a) to diffusion time (a^2/D_m) for a particular value of conversion. The Dean number and λ characterize the intensity of secondary flow, with an increase in Dean number or decrease in curvature ratio the secondary flow increases. The axial length for a particular conversion increases with increases in Dean number and with decreases in curvature ratio. So the ratio of Z/W_a for a particular conversion remains constant with

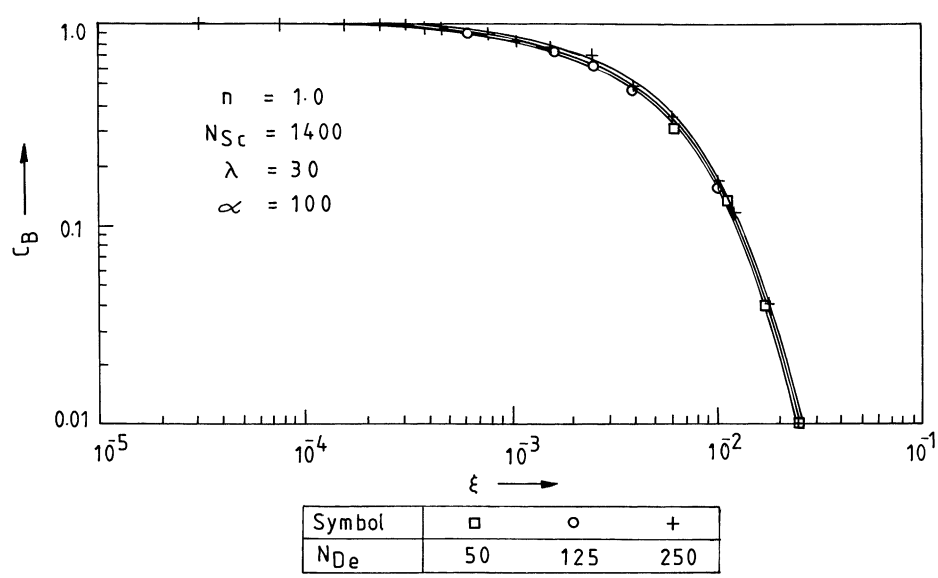

Fig. 3. Variation of bulk concentration along the dimensionless length (ξ) for different values of N_{De}.

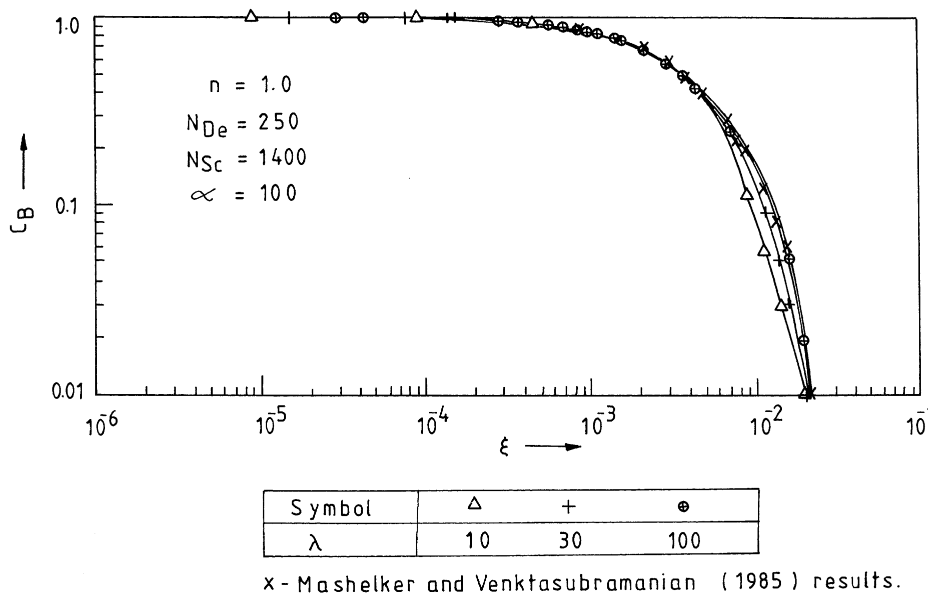

Fig. 4. Variation of bulk concentration along the dimensionless length (ξ) for the different values of λ.

increases in the secondary flow. Hence, for a given fluid and reaction parameter, the ratio of convective time and diffusive time for a particular conversion does not change with increases in secondary flow.

The effect of Schmidt number on the variation of bulk mean concentration along the dimensionless axial distance is shown in Fig. 5. It is clear from the figure that the variation of bulk concentration along the dimensionless length does not depend on N_{Sc} at given values of α, N_{De} and λ. This phenomenon can also be explained on the same logic as discussed above. With increases in the values of N_{Sc}, the diffusion time increase and, hence, the length required for a particular conversion increases for a given value of α. Therefore, the ratio of convective time to diffusive time for a particular conversion remains the same at given values of N_{De}, λ and α.

