Modeling of Non-Newtonian Reactive systems in Tubular Reactor

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Introduction

A vast majority of material processing in industry involves homogeneous phase reactions. These reactions are carried out in batch mode as well as continuous mode. The empty tubular reactors are widely used reactor systems for continuous processing in chemical and allied industry. The heat effects due to these reactions necessitate the use of some heat removal/addition system with these reactors. Tubular reactors for Newtonian fluids have been studied extensively experimentally as well as through modeling. A vast majority of reactions involved in polymer processing, food processing, biochemical industries etc. typically involve non-Newtonian behaviour. The modeling studies dealing with non-Newtonian fluids are very limited. The modeling and simulation study of non-Newtonian fluid reactions can lead to obvious benefits over experimental methodology.

Most of the studies in non-Newtonian fluids are either based on convective models or on isothermal conditions. Novosad & Ulbrecht (1966) have modeled the reaction of power law fluids under laminar flow conditions, using residence time distribution concept to get conversions, neglecting the diffusional effects. Osborne (1975) studied convective model for non-Newtonian fluid tubular reactor under isothermal conditions. Tracer technique has been used for the systems with unknown rheological properties. For constant wall temperature conditions and adiabatic conditions, non-isothermal tubular polymerizers have been studied using finite volume method, runaway condition having been found (Kleinstreuer & Agarwal, 1986). These studies do not account for non-adiabatic operation and the radial dispersion effects. In actual systems, due to heat exchange from the reactor wall, there is existence of temperature gradients in radial direction. These gradients in temperature influence reaction rates in a given cross section, setting up concentration gradients and the effect further gets magnified due to rheological parameters.

In this study, modeling of reactions of non-Newtonian fluids in tubular reactors with radial dispersion has been done. The reaction of non-Newtonian fluids has been modeled in non-isothermal non-adiabatic tubular reactor. Assuming a first order irreversible endothermic reaction of Ostwald-de-Waele power law fluids for the assumptions of constant wall temperature and axial symmetry, the 2-D model is used to generate concentration and temperature profiles in axial and radial directions.

Model Equations

The cylindrical elemental shell is used for analysis of the reactor. The balance equations are formed for this shell. The coupled mass balance, heat balance and velocity distribution equation have been considered as set of model equations. The equations are converted to non-dimensional form by suitable transformations. The model equations in the dimensionless form are given below.

Mass balance

$$\alpha_1\left[\frac{\partial^2 C^1}{\partial y^2}+\frac{1}{y}\frac{\partial C^1}{\partial y}\right]-V(y)\frac{\partial C^1}{\partial X}-\beta_1 e^{\frac{-E_A}{R_g(T+273))}}C^1=0 \quad (1)$$

Energy balance

$$\alpha_2\left[\frac{\partial^2 T^1}{\partial y^2}+\frac{1}{y}\frac{\partial T^1}{\partial y}\right]-V(y)\frac{\partial T^1}{\partial X}-\beta_2 e^{\frac{-E_A}{R_g(T+273))}}C^1=0 \quad (2)$$

Velocity distribution

$$V(y)=\frac{\left[\int_y^1 (y)^{1/n}\left[1+\beta\left(T^1-1\right)\right]dy\right]}{2\left[\int_0^1 y\left\{\int_y^1 (y)^{1/n}\left[1+\beta\left(T^1-1\right)\right]dy\right\}dy\right]}=\frac{I_1(y)}{2I_2} \quad (3)$$

where

C^1 – dimensionless concentration (=C/C_0) [-]
C_p – specific heat (J/kg^{o}C)
D_m – diffusivity of species (m^2/s)
E_A – activation energy (J/mol)
k_{th} – thermal conductivity (J/m ^{o}C)
L – reactor length (m)
n – rheological parameter
r – radial distance (m)
R – tube radius (m)
T^1 – dimensionless temperature (=T/T_0) [-]
X – dimensionless axial distance (=z/L) [-]
y – dimensionless radial distance (=r/R) [-]
ΔH_r – heat of reaction (J/mol)
α_1 – dimensionless parameter (= D_mL/ $v_b R^2$) [-]
α_2 – dimensionless parameter (=Lk_{th} /$\rho C_p v_b R^2$) [-]
β – dimensionless parameter (=β_0/T_0) [-]
β_0 – rheological constant ($^oC^{-1}$)
β_1 – dimensionless parameter (=k_0L/v_b) [-]
β_2 – dimensionless parameter (=k_0 $\Delta H_r C_{A0}$L/$\rho C_p v_b T_0$) [-]

The boundary conditions in dimensionless form are

1. At axis of the reactor

   y=0, $0\le X\le 1$, $\frac{\partial C^1}{\partial y}=0, \frac{\partial T^1}{\partial y}=0$ (4a)

2. At reactor wall

   y=1, $0\le X\le 1$, $\frac{\partial C^1}{\partial y}=0$,T^1=1 (4b)

3. The conditions at the reactor entrance are

   $0\le y\le 1$, X=0, $C^1=1$, $T^1=T_0/T_w$ (4c)

These equations (1)-(4) constitute the model equations for the tubular reactor in which a power law fluid undergoes first order reaction under non-isothermal conditions.

