Thermal and Mass Transients in the Developing Region of a Homogeneous Tubular Chemical Reactor

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The current investigation presents a finite difference simulation of a homogeneous tubular reactor under laminar flow conditions. The present simulation considers the unsteady operation where transients in flow hydrodynamics, temperature field, and species concentrations have been considered. Flow development in the entrance region of the present reactor has been considered. Present results exhibit reactant concentration and mixing cup temperature profiles for a variety of operating conditions. Effects of several parameters on the performance of the current reactor have been examined, including, reaction parameter, order of reaction, and Schmidt number. © 2009 American Institute of Chemical Engineers *AIChE J,* 56: 749–755, 2010

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Introduction

Recent global notion of clean environment has strongly motivated extensive research in the area of reactive flow. Reactive flow problems can be encountered in many engineering applications, such as, chemical destruction of industrial liquid waste, behavior of biological systems, petroleum refinery and industry, and chemical reactors such as chemical vapor deposition (CVD) that are used for the manufacturing of semi conductors chips. Problems that involve homogeneous tubular reactive flow under laminar conditions, in particular, have applications in chemical, petrochemical, and biochemical industries. These applications include; thermal pasteurization of liquid food, tubular polymerization reactors, polychlorination of methane, thermal cracking of hydrocarbons, and ethylene manufacturing by ethane pyrolysis.

The literature shows several investigations in the area of tubular reactive flow. In these investigations, there is a wide variation in the degree of sophistication as well as the applicability of their analysis to various engineering problems. Solomon and Hudson[1] investigated an irreversible, first order simultaneous heterogeneous and homogenous reactor. In their study, the authors considered a single reaction in an isothermal tubular reactor under fully developed Newtonian laminar flow conditions. They presented a numerical solution for study cases where the homogenous reaction might be neglected with respect to the heterogeneous reaction and vice versa. In 1976, the orthogonal collocation method was used by Young and Finlayson[2] in order to solve the mathematical model of a catalytic converter, where reaction takes place within a porous catalytic layer deposited on the wall of the tube. Nigman and Vasudeva[3] presented an experimental investigation of a one-dimensional transient laminar flow reactor with first order homogeneous reaction. The obtained experimental data was compared to computations based on the dispersion model. Kulkarni and Vasudeva[4] studied the performance of an isothermal laminar flow reactor where an empirical expression for the effective dispersion coefficient was introduced. The same setup investigated by Kulkarni and Vasudeva[4] was investigated by Nigman and Vasudeva[5] for non-Newtonian fluids. In 1977, the dispersion model with two dispersion coefficients was applied by Nigman and Vasudeva[6] to model a laminar flow reactor under a set of first order consecutive reactions. The problem studied by Kulkarni and Vasudeva[4] was revisited by Dang and Steinberg[7] for reversible reactions. Apelblat[8] investigated a

