

SELF-SIMILAR PROBLEMS OF CONVECTIVE DIFFUSION IN THE PRESENCE OF HETEROGENEOUS CHEMICAL REACTIONS WITH ALLOWANCE FOR THERMAL DIFFUSION EFFECTS

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ABSTRACT: A number of studies have been made of the problem of the effect of a temperature gradient on mass transfer in a forced viscous fluid flow. The question of allowing for thermal diffusion effects has been examined in connection with flow around bodies [1-4], duct flow [5], and jet flows [6, 7]. Recently, in addition to the problem of thermal diffusion separation, the attention of investigators has been claimed by the problem of taking into account the effect of thermal diffusion on mass transfer in a convective flow in the presence of chemical reactions on the flow surfaces [4].*

1. Let a laminar flow of a viscous incompressible fluid containing a certain substance A flow around a body with a chemically active surface, on which the substance A engages in a heterogeneous chemical reaction with the material of the surface [8]. If the flow temperature T_0 and the surface temperature T_1 are different, mass transfer by thermal diffusion will occur.

We will consider the problem of taking into account thermal diffusion effects in the presence of heterogeneous chemical reactions with mixed kinetics. For flows in which the velocity component normal to the surface depends only on the coordinate normal to the surface this problem has a similar solution. We introduce an orthogonal coordinate system tied to the body, letting the coordinate surface $y = 0$ coincide with the surface of the body. The self-similar problem investigated is described by the following system of equations and boundary conditions:

$$\begin{aligned} -M\varphi\left(\frac{y}{N}\right)c_y' &= D\{c_{yy}'' + [\sigma c(1-c)T_y']_y\}, \\ -M\varphi\left(\frac{y}{N}\right)T_y' &= \chi T_{yy}'', \\ c(y) &= c_0, \quad T(y) = T_0 \quad \text{at } y = \infty, \end{aligned}$$

$$D\left[\frac{\partial c}{\partial y} + \sigma c(1-c)\frac{\partial T}{\partial y}\right] = kc^n, \quad T(y) = T_1 \quad \text{at } y = 0. \quad (1.1)$$

Here $c(y)$, $T(y)$ are the temperature and concentration at a given point in the flow, D , χ are the diffusion coefficient and thermal diffusivity, c_0 is the concentration remote from the body, k is the rate constant of the chemical reaction [$k = k_0 \exp(-S_a/T)$], the constants k_0 and S_a being determined by the specific form of the chemical reaction; σ is the Soret coefficient. The function $\varphi(y/N)$ and the constants M and N are found from the solution of the corresponding problem of the hydrodynamics of a viscous fluid. For the case of rotation of a disc at constant angular velocity ω (Karman problem) we have $M = (\omega\nu)^{1/2}$, $N = (\nu/w)^{1/2}$. The velocity component normal to the surface of the disc has the form $v_y = -M\varphi(y/N)$. The function $\varphi(y/N)$ is found by numerical solution of a system of ordinary differential equations [8].

In studying the problem of thermal-diffusion separation on impermeable surfaces, the author compared small-parameter methods and the method of approximation of the temperature distribution by a linear function [2, 3]. In the present case it is convenient to use the method of a linear approximation of the temperature distribution. In fluids the thermal Prandtl number is usually much smaller than the diffusion value; therefore it is natural to assume that the thermal layer is much thicker than the diffusion layer.

The heat transfer equation of system (1.1) is integrated in quadratures. We expand the solution obtained for the temperature distribution in a Maclaurin series, confining ourselves to the first two terms. After substituting this linear function in the diffusion part of problem (1.1), we obtain for low-concentration solutions [$c(1-c) \approx c$]

$$\begin{aligned} -S\varphi(\eta)c'_{\eta} &= c^n_{\eta\eta} + qc'_{\eta}; \quad c'_{\eta} + qc = pc^n \quad \text{for } \eta = 0, \\ c(\eta) &= c_0 \quad \text{for } \eta = \infty \\ \left(S = \frac{MN}{D}, \quad \eta = \frac{y}{N}, \quad q = \sigma(T_0 - T_1)\alpha(Q)\right), \\ Q &= \frac{MN}{\chi}, \quad p = \frac{kN}{D}, \\ \alpha(Q) &= \left[\int_0^{\infty} \exp\left(-Q \int_0^{\xi} \varphi(h) dh\right) d\xi\right]^{-1}. \end{aligned} \quad (1.2)$$