Model Solution

The model equations are solved by discretising at various grid locations (I,J), using backward semi-implicit finite difference numerical technique (Srivastava, 1983). The

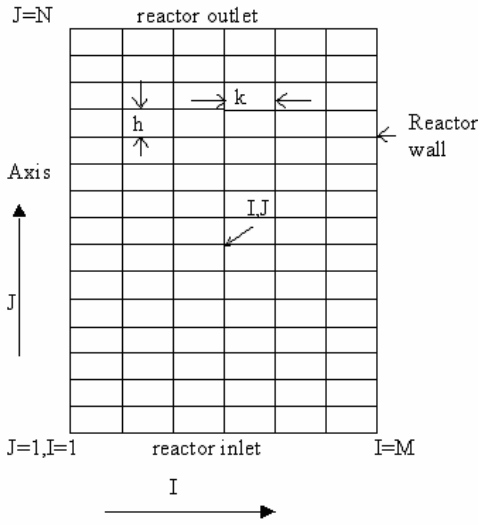

Fig 1: Reactor domain grid geometry

discretised reactor domain consists of M-1 divisions on radial scale and N-1 divisions on axial scale as shown in Fig 1. The discretised set of equations for concentration and temperature as unknowns, form a set of simultaneous equations at each axial position in the reactor. These sets of equations can be written in form of matrix equation **A.B = C** for each case**.** The coefficient matrix **A** is tridiagonal banded matrix of MxM dimension. This matrix equation is transformed such that the tridiagonal banded matrix is converted to an equivalent matrix of Mx3 dimension through Srivastava's technique (1983). This transformation reduces computing space and time. The transformed set of coupled equations is solved by developing a program in FORTRAN by making use of algorithm given by Srivastava (1983), choosing an appropriate grid. The simulated results give the profiles for concentration and temperature in the reactor in both the radial and axial directions under various conditions.

Simulation Results

As shown in Fig 2, the wall temperature is higher than the core flow zone. This leads to higher reaction rate in the zone near wall than in the bulk. Thus, the concentration in the zone near centre of tube is higher than that in the wall zone. Thus, typical radial variations in concentration and temperature are available in the reactor with heat flow from the reactor walls.

The axial profiles for concentration and temperature are depicted in Fig 3. It is found that as the stream moves through the reactor, more of conversion takes place leading to a decrease in concentration along the axis. On the contrary, the temperature of the stream increases in traversing the reactor length, despite endothermic reaction. This is due to the fact that wall temperature is kept constant, which leads to the rise in temperature.