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problem of mass transfer coupled with an irreversible chemical reaction of the first order. In his investigation, the author presented four flow cases namely, plug flow, Couette flow, Couette flow with moving interface, and fully developed boundary layer flow. The author introduced analytical solutions and asymptotic expressions for homogeneous and heterogeneous chemical reactions. He also presented some extensions for mass transfer in non-Newtonian liquids and for cases with permeable surfaces. In the same year, homogenous chemical reactors with diffusion under different conditions were studied by Dang and Steinberg.[9] They considered a steady state two-dimensional reversible Newtonian fully developed laminar flow with an irreversible chemical reaction. In 1982, the diffusion role in the direction of convective transport investigated by Apelblat.[10] He derived analytical solutions and asymptotic expressions for cases of mass transfer coupled with first order homogeneous and heterogeneous irreversible chemical reactions. Nigam et al.[11] studied the convective diffusion transport phenomena with a heterogeneous reaction at the walls. The authors obtained a mathematical solution in terms of an eigenfunction series expansion. In 1983, a convective diffusion non-Newtonian tubular flow under developing flow conditions was investigated by Venkatsubramanian and Mashelkar.[12] A year later, McLaughlin et al.[13] studied the effect of radial velocity in a tubular laminar flow reactor. They showed that the radial velocity should not be neglected when the convective diffusion of heat and mass is considered. Chang and Chern[14] numerically investigated a tubular isothermal reactor under laminar flow diffusion with simultaneous heterogeneous and homogeneous reactions. In their study, the authors considered non-Newtonian power-law fluids with arbitrary order reactions. Barouh and Mikhailov[15] investigated a gas phase homogeneous tubular reactor subjected to a wall-catalytic effect. In 1992, the dynamic behavior of an adiabatic tubular reactor during the startup and the feed pump failure conditions was studied by Verwijs et al.[16] They showed that for industrial tubular reactors, a much higher initial temperature is required during startup compared to the reactor inlet temperature during normal steady-state operation. Elperin and Fominykh[17] have obtained a closed form solution for the problem of mass transfer in a two-dimensional submerged wall jet flow with a chemical reaction of the first order at the surface. Lawal[18] has presented analytical solutions for the convective diffusion of power-law fluids in parallel plate and tubular reactors with single homogeneous and catalytic wall reactions. In 1996, heat transfer and reaction characteristics of a chemically reactive flow near the stagnation point of a catalytic porous bed with finite thickness were theoretically investigated by Chao et al.[19] Park and Cho[20] developed a new method to obtain a low dimensional dynamic model of flow reactors governed by non-linear partial differential equations. This is based on the Karhunen-Loeve decomposition that is a technique of obtaining empirical eigenfunctions from experimental or numerical data of a system. An integral-spectral formulation for laminar reacting flows in tubular geometry was introduced by Arce et al.[21] Sarrafi et al.[22] studied a gas-liquid bubble reactor. In their study, the authors discussed the basis for the prediction of heat and mass transfer coefficients. Al-Khateeb[23] has numerically investigated a homogeneous- heterogeneous annular chemical reactor. In his study, Al-Khateeb considered transients in temperature and species concentrations while flow hydrodynamics were assumed steady. The author presented detailed parametric study of the thermal performance of the reactor under investigation. One year later, Almuhtasib[24] numerically studied the transient behavior of a homogeneous-heterogeneous tubular chemical reactor. In this study, flow hydrodynamics were assumed fully developed. Balasubramanian et al.[25] studied the influence of a secondary flow on diffusion with heterogeneous reaction. In their study, the authors obtained the concentration distribution in a Newtonian fluid for the secondary flow in a curved tube with bulk/wall reaction for a range of parameter values using an axially marching spectral finite difference scheme. Their results showed that for fixed extent of secondary flows there was an improvement in the performance of the reactor as the effect of bulk and wall reaction mechanisms were intensified in the system.

Churchill and Yu[26] have numerically investigated a fully developed, steady, homogeneous, tubular reactor. Their model has adopted a global, single step, first-order, irreversible reaction. In a more recent study, Moustafa et al.[27] have numerically investigated the steady non-isothermal operation of the catalytic partial oxidation of methanol in a laminar tubular reactor. The author performed a parametric study in order to investigation the optimum operating conditions of the reactor under investigation.

Accurate simulation of the unsteady operation of homogeneous, tubular, nonisothermal chemical reactors requires the inclusion of many complex thermo-chemical phenomena in the analysis. The present simulation considers many of these phenomena including: 1) transient flow hydrodynamics, 2) transient temperature flied, 3) transients in species concentrations. These three items provides a tool to study the start up conditions of the reactor under consideration, as well as the steady state behavior of the reactor after a relatively long time of operation, 4) hydrodynamic, thermal and mass development within the entrance region of the reactor, and 5) the two-dimensional character of the flow. The problem has been cast in a generalized dimensionless form. This makes it applicable to a wide range of industrial applications and not limited to a specific reactor with specific dimensions and specific type of working fluid. To the best of the authors' knowledge, tubular reactors involving all aforementioned complex phenomena have not been simulated yet.