Integrating (1.2), we have

$$c(\eta) = c_0 \left[A \int_0^{\eta} \exp\left(-S \int_0^{\xi} \varphi(h) dh - q\xi\right) d\xi + B \right], \quad (1.3)$$

where the constants A and B are given by

$$\begin{aligned} A &= (1 - B)\beta(S, q), \quad \lambda B^n = B[q - \beta(S, q)] + \beta(S, q) \\ \beta(S, q) &= \left[\int_0^{\infty} \exp\left(-S \int_0^{\eta} \varphi(\xi) d\xi - q\eta\right) d\eta\right]^{-1}, \quad \lambda = pc_0^{n-1}. \end{aligned}$$

The algebraic equation for B can be solved rapidly. The mass flux at the surface is given by

$$j = kc^n|_{y=0} = kc_0^n B^n. \quad (1.5)$$

At large values of the thermal and diffusion Prandtl numbers, assuming $\varphi(\eta) = E\eta^2$ and taking into account the smallness of the quantity q , we obtain

$$\begin{aligned} \alpha(Q) &= \frac{QE^{1/3}}{3^{1/3}\Gamma(4/3)}, \\ \beta(S, Q) &= \frac{(SE)^{1/3}}{3^{1/3}\Gamma(4/3)} \left[1 + \frac{3^{1/3}\Gamma(5/3)q}{2\Gamma(4/3)(SE)^{1/3}} \right]. \end{aligned} \quad (1.6)$$

As an example of the use of the results obtained above we will consider the problem of allowing for thermal diffusion effects in the presence of first-order ($n = 1$) heterogeneous chemical reactions. From (1.4) and (1.5) it follows that

$$j = kc|_{y=0} = \frac{kc_0\beta(S, q)}{\lambda - q + \beta(S, q)}. \quad (1.7)$$

For large thermal and diffusion Prandtl numbers, considering the smallness of the quantity q , in the case of small λ we obtain

$$\frac{j - j_0}{j_0} = \sigma(T_0 - T_1)\gamma^{1/3} \quad \left(\gamma = \frac{D}{\chi}\right), \quad (1.8)$$

where j_0 is mass flux at the surface under isothermal conditions.

For large values of λ from (1.7) we have

$$\frac{j - j_0}{j_0} = \frac{\sigma(T_0 - T_1)\gamma^{1/3}\Gamma(5/3)}{2\Gamma^2(4/3)}. \quad (1.9)$$

*The author dealt with similar problems in his dissertation (Moscow State University, 1964).

A comparison of (1.8) and (1.9) shows that the relative influence of thermal diffusion on the mass flux is more strongly manifested at small values of the parameter λ , i.e., under conditions close to purely kinetic. Relations (1.8) and (1.9) show that at large values of the thermal and diffusion Prandtl numbers for cases of purely diffusion and purely chemical kinetics the relative variation of the mass flux at the surface does not depend on the shape of the surface and the hydrodynamic characteristics of the flow. The case of impermeable surfaces, the limiting case for small λ , was examined in [2, 3]. Below we consider the case of purely diffusion kinetics, the limiting case for large λ .

2. We will consider the problem of mass transfer in a plane laminar boundary layer in the presence of thermal diffusion effects. The diffusion and thermal Prandtl numbers will be assumed to be large. We introduce an orthogonal coordinate system tied to the body, letting the line $y = 0$ coincide with the contour of the body. This problem is described by the equations

$$u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \chi \frac{\partial^2 T}{\partial y^2},$$

$$u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} = \frac{\partial}{\partial y} \left\{ D \left[\frac{\partial c}{\partial y} + \sigma c (1 - c) \frac{\partial T}{\partial y} \right] \right\}, \quad (2.1)$$

the relations

$$u(x, y) = \tau(x) y / \mu, \quad v = -\tau'(x) y^2 / 2\mu, \quad (2.2)$$

and the boundary conditions

$$\begin{aligned} T(x, 0) &= T_1, & c(x, 0) &= 0, \\ c(x, \infty) &= T_0, & c(x, \infty) &= c_0, \\ T(0, y) &= T_0, & c(0, y) &= c_0. \end{aligned} \quad (2.3)$$

