Homogeneous-heterogeneous reactions in boundary-layer flow of a nanofluid near the forward stagnation point of a cylinder

Qingkai Zhao

Collaborative Innovation Center for
Advanced Ship and Deep-Sea
Exploration(CISSE),
State Key Lab of Ocean Engineering,
School of Naval Architecture,
Ocean and Civil Engineering,
Shanghai Jiao Tong University,
Shanghai 200240, China
Email: qkzhao@sjtu.edu.cn

Hang Xu*

Collaborative Innovation Center for
Advanced Ship and Deep-Sea
Exploration(CISSE),
State Key Lab of Ocean Engineering,
School of Naval Architecture,
Ocean and Civil Engineering,
Shanghai Jiao Tong University,
Shanghai 200240, China
Email: hangxu@sjtu.edu.cn

Longbin Tao

School of Marine Science and Technology,
Newcastle University, Newcastle NE1 7RU, U.K.
Email: l.tao@ncl.ac.uk

A mathematical model describing the homogeneous-heterogeneous reactions in the vicinity of the forward stagnation point of a cylinder immersed in a nanofluid is established. We assume that the homogeneous reaction is given by isothermal cubic autocatalator kinetics, while the heterogeneous reaction is chosen as first order kinetics. The existence of multiple solutions through hysteresis bifurcations is discussed in detail for the various diffusion coefficients of reactant and autocatalyst.

1 Introduction

The homogeneous and heterogeneous reactions are often encountered in many chemically reacting processes such as combustion, catalysis and biochemical systems. In such procedures, the homogenous reaction take places in the bulk and the heterogeneous reaction occurs on the catalyst surface. A common assumption for this flow problem is that the reaction only takes place in the boundary layer region of a body surface with an external flow being imposed on the outer edge of the boundary layer [1–3]. The problem can thus be simplified by using the boundary layer flows, usually stagnation-point flows [4–6]. Several experimental studies on methane/ammonia and propane oxidation flow-

ing over platinum have been given by Williams and his collaborators [7, 8], which clearly exhibit the existence of such homogeneous-heterogeneous reactions. Some theoretical works have been done to testifying the maturity of this model by some researchers [9–12].

Recently, nanofluids received considerable attractions owing to their better heat transfer capabilities. Several mathematical models have been proposed to predict nanofluids' behaviours such as the homogenous flow model [13], the dispersion model [14], the Buongiorno's model [15]. Among those models, the Buongiorno's model [15] received applausively attention since it well explained the slip mechanisms between the nanoparticles and the base fluid. In literature, few researchers have considered the homogeneous and heterogeneous reactions in nanofluids. Until now, only Kameswaran *et al.* [16] considered such chemical reactions in nanofluids. While their approach was based on the homogenous flow model, that was criticized by Magyari [17] that the governing equations of the homogeneous flow models can be reduced with the help of scaling transformations to the regular fluids. As a result, the corresponding nanofluid results can be recovered from the solutions of the Newtonian fluid problems via simple arithmetic operations. Different from the work of Kameswaran *et al.* [16], we use the Buongiorno's model [15] to model the nanofluid flow behaviours in the stagnation-point region of a two-dimensional body in the presence of the homogeneous-heterogeneous reactions.

*Address all correspondence related to ASME style format and figures to this author.

As far as we know, few studies have been done on such homogeneous-heterogeneous reaction problems in nanofluids by this model so that our work is unique and original.