Mathematical Model

The present problem consists of an insulated tubular chemical reactor as demonstrated in Figure 1. Initially, the working fluid is stagnant. For times larger than zero, a sudden constant inlet velocity is applied to the working fluid at the reactor entrance. The working fluid consists of a carrier fluid loaded with a contaminated material that will be referred to as the fuel. At the reactor entrance, the fluid temperature is kept uniform at T_o. Chemical reaction is launched for times larger than zero. The present study focuses on the thermal developing region of the reactor. The dimensionless governing equations have been formulated in view of a set of simplifying assumptions and operating conditions including, 1) boundary layer flow where axial diffusion is

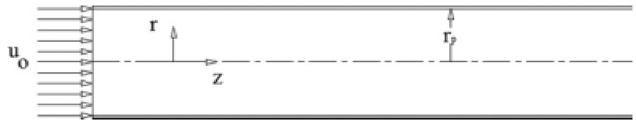

Figure 1. Schematic diagram of the problem under consideration.

neglected compared to axial convection, 2) transient incompressible flow with constant physical properties, 3) relatively low fuel concentration, 4) global, single step, Arrhenius type, exothermic chemical reaction of the form $\upsilon_f F + \upsilon_o O \xrightarrow{k} \upsilon_c C$, and 5) equal mass diffusivities of the fuel and the oxidant.

According to the aforementioned listed operating conditions and simplifying assumptions, and using a cylindrical coordinate system, the present dimensionless governing equations take the following form,

Continuity equation:

$$\frac{\partial U}{\partial Z} + \frac{1}{R}\frac{\partial (RV)}{\partial R} = 0 \tag{1}$$

Axial momentum equation:

$$\frac{\partial U}{\partial \tau} + U\frac{\partial U}{\partial Z} + V\frac{\partial U}{\partial R} = -\frac{dP}{dZ} + \frac{1}{R}\frac{\partial\left(R\left(\frac{\partial U}{\partial R}\right)\right)}{\partial R} \tag{2}$$

Energy equation:

$$\frac{\partial \theta}{\partial \tau} + U\frac{\partial \theta}{\partial Z} + V\frac{\partial \theta}{\partial R} = \frac{1}{Pr}\frac{1}{R}\frac{\partial\left(R\left(\frac{\partial \theta}{\partial R}\right)\right)}{\partial R} + (T_c)\left(e^{\left(\frac{-\theta_i}{\theta}\right)}\right)\left(Y_f^{nf}\right)\left(Y_o^{no}\right) \tag{3}$$

Fuel species equation:

$$\frac{\partial Y_f}{\partial \tau} + U\frac{\partial Y_f}{\partial Z} + V\frac{\partial Y_f}{\partial R} = \frac{1}{Sc}\frac{1}{R}\frac{\partial\left(R\left(\frac{\partial Y_f}{\partial R}\right)\right)}{\partial R} - (F_c)\left(e^{\left(\frac{-\theta_i}{\theta}\right)}\right)\left(Y_f^{nf}\right)\left(Y_o^{no}\right) \tag{4}$$

Oxidant species equation:

$$\frac{\partial Y_o}{\partial \tau} + U\frac{\partial Y_o}{\partial Z} + V\frac{\partial Y_o}{\partial R} = \frac{1}{Sc}\frac{1}{R}\frac{\partial\left(R\left(\frac{\partial Y_o}{\partial R}\right)\right)}{\partial R} - (O_c)\left(e^{\left(\frac{-\theta_i}{\theta}\right)}\right)\left(Y_f^{nf}\right)\left(Y_o^{no}\right) \tag{5}$$

Initial and Boundary Conditions:

At $\tau = 0$, $Z \geq 0$, and $0 \leq R \leq 1$:

$$U = 0,\ \theta = 1,\ Y_f = 1,\ Y_o = \mathrm{of}$$

For $\tau > 0$, $Z = 0$, and $0 \leq R \leq 1$:

$$U = 1,\ \theta = 1,\ P = 0,\ Y_f = 1,\ Y_o = \mathrm{of}$$

At $\tau > 0$, $Z > 0$, and $R = 0$:

$$\frac{\partial U}{\partial R} = 0,\ \frac{\partial \theta}{\partial R} = 0,\ \frac{\partial Y_f}{\partial R} = 0,\ \frac{\partial Y_o}{\partial R} = 0$$

At $\tau > 0$, $Z > 0$, and $R = 1$:

$$U = 0,\ V = 0,\ \frac{\partial \theta}{\partial R} = 0,\ \frac{\partial Y_f}{\partial R} = 0, \frac{\partial Y_o}{\partial R} = 0$$