Here $u(x, y)$, $v(x, y)$ are the velocity components, $T(x, y)$ the temperature, $c(x, y)$ the concentration, $\tau(x)$ the friction stress at the surface, and μ the coefficient of dynamic viscosity. Problem (2.1)–(2.3) is self-similar. Setting

$$T = T(\eta), \quad c = c(\eta), \quad \eta = \varphi t^{-1/3}, \quad \varphi = \frac{\tau^{1/2}(x) y}{2^{1/2} \mu^{1/2}},$$

$$t = (8\mu)^{-1/2} \int_0^x \tau^{1/2}(\xi) d\xi, \quad M = (3D)^{-1}, \quad N = (3\chi)^{-1} \quad (2.4)$$

we obtain the following system:

$$-M\eta^2 c_{\eta\eta}' = [c_{\eta\eta}' + \sigma c(1-c)T_{\eta\eta}']_{\eta}, \quad -N\eta^2 T_{\eta\eta}' = T_{\eta\eta}''$$

$$c(0) = 0, \quad T(0) = T_1; \quad c(\infty) = c_0, \quad T(\infty) = T_0. \quad (2.5)$$

At low concentrations we may assume that $c(1-c) \approx c$.

We introduce the new variable $z = N^{1/3} \eta$; we expand the function $T(z)$, giving the solution of the thermal part of the problem (2.5), in a Maclaurin series, confining ourselves to the first two terms. After substituting the thus determined linear approximation of the temperature distribution function in the diffusion part of problem (2.5), we obtain

$$\gamma^{-1} z^2 c_z' = c_{zz}'' + q c_z', \quad c(0) = 0, \quad c(\infty) = c_0$$

$$\left(\gamma = \frac{H}{M} = \frac{D}{\chi}, \quad q = \frac{\sigma(T_0 - T_1)}{3^{1/2} \Gamma(4/3)} \right). \quad (2.6)$$

Integrating (2.6), we find

$$c(z) = c_0 \delta(\gamma, q) \int_0^z \exp\left(-\frac{\xi^3}{3\gamma} - q\xi\right) d\xi,$$

$$\delta(\gamma, q) = \left[\int_0^{\infty} \exp\left(-\frac{\xi^3}{3\gamma} - q\xi\right) d\xi \right]^{-1}. \quad (2.7)$$

The mass flux at the surface

$$j = \frac{D c_0 \delta(\gamma, q) \sqrt{\tau(x)}}{\sqrt{2\mu} (3\chi)^{1/3}} \left(\frac{1}{\sqrt{8\mu}} \int_0^x \sqrt{\tau(\xi)} d\xi \right)^{-1/3}. \quad (2.8)$$

We form the ratio of the mass flux at the surface with allowance for thermal diffusion to the mass flux under isothermal conditions. From (2.8) we have

$$j/j_0 = \delta(\gamma, q) / \delta(\gamma, 0). \quad (2.9)$$

It follows from (2.9) that the ratio j/j_0 does not depend on the shape of the surface and the hydrodynamic characteristics of the flow. In view of the smallness of the quantity q , we obtain

$$\frac{j-j_0}{j_0} = \frac{\sigma(T_0 - T_1) \gamma^{1/3} \Gamma(2/3)}{2\Gamma^2(4/3)}. \quad (2.10)$$

Thus, relation (1.9) is valid over a quite wide range of flows. The author thanks G. I. Barenblatt for his interest and advice.

REFERENCES

1. V. C. Liu, "On the separation of gas mixtures by suction of thermal-diffusion boundary layer," *Quart. J. Mech. and Appl. Math.*, vol. 12, part 1, 1959.
2. A. M. Suponitskii, "Calculation of thermal diffusion in a laminar incompressible viscous fluid flow at large Prandtl numbers," *PMTF*, no. 2, 1962.
3. A. M. Suponitskii, "Calculation of thermal diffusion in a laminar viscous fluid flow at moderate values of the thermal and diffusion Prandtl numbers," *PMTF*, no. 5, 1963.
4. V. G. Levich, V. S. Markin, and Yu. S. Chirkov, "Thermal diffusion in liquids at the surface of a rotating disc," *Elektrokimiya*, 1, no. 12, 1965.
5. J. C. R. Turner, "Thermal diffusion with laminar flow in a duct. A theoretical solution and practical results," *Chem. Eng. Sci.*, vol. 17, Febr. 1962.
6. V. P. Kashkarov, "Diffusion boundary layer in a semibounded jet," *Izv. AN SSSR, Mekhanika i mashinostroenie*, no. 6, 1964.
7. H. Thomann and J. R. Baron, "Experimental investigation of thermal diffusion effects in laminar and turbulent shear flow," *Heat and Mass Transfer.*, vol. 8, 1965.
8. V. G. Levich, *Physico-Chemical Hydrodynamics* [in Russian], Fizmatgiz, 1959.

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