2 Mathematical descriptions

Inspired by Merkin [18], we develop a model on boundary layer flow of a nanofluid in the forward stagnation-point region of a two-dimensional cylinder in the presence of the homogeneous and heterogeneous reactions. The sketch of this problem is shown in Fig.1. In the forward stagnation point, we assume that the reaction in the bulk is isothermal cubic autocatalytic, given by

while on the catalyst surface we have the single, isothermal, first-order reaction

Here it is assumed that there is only reactant A in the external flow, which has a uniform concentration C_∞ . Due to Eq.(1), we assume that the reaction rate is zero at the outer edge of the boundary layer. Based on those assumptions, the governing equations for boundary layer flow of a nanofluid in the forward stagnation-point region are written by

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad (3)$$

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \quad (4)$$

$$u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \tau D_B \left(\frac{\partial C_b}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial C_b}{\partial y} \frac{\partial T}{\partial y} \right) + \tau \frac{D_T}{T_\infty} \left[\left(\frac{\partial T}{\partial x} \right)^2 + \left(\frac{\partial T}{\partial y} \right)^2 \right], \quad (5)$$

$$u \frac{\partial C_a}{\partial x} + v \frac{\partial C_a}{\partial y} = D_A \left(\frac{\partial^2 C_a}{\partial x^2} + \frac{\partial^2 C_a}{\partial y^2} \right) - k_1 C_a C_b^2, \quad (6)$$

$$u \frac{\partial C_b}{\partial x} + v \frac{\partial C_b}{\partial y} = D_B \left(\frac{\partial^2 C_b}{\partial x^2} + \frac{\partial^2 C_b}{\partial y^2} \right) + \frac{D_T}{T_\infty} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + k_1 C_a C_b^2. \quad (7)$$

subject to the boundary conditions

$$u = 0, \quad v = 0, \quad T = T_w, \quad D_A \frac{\partial C_a}{\partial y} = k_s C_a,$$

$$D_B \frac{\partial C_b}{\partial y} = -k_s C_a \quad \text{at} \quad y = 0, \quad (8)$$

$$u \rightarrow u_e = ax \quad (a > 0), \quad T \rightarrow T_\infty, \quad C_a \rightarrow C_\infty, \quad C_b \rightarrow 0 \quad \text{as} \quad y \rightarrow \infty. \quad (9)$$

Fig. 1. Physical model and coordinate system

Within the boundary layer assumptions, we introduce the following similarity transformations and non-dimensional quantities

$$\begin{aligned} \psi(x, y) &= (av)^{1/2} x f(\eta), \quad u = ax f'(\eta), \\ v &= -\frac{\partial \psi}{\partial x} = -(av)^{1/2} f(\eta), \quad \theta(\eta) = \frac{T - T_\infty}{T_w - T_\infty}, \\ \xi(\eta) &= \frac{C_a}{C_\infty}, \quad \phi(\eta) = \frac{C_b}{C_\infty}, \quad \eta = \left(\frac{a}{v} \right)^{1/2} y. \end{aligned} \quad (10)$$

into Eqs.(3)-(7), the continuity equation(3) is satisfied automatically, and other equations are reduced to

$$f''' + f f'' + 1 - f'^2 = 0, \quad (11)$$

$$\frac{1}{Pr} \theta'' + Nb \phi' \theta' + Nt \theta'^2 + f \theta' = 0, \quad (12)$$

$$\frac{1}{Sc_A} \xi'' + f \xi' - K \xi \phi^2 = 0, \quad (13)$$

$$\frac{1}{\epsilon Sc_A} \left(\phi'' + \frac{Nt}{Nb} \theta'' \right) + f \phi' + K \xi \phi^2 = 0. \quad (14)$$

subject to the boundary conditions

$$\begin{aligned} f'(0) &= 0, \quad f(0) = 0, \quad \theta(0) = 1, \\ \xi'(0) &= K_s \xi(0), \quad \phi'(0) = -\epsilon K_s \xi(0), \\ f'(\infty) &= 1, \quad \theta(\infty) = 0, \quad \xi(\infty) = 1, \quad \phi(\infty) = 0, \end{aligned} \quad (15)$$

where

$$\begin{aligned} Pr &= \frac{\nu}{\alpha}, \quad Nb = \frac{\tau C_\infty D_B}{\nu}, \quad Nt = \frac{\tau D_T \Delta T}{\nu T_\infty}, \quad Sc_A = \frac{\nu}{D_A}, \\ \epsilon &= \frac{D_A}{D_B}, \quad K = \frac{k_1 C_\infty^2}{a}, \quad K_s = \frac{k_s}{D_A} \left(\frac{a}{v} \right)^{-1/2}. \end{aligned}$$