Numerical Computation

The present governing equations have been solved numerically according to the boundary and initial conditions listed earlier. The present solution employs an implicit finite difference technique in which central differencing has been applied to all radial derivatives while first order backward differencing has been applied to axial and temporal derivatives. The resulting finite difference equations have been applied to a three-dimensional Cartesian mesh that sweeps the entire domain of interest. This, typically, results in converting the present partial differential equations into a set of algebraic equations. These equations inherit the nonlinear character of the original differential equations; however, the lagging technique has been used in order to linearize the present group of algebraic equations. A standard linear solver has been used to solve the system of linear equations under consideration. The present scheme has appeared several times in the literature. Details of this scheme could be found in El-Shaarawi and Alkam[28], and Haddad et al.[29]

Grid Analysis

The sensitivity of the present numerical solution to the grid size has been investigated. This has been carried out in order to select the appropriate grid size for the entire computations. The sensitivity of the fuel concentration radial gradient (FCRG) at the centerline to the grid size has been used in the present grid refinement analysis. First of all, the sensitivity of FCRG to the number of grid points in the radial direction (NR) has been studied at $Z = 0.5$, and $\tau = 0.5$ with $\Delta Z = 0.01$, and $\Delta\tau = 0.001$. The result of this study showed that increasing the value of NR above 40 produced no appreciable change in the calculation of FCRG, hence the optimum radial step size has been fixed at 0.025 throughout the present computations. Having fixed the value of ΔR at 0.025, similar sensitivity analysis has been carried out to optimize the axial step size (ΔZ). This analysis resulted in an optimum axial step size of $\Delta Z = 0.002$. Finally, the sensitivity of the FCRG to the temporal step size ($\Delta\tau$) has been studied in a similar fashion. This specific study is exhibited in Figure 2. Based on this figure, the optimum temporal step size has been fixed at a value of 0.001.

Parametric Study

In this section, a parametric study is presented to discuss effects of several operating and design conditions on the performance of the reactor under consideration. A base case study has been chosen to carry out the numerical solution for the set of finite difference equations that correspond to the present governing equations. The base case study

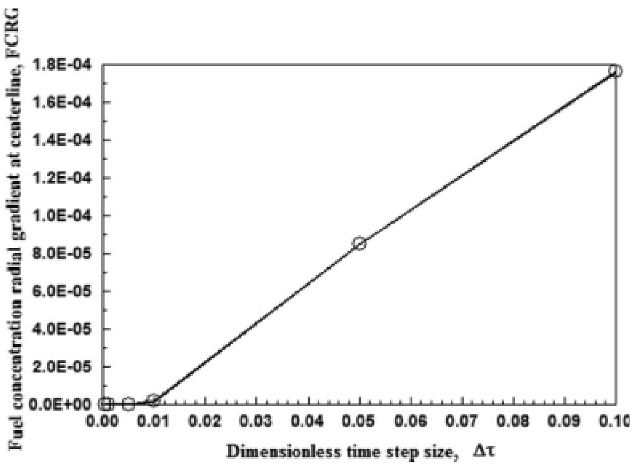

Figure 2. Effect of the time step size on the computation of the fuel concentration gradient at the tube centerline evaluated at $Z = 0.5$, and $\tau = 0.5$.

represents a typical laminar flow tubular reactor with a global single step Arrhenius first order reaction. The following input data to the mathematical model has been used as the default values to plot the figures of the present parametric study unless mentioned otherwise for a specific figure,

$$\mathrm{Pr} = 2.6,\ \mathrm{Sc} = 1,\ \mathrm{F_c} = \mathrm{T_c} = 10,\ \mathrm{O_c} = 15,\ \mathrm{nf} = 1,$$
$$\mathrm{no} = 0,\ \theta_i = 1$$

Among the parameters of interest to the present parametric study is the mean fuel concentration, θ_f, and the mixing cup temperature, T_mc. The mean fuel concentration represents the average value of the dimensionless fuel concentration over the cross sectional area of the reactor at a prescribed axial location. θ_f is defined as:

$$\theta_\mathrm{f} = \frac{\int_0^1 URY_\mathrm{f}dR}{\int_0^1 URdR} \tag{6}$$

While the mixing cup temperature represents the average of the dimensionless temperature over the cross sectional area of the reactor calculated at a certain axial location. T_mc is defined as:

$$T_\mathrm{mc} = \frac{\int_0^1 UR\theta dR}{\int_0^1 URdR} \tag{7}$$

Having chosen an optimum grid setup for the present problem, computations of the present code have been verified by comparing the present computations to previous published work by Venkatsubramanian and Mashelkar.[12] In this regard, the axial distribution of the steady-state mean fuel concentration, θ_f, has been plotted and compared to corresponding results by Venkatsubramanian and Mashelkar[12] in Figure 3.