These are the striking results which simplified the phenomenon of convective diffusion with reaction in coiled tube for Newtonian fluids. The variation of bulk mean concentration along the axial length of the reactor can be simulated as a function of α and ξ. The performance of coiled tube reactors for power law fluids has also been analyzed. Fig. 6 shows the variation of bulk mean concentration with dimensionless axial distance for power law indices 0.75 and 0.5 for value of $N_{De} = 125$, $N_{Sc} = 14,000$, $\lambda = 30$ and $\alpha = 100$. The effect of reaction parameter on the variation of bulk concentration with axial distance for power law fluids is similar to the case of Newtonian fluids. The length

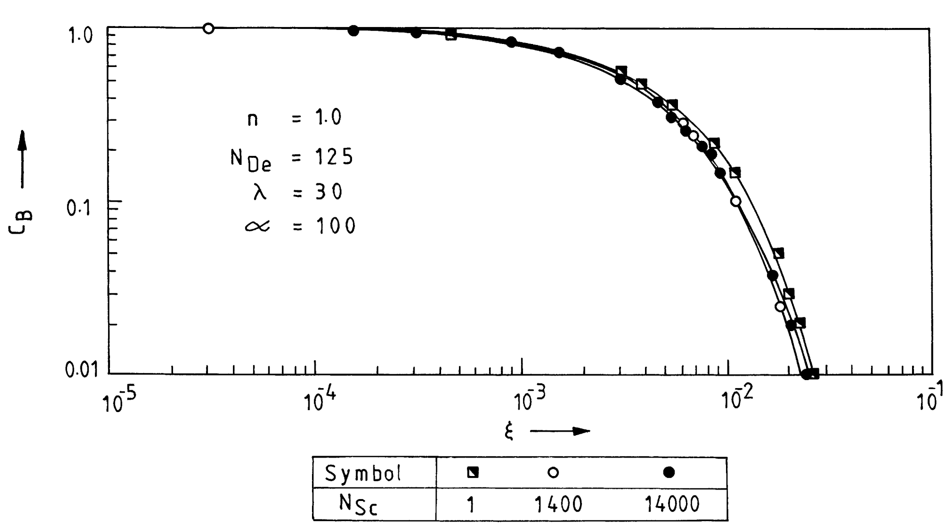

Fig. 5. Variation of bulk concentration along the dimensionless axial distance (ξ) for different values of N_{Sc}.

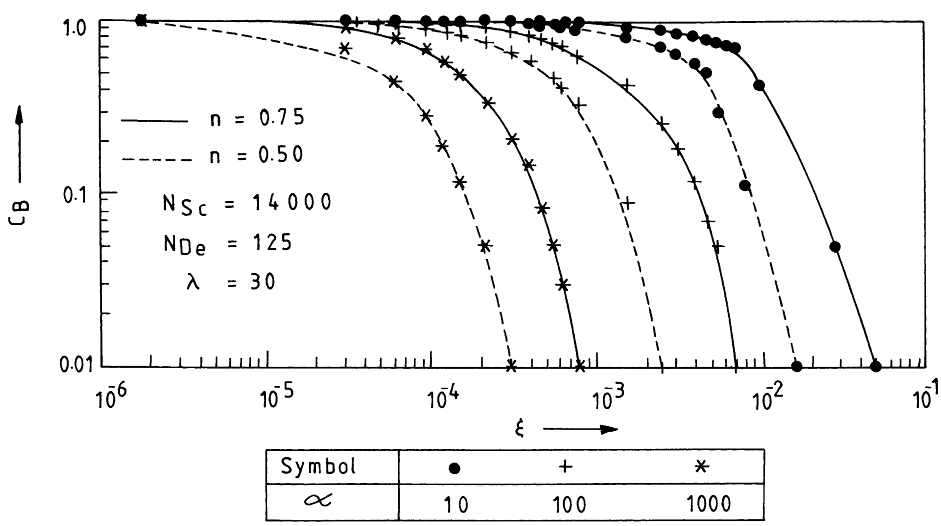

Fig. 6. Variation of bulk concentration along the dimensionless distance (ξ) for power law fluids at different values of α.

required for a particular conversion decreases with increases in α for the given N_{De}, N_{Sc}, and λ.

The dependence of power law index on the variation of concentration along the dimensionless axial distance (ξ) is shown in Fig. 7 for $N_{De} = 125$, $N_{Sc} = 1.4 \times 10^4$, $\lambda = 30$ and $\alpha = 100$. The conversion increases with decrease in the power law index at a particular dimensionless axial distance. For given values of Dean and Schmidt number, the secondary flow decreases with increasing pseudoplasticity of the fluid. The constitutive equation of power law fluids reveals that the effect of convection become less with increases in pseudoplasticity of the fluid and, hence, the velocity profile becomes progressively more blunt which causes a decrease in the intensity of secondary flow. Therefore, the length required for a given conversion increases with increases in the power law index.

