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Mathematics of thermal diffusion in an exponential temperature field

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ABSTRACT

The Ludwig-Soret effect, also known as thermal diffusion, refers to the separation of gas, liquid, or solid mixtures in a temperature gradient. The motion of the components of the mixture is governed by a nonlinear, partial differential equation for the density fractions. Here solutions to the nonlinear differential equation for a binary mixture are discussed for an externally imposed, exponential temperature field. The equation of motion for the separation without the effects of mass diffusion is reduced to a Hamiltonian pair from which spatial distributions of the components of the mixture are found. Analytical calculations with boundary effects included show shock formation. The results of numerical calculations of the equation of motion that include both thermal and mass diffusion are given.

1. Introduction

Thermal diffusion, also known as the Soret effect or Ludwig-Soret effect is a process whereby mixtures separate in response to an imposed temperature gradient [1,2]. The separation is known to take place in gases, liquids, and even solids, but is typically small. When the temperature distribution in space is specified and the contribution of the Dufour effect to the dynamics of thermal diffusion is ignored [3], the equation governing the time dependence of one of the normalized density fractions c in a binary mixture is given by

$$\frac{\partial c}{\partial t} = \nabla \cdot [c(1-c)D_T \nabla T] + D\nabla^2 c, \tag{1}$$

where D_T is the thermal diffusion coefficient, D is the mass diffusion coefficient, T is the temperature, and t is the time [3]. The solution to this equation for a sinusoidal temperature gradient, as has been discussed in Ref. [4–6], shows that the underlying motion of c for a positive thermal diffusion coefficient is accumulation at regions where there are temperature minima followed by formation of a pair of counter-propagating shocks whose fronts are smoothed by the effects of mass diffusion. The extent to which the shocks are qualitatively discernible was shown to be dependent on the relative magnitudes of D_T and D. Further investigation of the Ludwig-Soret effect for a linear temperature field in one dimension [7,8] showed that Eq. (1) can be reduced to the heat diffusion equation through use of the Hopf-Cole transformation, thus giving an exact, closed form solution for the motion of the components of a binary mixture.

This paper shows in the first section, Analytical Solutions with Mass Diffusion Neglected, that the Ludwig-Soret equation can be reduced to a Hamiltonian pair and that the motion of the components can be determined away from the origin. As well, the effects of a boundary at the origin are treated showing formation of shock waves. The section entitled Numerical Calculation gives solutions to the nonlinear Ludwig-Soret equation using the discontinuous Galerkin finite element method with mass diffusion included. The time evolution of density fractions which are initially Gaussian in space, distant from the origin is given as well.

2. Analytical solutions with mass diffusion neglected

Consider thermal diffusion acting on an initially uniform density fraction distribution in space having a value c_0 in an exponential temperature field that extends from the origin along the positive z axis according to $T = T_0 e^{-\bar{\alpha} z}$, where $\bar{\alpha}$ is a spatial decay constant and T_0 is a temperature. The temperature T can be written in terms of a dimensionless temperature $\widehat{T} = e^{-\zeta}$, where ζ is a dimensionless coordinate defined as $\zeta = \bar{\alpha} z$. Eq. (1) for the Ludwig-Soret effect in one dimension for $\zeta > 0$ thus reduces to

$$\frac{\partial c}{\partial \tau} = -\alpha \frac{\partial}{\partial \zeta}[c(1-c)e^{-\zeta}] + \frac{\partial^2 c}{\partial \zeta^2}, \tag{2}$$

where the thermal diffusion factor α is given as $\alpha = S_T T_0$ ($S_T = D_T/D$ is the Soret coefficient) and a dimensionless time has been defined as $\tau = D\bar{\alpha}^2 t$.

To determine the underlying motion of c, Eq. (2) can be studied without the effects of mass diffusion which corresponds to the sec-

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ond spatial derivative of c, giving the equation of motion for $\zeta > 0$ as

$$\frac{\partial c}{\partial \tau} = -\alpha \frac{\partial}{\partial \zeta}[c(1-c)e^{-\zeta}], \tag{3}$$

which, by introducing the flux function

$$f(c,\zeta) = \alpha c(1-c)e^{-\zeta}, \tag{4}$$

gives

$$\frac{\partial c}{\partial \tau} = -\frac{\partial f}{\partial c}\frac{\partial c}{\partial \zeta} - \frac{\partial f}{\partial \zeta}. \tag{5}$$

Eq. (5) can be solved by regarding c and ζ as two independent variables, that is, $c = c(\zeta(\tau),\tau)$ and $\zeta = \zeta(\tau)$. The total differential of c can be written as

$$\frac{\partial c}{\partial \tau} = -\frac{\partial c}{\partial \zeta}\frac{d\zeta}{d\tau} + \frac{dc}{d\tau}. \tag{6}$$

Equating various terms in Eqs. (5) and (6) gives the Hamiltonian system,

$$\frac{d\zeta}{d\tau} = \frac{\partial f(c,\zeta)}{\partial c}$$
$$\frac{dc}{d\tau} = -\frac{\partial f(c,\zeta)}{\partial \zeta}, \tag{7}$$

where (ζ, c) constitutes a pair of canonical coordinates and f acts as the Hamiltonian. For the present problem, Eq. (7) gives the equations of motion for the position ζ and the density fraction c as

$$\frac{d\zeta}{d\tau} = \alpha(1-2c)e^{-\zeta}$$
$$\frac{dc}{d\tau} = \alpha c(1-c)e^{-\zeta}. \tag{8}$$

A Hamiltonian field plot for f is given in Fig. 1. The slopes of the vectors $dc/d\zeta$can be found by division of the second of Eq. (8) by the first giving