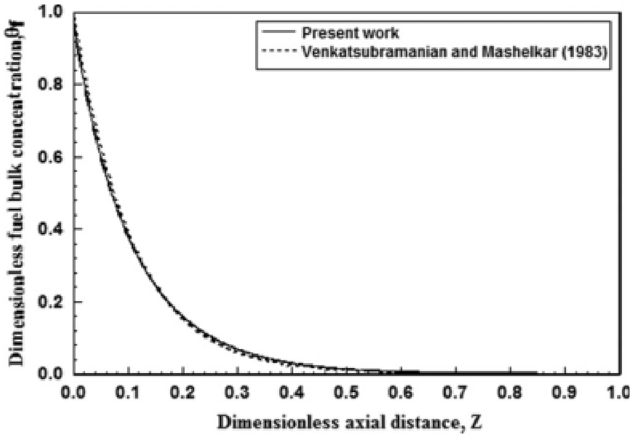

Figure 3. Variation of the steady-state dimensionless mean fuel concentration, θ_f, with axial distance.

Comparison with computations obtained by Venkatsubramanian and Mashelkar (1983).

In the following current parametric study, the main features of the thermo-chemical behavior of the present reactor are displayed. A discussion of the effects of several parameters on the thermal performance of the current reactor is presented. These parameters include, the fuel constant (F_c), Schmidt number (Sc), and reaction order with respect to the fuel (nf).

Using the default model input for the base case study mentioned earlier, the axial distribution of the dimensionless fuel bulk concentration, θ_f, has been plotted in Figure 4. The figure shows several profiles corresponding to different values of dimensionless time, τ, namely, $\tau = 0.2$, 0.4, 0.6, 0.8, and 1. No significant variation of θ_f was noticed for $\tau > 1$, and hence, $\tau = 1$ is considered the steady state time for this specific test case. The figure shows also the asymptotic destruction of the fuel with Z, typically observed for first order reactions. At, $Z = 1$, more than 99% destruction of the fuel took place at steady state condition. The dimensionless

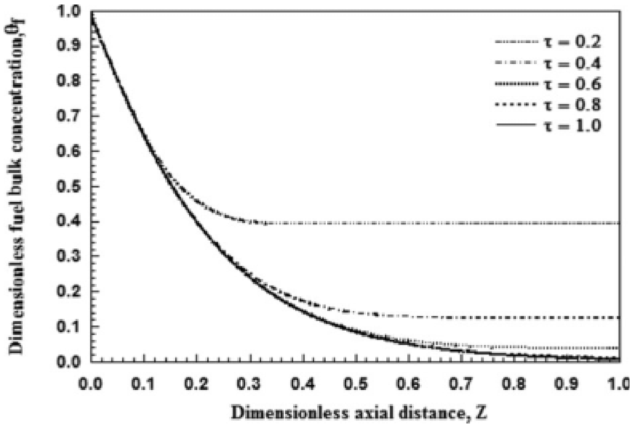

Figure 4. Axial distribution of the dimensionless fuel bulk concentration, θ_f, at different dimensionless times.

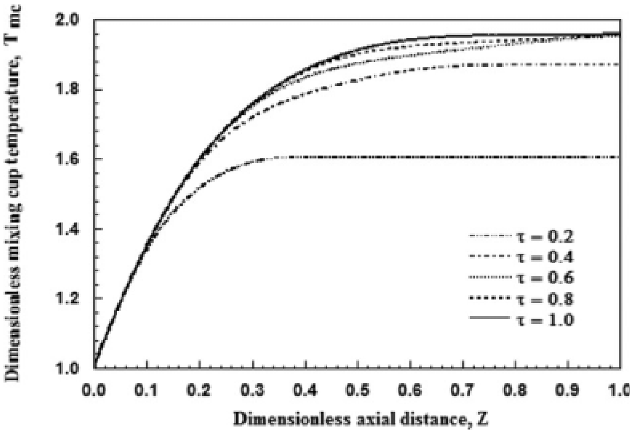

Figure 5. Axial distribution of the dimensionless mixing cup temperature, T_{mc}, at different dimensionless times.