3 Results

In this part, the solution diversities are examined in detail. In the computation, we assume that the diffusion coefficients of chemical species A and B are of a comparable size,

which is not against real circumstance. In addition, the momentum equation and the energy equation have been studied by other researchers [19, 20]. And note that we can use the approximate relation $C_a + C_b = 1$ to get all results for $\phi(\eta)$, we therefore only consider $\xi(\eta)$ in this note.

In this paper, the reduced governing equations(11)-(14) with the boundary conditions(15) are solved by means of the shooting method associate with fourth order Runge-Kutta Scheme. The step size $\Delta\eta$ has to be adjusted for different values of the parameters to maintain the necessary accuracy. In our study, the value of $\Delta\eta$ between 0.001 and 0.01 were used, in order that the numerical values obtained are mesh in-dependent. On the other hand, a uniform grid of $\Delta\eta = 0.001$ was found to be satisfactory for a convergence criterion of 10^{-8} which gives accuracy to seven decimal place, in nearly all case.

As shown in Fig.2, the multiple solutions can be in existence for particular sets of the heterogeneous reaction rate K_s and the homogenous reaction rate K . As K_s is considerably small, the multiple solutions are possible for some values of K . When K_s increases gradually, the multiple solutions vanish. In other words, the range of K for existence of multiple solutions begins to appear and grows significantly as K_s continuously diminishes. Particularly, for $K = 0$, we notice that the maximum value of $\xi(0)$ approaches to 1 as K_s becomes negligibly small. We then examine the influence of the ratio of N_t/N_b on solution multiplicities. As shown in Fig.3, N_t/N_b can alter solution behaviour distinctly. For example, at $K_s = 0.025$, the multiple solutions could be possible (see Fig.2). While as N_t/N_b increases to a sufficiently large value, the multiple solutions start to be disappeared. We also notice that the maximum value of $\xi(0)$ increases as N_t/N_b enlarges. It is worth noting that we choose the parameter $\varepsilon = 1$ in Fig.3. When $N_t/N_b = 0$, our problem is simplified to Chaudhary and Merkin's work [2], and we can find that our figure is the same as Fig.1(c) of Chaudhary and Merkin's

Fig. 2. $\xi(0)$ against K with $Pr = 1, Nb = 1, Nt = 0.05, Sc = 1, \varepsilon = 1.5$ for some values of K_s .

Fig. 3. $\xi(0)$ against K with $Pr = 1, Nb = 1, K_s = 0.025, Sc = 1, \varepsilon = 1$ for different values of N_t .

Fig. 4. $\xi(0)$ against K_s with $Pr = 1, Nb = 1, Nt = 0.05, Sc = 1, \varepsilon = 1.5$ for different values of K .

work in the case $K_s = 0.025$.

Fig.4 exhibits the relation of K and K_s on solution diversifies. It is found that as the homogeneous reaction rate is weak enough, no multiple solutions are valid for any K_s . While as this value is considerably large, the solution bifurcations begin to appear. Note that the heterogeneous reaction rate K_s must be greater than or equal to zero to meet physical requirements. It is found from Fig.5, the ratio of the diffusion coefficient ε has effects on solution behaviours. For prescribed values of K , the multiple solutions come out for small ε . When ε becomes sufficient large, the multiple solutions vanish. We further notice that a tiny variation of ε can causes a significant increase of $\xi(0)$ when ε is sufficiently small. As ε is considerably large, $\xi(0)$ diminishes rapidly as

Fig. 5. $\xi(0)$ against ε with $Pr = 1$, $N_b = 1$, $N_t = 0.05$, $Sc = 1$, $K_s = 0.025$ for different values of K .