5.2. Comparison of coiled tube reactor with plug and tubular flow reactor

The performance of helical coils lies between that of plug flow and laminar flow as shown in Fig. 8. The variation of bulk mean concentration with dimensionless axial distance is given by the following equations for plug flow [15].

$$C_{\mathrm{B}} = C^{-2\xi'} \tag{6}$$

where

$$\xi' = \xi\alpha$$

and for tubular flow

$$C_{\mathrm{B}} = \mathrm{e}^{-\xi'}(1-\xi') + \xi'^2 \int_{-\xi'}^{\alpha} \frac{\mathrm{e}^{-x}}{x}\,\mathrm{d}x$$

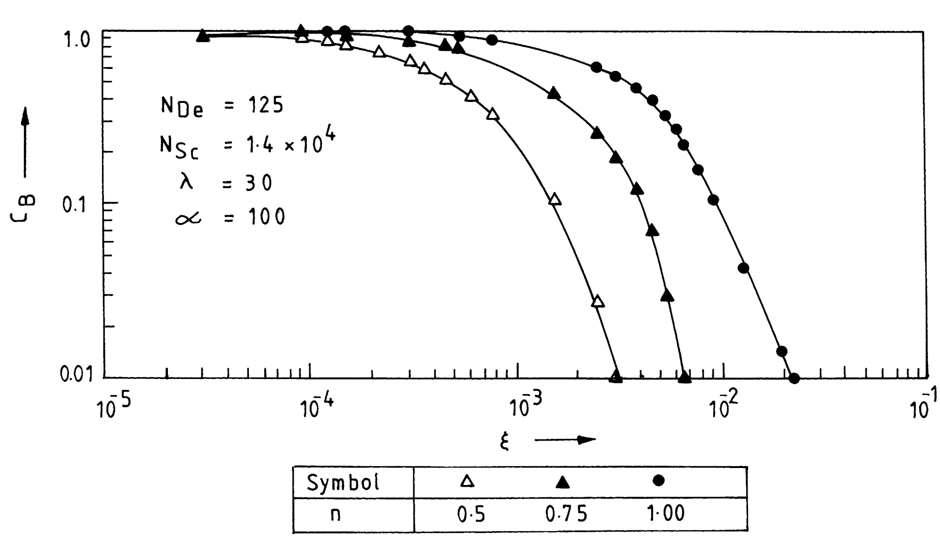

Fig. 7. Variation of bulk concentration along the dimensionless axial distance (ξ) for Newtonian and Power law fluids.

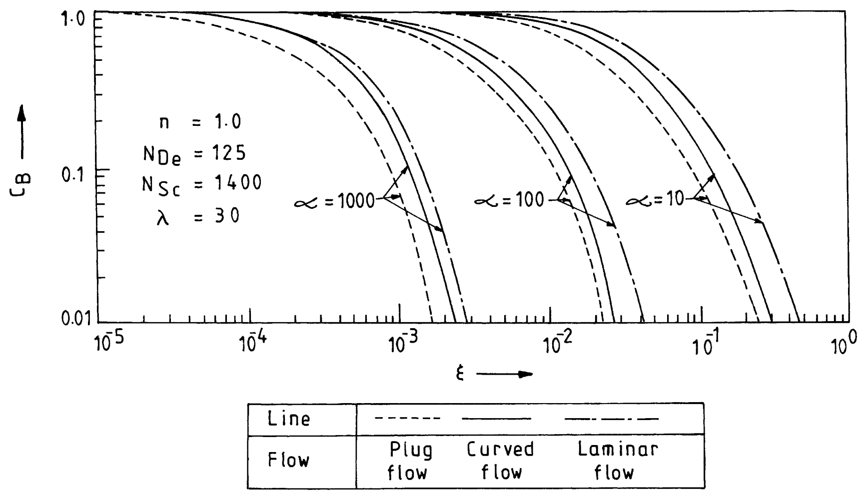

Fig. 8. Comparison of bulk average concentration of laminar tubular, helical coil and plug flow reactors.

The variation of bulk mean concentration C_B along the dimensionless length ξ for coiled tube flow, plug flow and laminar flow reactor is shown in Fig. 8 for different values of $\alpha = 10$, 100 and 1000 at Dean number of 125, $N_{Sc} = 1400$ and $\lambda = 30$. It is clear from Fig. 8 that the conversion obtainable in a coiled tube is higher than in a straight tube but less than that in plug flow reactor. Due to the existence of secondary flow the mixing takes place in a cross-sectional plane which improves the performance of coiled tube reactor to a plug flow reactor. As discussed by Mashelkar and Venkatasubramanian [30], it is also clear from Fig. 8 that the improvement due to coding diminishes with increases in α.

6. Conclusions

The present study described a numerical solution for convective diffusion with first order reaction in curved circular tubes. Newtonian and power law fluids in the range $1 < N_{De} < 250$, $1 < N_{Sc} < 1.4 \times 10^4$, $10 < \lambda < 100$ and $0.5 < n < 1$. The following conclusion may be drawn from the present analysis.

1. The phenomenon of convective diffusion with reaction for Newtonian and power law fluids flowing through curved circular tubes can be characterized by reaction parameter (α), dimensionless axial distance (ξ) and power law index (n).
2. The variation of bulk concentration along the dimensionless axial distance decreases with increases in values of α for particular values of n, N_{De}, N_{Sc}, and λ.
3. The performance of coiled chemical reactor lies between the performance of plug and laminar reactors.

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