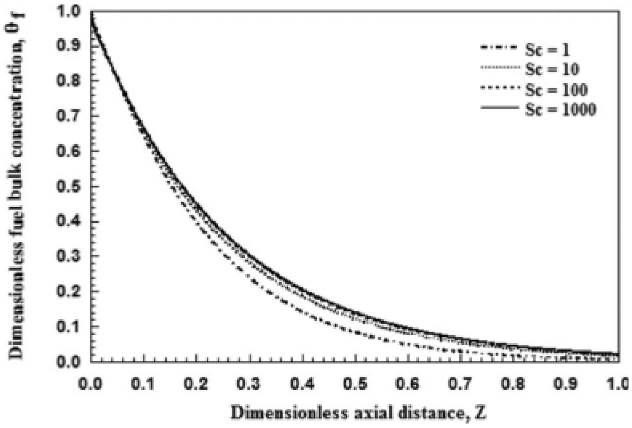

Figure 7. Effect of *Sc* number of the steady state axial distribution of the dimensionless fuel bulk concentration, θ_f.

mixing cup temperature, T_{mc}, axial profiles for the same test case have been plotted in Figure 5 for several values of τ. The figure shows that at $Z = 1$, a steady state rise in T_{mc} reaches 95.8 % over the value of T_{mc} at the reactor inlet, $Z = 0$. One can qualitatively observe the correlation between the asymptotic rise in T_{mc} (Figure 5) and the drop in θ_f (Figure 4) due to heat release. It is worth mentioning that Figures 4, 5 have been plotted within $Z = 1.0$ because flow activities could be represented within this length of the reactor.

At several axial locations, the steady state radial distribution of the dimensionless fuel concentration, Y_f, has been plotted in Figure 6. At a certain cross section of the reactor, the value of Y_f is a maximum at the reactor centerline and it drops with R as it approaches the inner wall of the reactor. This is due to the marked effect of the friction between the flow and the wall that results in flow retardation. This flow retardation closer to the wall provides longer residence time for the fuel particles inside the reactor which eventually results in more fuel destruction. As the flow moves along the reactor, radial transport plays a major role in flattening the radial profile gradually.

The effect of *Sc* number on the axial distribution of the steady state dimensionless bulk fuel concentration is shown in Figure 7. The figure shows computations corresponding to four values of *Sc* number ($Sc = 1$, 10, 100, and 1000). The figure shows the same behavior exhibited in a previous study by Venkatsubramanian and Mashelkar[12] in which lower *Sc* number, i.e., higher diffusion, produced faster development of the fuel concentration profile. The effect of the reaction order on the steady state axial distribution of the dimensionless fuel bulk concentration is shown in Figure 8. The figure shows three cases corresponding to zero order, first order, and second order reactions. For the zero order case, the fuel is completely destructed at $Z = 0.189$. Complete destruction is achievable for zero order reaction systems because the reaction rate is insensitive to the fuel concentration, while for first and second order systems, the reaction rate slows down as the fuel concentration decreases. Yet, the sensitivity of the reaction rate to the fuel concentration for second order reactions is higher than that for first order reactions. As a

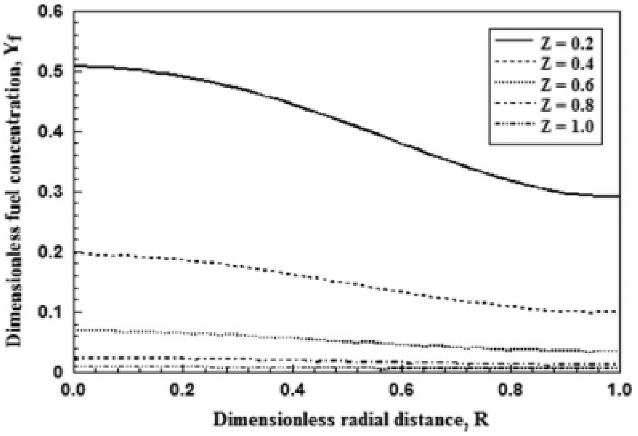

Figure 6. Radial distribution of the dimensionless fuel concentration, Y_f, at different values of *Z*, and at $\tau = 1$.