Fig. 6. $\xi(0)$ against N_t with $Pr = 1$, $Sc = 1$, $N_b = 1$, $\varepsilon = 1.5$, $K_s = 0.025$ for different values of K .

ε evolves. Fig. 6 illustrates the effect of N_t/N_b on $\xi(0)$. Similarly for some values of N_t/N_b , the multiple solutions are possible. While physically, N_t/N_b must be positive. Hence only dual solutions that could be physically realistic is expected for a range values of N_t/N_b . As N_t/N_b continuously grows, the multiple solutions disappear and only one solution can be found.

From the perspective of physical significance, we note that, the values of K, K_s and N_t/N_b have to be nonnegative. Moreover, the concentrations of C_a and C_b cannot be greater than 1. As a result, solutions in this range are physically realistic. On the other hand, as suggested by Chaudhary and Merkin [2, 3], for large value of K , the solution represents that the homogenous reactions are dominant. When K is s-

mall and K_s is positive, the heterogeneous (surface) reactions become important. We therefore can conclude both solutions are meaningful as all parameters are chosen physically realistic. In some special cases, for example $K = 0$, there is no homogeneous reaction, the system can still sustain a surface reaction with the concentration of reactant A having a value which below the ambient value C_∞ . When $K_s = 0$, there is no heterogeneous reaction on the surface, the homogeneous reaction is sufficiently strong to be self-sustaining even when there is a loss of reactant from the surface. This corresponds to having an endothermic homogeneous reaction. In other cases, both homogeneous reaction and heterogeneous reaction exist.

4 Conclusions

The homogeneous-heterogeneous reactions in boundary-layer nanofluid flow near a forward stagnation-point on a cylinder surface has been studied. The Chaudhary and Merkin's model [1] has been extended to nanofluids via Buongiorno's nanofluid model [15]. It is found that the homogeneous reaction rate parameter K , the heterogeneous reaction rate parameter K_s , the diffusivity ratio ε and the ratio N_t/N_b could leads to multiple solutions. In summary, the following conclusions can be reached:

1. The appropriate sets of K and K_s could produce multiple solutions. While solutions for negative K_s have no physical meanings;
2. The diffusivity ratio ε can affect solution behaviours to a large extent. For average values ε , triple solutions are expected;
3. N_t/N_b can cause solution diversifies. While the negative value of N_t/N_b has only mathematical meanings. Dual solutions can be found for positive values of N_t/N_b .

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Nomenclature

- A, B two different kinds of chemical species.
 C_a, C_b concentration of the chemical species A and B, respectively.
 C_∞ reference concentration of the chemical species A in external flow.
 D_A, D_B diffusion coefficient of chemical species A and B, respectively.
 D_T thermophoretic diffusion coefficient.
 f dimensionless velocity.
 k_1, k_s homogeneous and heterogeneous reaction rate constants, respectively.
 K homogeneous reaction rate parameter.
 K_s heterogeneous reaction rate parameter.
 Nb Brownian motion parameter.

Nt thermophoresis parameter.
 p pressure.
 Pr Prandtl number.
 T temperature.
 u, v velocity components in x and y directions, respectively.
 u_e free stream velocity.
 x, y coordinates.

Greek symbols

α thermal diffusivity.
 ε ratio of the diffusion coefficient
 ν kinematic viscosity.
 μ dynamic viscosity.
 ρ fluid density.
 τ ratio of the effective heat capacity of the nanoparticle to that of the fluid.
 τ_w shear stress.
 η similarity variable.
 $\theta(\eta)$ reduced temperature.
 $\xi(\eta)$ reduced concentration of chemical species A.
 $\phi(\eta)$ reduced concentration of chemical species B.
 ψ dimensionless stream function.

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