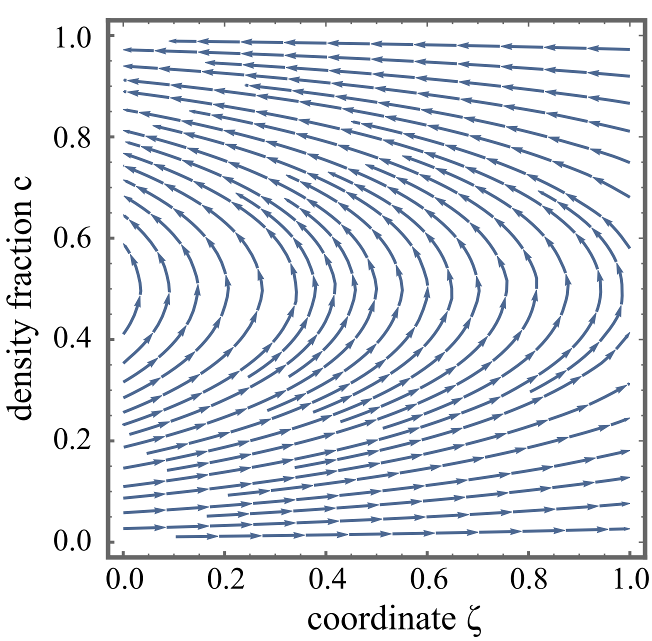

Fig. 1. Hamiltonian field plot $\{\partial f/\partial c, -\partial f/\partial \zeta\}$ of c versus ζ for the flux function f in Eq. (4) calculated with $\alpha = 10$. For negative values of α, the directions of arrows are reversed.

$$\frac{dc}{d\zeta} = \frac{c(1-c)}{1-2c}, \tag{9}$$

with the differential directions of the components in time of each vector determined by multiplication of Eq. (8) by $d\tau$. For any point in the (ζ, c) plane, the Hamiltonian field plot shows its direction in time, giving an indication of the time development of any initial distribution of c in space.

The total differential of the flux is $df = -\alpha(2c-1)\exp(-\zeta)dc - \alpha c(1-c)\exp(-\zeta)d\zeta$, which, when combined with Eq. (9), shows that f is a constant of the motion along the lines defined by Eq. (9), as expected for a Hamiltonian system since f does not explicitly depend on τ. Hence, any point in the (ζ, c) plane moves in time from an initial point (ζ_0, c_0) to a new point (ζ, c) as governed by

$$\alpha c(1-c)e^{-\zeta} = \alpha c_0(1-c_0)e^{-\zeta_0}. \tag{10}$$

By solving Eq. (10) for a point originally at (ζ_0, c_0), the new values of c and ζ can be found to obey the following expression

$$\zeta = -\ln\left[\frac{c_0(1-c_0)e^{-\zeta_0}}{c(1-c)}\right]. \tag{11}$$

As the flux function is a constant of the motion and is identical to the right hand side of the second of Eq. (8), it follows that $c - c_0 = k\tau$, where k is the value of f at some initial point and time. Hence, for any initial point (ζ_0, c_0), after a time τ the new density fraction and coordinate are given by

$$c(\tau) = c_0 + \alpha\tau\beta$$
$$\zeta(\tau) = -\ln\left[\frac{\beta}{[c_0+\alpha\tau\beta][1-(c_0+\alpha\tau\beta)]}\right], \tag{12}$$

where $\beta = c_0(1-c_0)e^{-\zeta_0}$. By eliminating β from Eq. (12), c can be expressed as a function of τ and ζ in the form

$$c(\zeta,\tau) = \frac{-e^{\zeta} + \alpha\tau + \sqrt{e^{2\zeta} + 4\alpha\tau(c_0 - \frac{1}{2})e^{\zeta} + \alpha^2\tau^2}}{2\alpha\tau}. \tag{13}$$

A density fraction distribution versus coordinate at a single value of τ calculated from Eq. (13) is shown in Fig. 2 (dotted curve). Note that the area beneath c at $\tau = 5$ is larger than the area of the initial

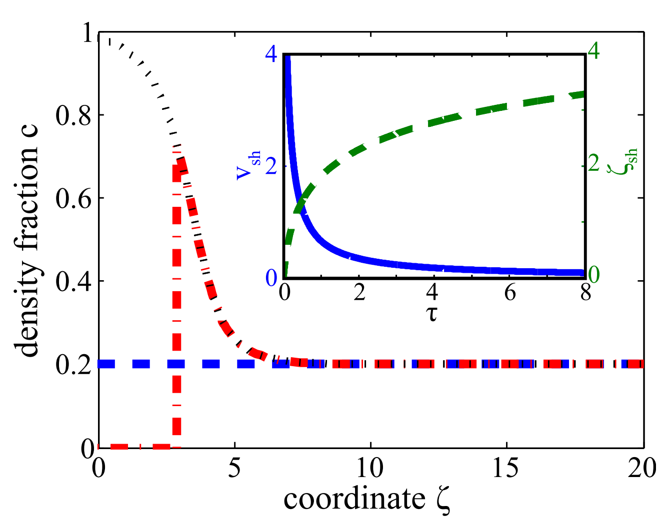

Fig. 2. Density fraction c versus coordinate ζ for an initially uniform density distribution with $c_0 = 0.2$ (flat line). The dotted curve shows the direct calculation result from Eq. (13) with $\alpha = 10$ at $\tau = 5$. The dashed curve shows shows c with shock formation originating from the effect of the boundary. Inset: Shock front position ζ_{sh} (dashed curve) and shock speed v_{sh} (solid curve) versus time τ with $\alpha = 10$.