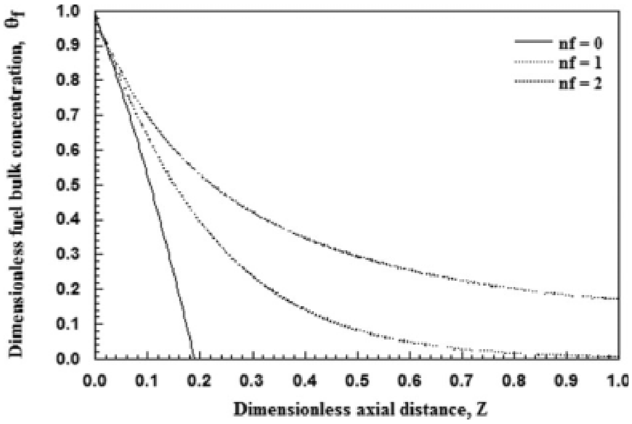

Figure 8. Effect of the reaction order, nf, of the steady state axial distribution of the dimensionless fuel bulk concentration, θ_f.

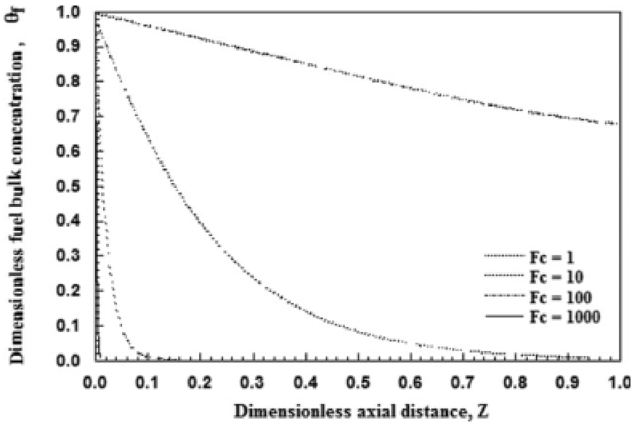

Figure 9. Effect of the fuel constant, F_c, on the steady state axial distribution of the dimensionless fuel bulk concentration, θ_f.

result of that, first order reaction systems experience faster destruction of the fuel than second order ones.

The effect of the fuel constant, F_c, on the performance of the present reactor is shown in Figure 9. The fuel constant is a dimensionless reaction parameter that reflects the speed of the reaction considered. F_c is the coefficient of the source term in the species equation for the fuel that represents the rate of destruction of the fuel due to the chemical reaction. It is quite clear that faster reactions, higher F_c, lead to faster fuel destruction as shown in Figure 9.

Conclusions

In the current paper, a numerical investigation has been presented to study the thermo-chemical behavior of a reactive flow in the developing region of a tubular chemical reactor. Transients have been considered in the flow hydrodynamics, temperature field, and species concentration profiles. A global, Arrhenius type, single, homogeneous reaction has been adopted. The present study has examined effects of several parameters on the performance of the reactor under consideration. These parameters included, order of the reaction (nf), *Sc* number, and the reaction parameter (F_c). The following qualitative and quantitative conclusions have been drawn:

1. As it is anticipated, the order of the reaction has a significant impact on the destruction rate of the reactant. For a zero order reaction, a dimensionless reactor length of 0.19 was long enough to achieve complete destruction of the reactant, while at this specific reactor length, the percentage of reactant destruction for the first order and the second order reactions were 57.1%, and 45.3%, respectively.
2. Quantitative results exhibited the role of increasing the reaction parameter, F_c, on destruction rate of the reactant. For the first order reaction case considered, 99% destruction of the reactant was achieved within dimensionless reactor lengths of 0.009, 0.015, and 0.918 for reaction parameters of 1000, 100, and 10, respectively.
3. Although it is known that the increase in Sc number reduces the destruction rate of the reactant, the present results showed that this effect was within a few percentages. For a dimensionless reactor length of 1, the reactant destruction rates were 99.3%, 98.3%, 97.9%, and 97.85% for *Sc* numbers of 1, 10, 100, and 1000.
4. Because of flow development, the radial variation of the reactant concentration was significant near the reactor entrance and it did not approach zero until the flow has reached a dimensionless axial distance of around 1.
5. During startup conditions, the time needed for the reactor to achieve steady state conditions depends on the reactor length. For the present reactor, the dimensionless times needed to achieve steady state conditions was 0.2, 0.6, and 1.0 for a reactor dimensionless lengths of 0.1, 0.5, and 1.0, respectively.
6. For the present reactor, the steady state mixing cup temperature at a dimensionless axial distance of 1 has experienced a 95.8 % increase over its value at the reactor entrance.