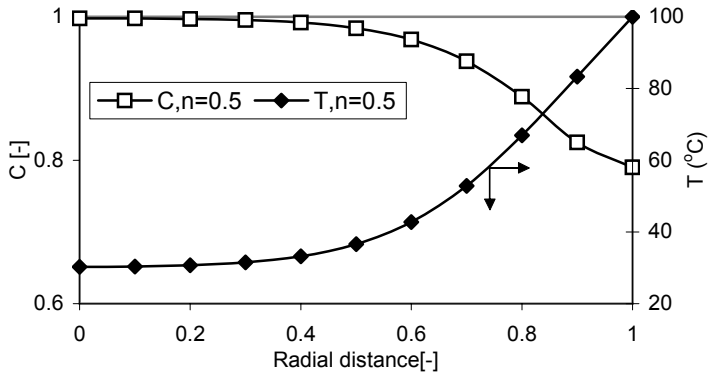

Fig 2: Radial concentration and temperature profiles

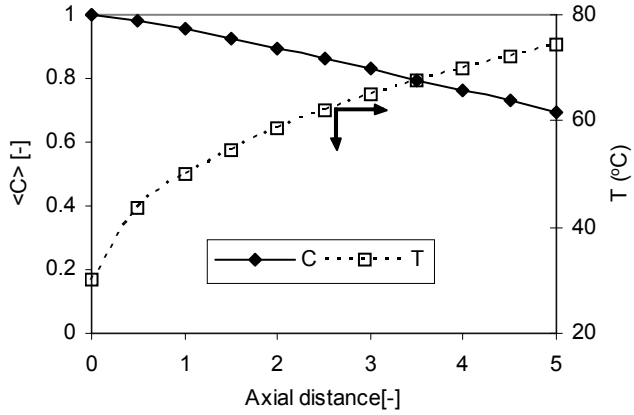

Fig 3: Axial concentration and temperature profiles

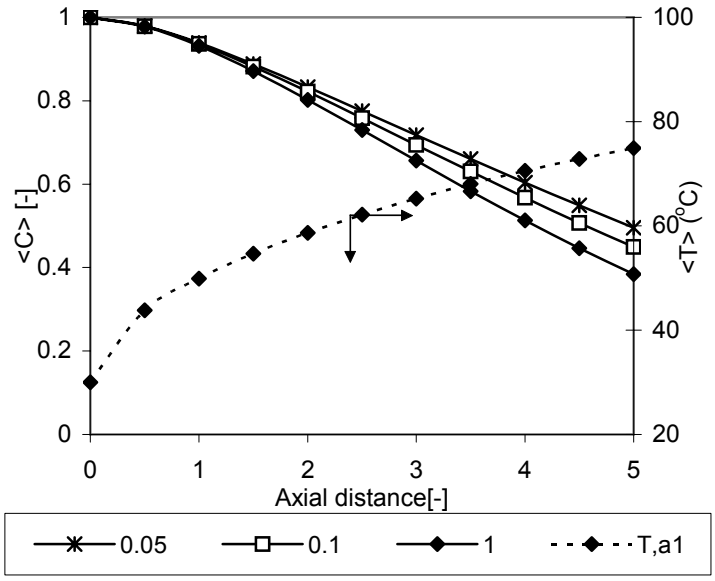

Fig 3: Effect of α_1 on axial profiles

In addition, the effect of various dimensionless parameters involved in the model, on these profiles is also investigated. As is clear from Fig 3, a higher value of α_1

gives a reduction in concentration at a given axial level. This signifies a higher conversion with increase in α_1. The effect of change in α_1 on temperature is negligible. A similar trend is shown for change in β_1. Thus, an increase in α_1 and β_1 leads to an increase in conversion whereas temperature is not affected appreciably.

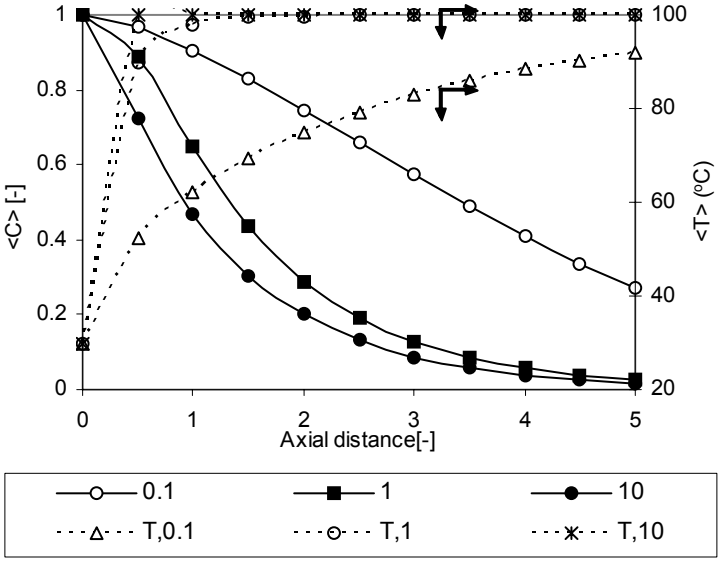

Fig 4: Effect of α_2 on axial profiles

An increase in α_2 leads to increase in conversion and temperature gain as shown in Fig 4. As α_2 increases, concentration values reduce at the same axial location. Also, simultaneously the temperature for given axial position of the stream is increased for increase in α_2. The increase in conductive heat or decrease of convective heat with increase in α_2 is the reason for this behaviour. On the other hand, an increase in β_2 gives a reduced conversion and temperature gain. The rheological parameter n also affects the reactor performance. An increase in rheological parameter leads to decrease in conversion and temperature. Also, the effect of n on velocity profile is also predicted. The distortion in velocity profile in moving along the reactor axis is higher for higher value of n. The model generates the reactor behaviour in both radial and axial directions. Also, the effect of variation in parameters on the reactor performance is also simulated by using this model.

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