Notation

A = pre-exponential factor
C = products of the chemical reaction
c_p = constant pressure specific heat (J/kg K)
D = diffusion coefficient (m^2/s)
E = activation energy (J/Kmol)
F = fuel
F_c = fuel constant, $\frac{\upsilon_f A r_p^2 w_f^{1-nf}\left(\rho^{nf+no-1}\right)\left(y_{fo}^{nf+no-1}\right)}{\upsilon w_o^{no}}$
FCRG = fuel concentration radial gradient at the centerline, $\frac{\partial Y_f}{\partial R}$
k = specific reaction rate constant, $Ae^{\frac{-E}{RuT}}$
nf = reaction order with respect to the fuel
no = reaction order with respect to the oxidant
O = oxidant
of = initial oxidant-fuel ratio, $\frac{y_{oo}}{y_{fo}}$
O_c = oxidant constant, $\frac{\upsilon_o A r_p^2 w_o^{1-no}\left(\rho^{nf+no-1}\right)\left(y_{fo}^{nf+no-1}\right)}{\upsilon w_f^{nf}}$
P = Dimensionless pressure, $\frac{p}{\rho u_o^2}$
Pr = Prandtl number, $\frac{\upsilon}{\alpha}$
p = fluid pressure at any point (Pa)
Q = heat of reaction (J/kmol)
R = dimensionless radius, $\frac{r}{r_p}$
Re = Reynolds number, $\frac{2\rho r_p u_o}{\mu}$
Ru = universal gas constant (J/kmol K)
r = radial distance (m)
r_p = pipe radius (m)
Sc = Schmidt number, $\frac{\upsilon}{D}$
T = temperature (K)
T_o = initial temperature (K)
T_c = temperature constant, $\frac{Q\upsilon_f A r_p^2 w_f^{1-nf}\left(\rho^{nf+no-1}\right)\left(y_{fo}^{nf+no}\right)}{C_p \upsilon T_o w_o^{no}}$
T_{mc} = dimensionless mixing cup temperature, $\frac{\int_0^1 UR\theta dR}{\int_0^1 URdR}$
t = time (s)
U = dimensionless axial velocity, $\frac{u}{u_o}$
u = axial velocity (m/s)
u_o = axial velocity at the reactor inlet (m/s)
V = dimensionless radial velocity, $\frac{\rho r_p v}{\mu}$
v = radial velocity (m/s)
w_f = fuel molecular weight (kg/kmol)
w_o = oxidant molecular weight (kg/kmol)
Y_f = dimensionless fuel concentration, $\frac{y_f}{y_{fo}}$
Y_o = dimensionless oxidant concentration, $\frac{y_o}{y_{fo}}$
y_f = fuel mass fraction
y_{fo} = initial fuel mass fraction
y_o = oxidant mass fraction
y_{oo} = initial oxidant mass fraction
Z = dimensionless axial distance, $\frac{2z}{Re\, r_p}$
z = axial distance (m)

Greek letters

α = thermal diffusivity (m^2/s)
$\Delta\tau$ = dimensionless time step size
ΔR = dimensionless radial step size
ΔZ = dimensionless axial step size
μ = dynamic viscosity (Pa s)
υ = kinematic viscosity (m^2/s)
υ_c = stoichiometric coefficient of the reaction product
υ_f = stoichiometric coefficient of the fuel
υ_o = stoichiometric coefficient of the oxidant
θ = dimensionless temperature, $\frac{T}{T_o}$
θ_i = dimensionless activation energy, $\frac{E}{RuT_o}$
θ_f = dimensionless bulk fuel concentration, $\frac{\int_0^1 URY_f dR}{\int_0^1 URdR}$
ρ = fluid density (kg/m^3)
τ = dimensionless time, $\frac{\upsilon t}{r_p^2}$

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