

Evaporation and Condensation Flows of a Vapor-Gas Mixture from or onto the Condensed Phase with an Internal Structure

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Abstract. Transient motions of a vapor-gas mixture due to the evaporation and condensation processes from or onto the plane condensed phase with a temperature field as its internal structure have been studied numerically based on the Boltzmann equation of BGK type for a binary gas mixture. The condition of the continuity of the energy flow across the interface surface has to be imposed in addition to the conditions at the surface of the condensed phase without the internal structure because the temperature of the surface in this case becomes an unknown parameter to be determined as part of the solution. The transient flow fields of the mixture occur owing to the phase change processes caused by the continuous change in temperature of the surface of the condensed phase. The effects of the internal structure of the condensed phase coupled with the presence of a noncondensable gas, which is small in amount here, on the transition process of the transient flow fields and, hence, the formation and the propagation of the shock waves and the contact regions may clearly be recognized. Some of the features of the present flows are that 1) the maxima of the mass and energy flows may exist at a certain value of the latent heat parameter, the phenomenon of which may be ascribed to the coupling effects of the latent heat parameter and the existence of the internal structure of the condensed phase; 2) the *negative mass flow* appears in a short period of time during the transitional state of the flow fields when the latent heat parameter is extremely small. However, it disappears soon as time goes on. These two phenomena, which are affected here by the presence of a noncondensable gas, are also found in a pure-vapor case.

INTRODUCTION

Phase-change phenomena and flow problems associated with these processes are not only of theoretical interest in gas dynamics but also of practical importance because they do have wide applications in various thermo-fluid engineering fields. Such problems, however, are the ones to which the ordinary continuum-based fluid dynamics is not directly applicable because of the existence of a nonequilibrium region called the Knudsen layer in the close vicinity of the condensed phase. The existence of this region can never be neglected in any problems of such kind even in the continuum limit. The analyses of these problems, therefore, must necessarily be based on the kinetic equation because it is this nonequilibrium region that is responsible for the phase-change processes to occur. However, the kinetic equation is complex and difficult to deal with and the analyses based on this equation, regardless of whether they are theoretical or numerical, impose us a great burden. Moreover, when the gas phase is a mixture consisting of a condensable and noncondensable gases, the problems become more complex. In spite of this, a large number of evaporation and condensation problems have been studied so far not only for pure-vapor cases but also for gas mixture cases (see e.g., the proceedings of the Rarefied Gas Dynamics Symposia) based on the kinetic equation and a fairly large amount of the useful information and knowledge has been obtained. Among others, it would be worth noting from the practical point of view that the noncondensable gas, especially when it is of small amount, is driven toward the interface and accumulate near there, forming an extremely large spacial gradient of the density leading to the great hindrance of the phase change processes [1]. However, the analyses so far are all confined to systems in which the condensed phases have no internal structures except a recent work by Onishi and Yamada [2], who treated a half-space problem of a pure-vapor case based on the Boltzmann equation of BGK type [3]. They considered a temperature field as the internal structure of the condensed phase and studied its effects on the flow fields of the vapor. The consideration of the internal structure within the condensed phase may give us practically important information on flow fields within heat and energy exchange or transfer systems such as heat pipes. Especially for mixture cases containing a small amount of noncondensable gas, the effects of the internal structure coupled with the presence of the

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noncondensable gas would become very important and should be studied because the practical heat and energy transfer systems, initially free from noncondensable gases, would eventually be contaminated by them during the course of their operation.

Therefore, we here try to study the effects of the internal structure of the condensed phase on the flow fields of a mixture, particularly the flow fields of a condensable gas in the presence of a small amount of noncondensable gas. Actually, we take up simple flow fields of a mixture due to evaporation and condensation processes from or onto the plane condensed phase with a temperature field as its internal structure. For this analysis, the equation of heat conduction with constant substance properties is used for the temperature field within the condensed phase, and for the motions of the mixture gas phase the Boltzmann equation of BGK type proposed by Hamel [4] is used subject to the diffusive type of boundary conditions with the parameter (called the *imperfection parameter* here) first introduced by Wortberg and his co-workers [5] incorporated together with the condition of the continuity of energy flow across the interface.

GOVERNING KINETIC EQUATIONS

Consider a two phase system of a gas phase and the condensed phase with finite thermal conductivity. Let the interface surface of the condensed phase be at $x = 0$ and the other end surface at $x = -D$. The gas phase, which occupies the half-space ($x > 0$), consists of a condensable gas (*A*-gas) and a noncondensable gas (*B*-gas). Initially, the condensed phase and the mixture gas phase are in complete equilibrium at a temperature T_0 . Let the pressure and the number density (or density) of the component gas at this state be P_0^s and N_0^s (or ρ_0^s), respectively. The superscript s denotes *A*-gas for $s = A$ and *B*-gas for $s = B$. Suppose that at a certain time, say $t = 0$, the temperature of the edge surface of the condensed phase at $x = -D$, which is initially T_0 , is suddenly changed to T_c . The heat flow then occurs through the condensed phase and after a certain elapse of time the temperature of the interface surface starts to be changing with time. This leads to the onset of the phase change process at the interface of the condensed phase, giving then rise to a transient motion of the mixture gas phase.

Now, for the temperature field within the condensed phase, the equation of heat conduction with constant substance properties

$$\frac{\partial \tilde{T}}{\partial t} - \kappa_c \frac{\partial^2 \tilde{T}}{\partial x^2} = 0 \quad (1)$$

holds for $-D < x < 0$, where t is the time; x is the coordinate; κ_c is the thermal diffusivity of the condensed phase, which is here assumed to be constant for simplicity, and \tilde{T} represents the temperature field within it. For the description of the motions of the gas mixture in the present problem, on the other hand, the Boltzmann equation of BGK type [4] is used, which may be written as

$$\frac{\partial f^s}{\partial t} + \xi_x \frac{\partial f^s}{\partial x} = N^s \kappa_{ss} (F_e^s - f^s) + N^t \kappa_{st} (F_e^{st} - f^s) \quad (2)$$

$$\left[\begin{array}{c} N^s \\ N^s u^s \\ \frac{3}{2} N^s k T^s \end{array} \right] = \iiint \left[\begin{array}{c} 1 \\ \xi_x \\ \frac{1}{2} m_s [(\xi_x - u^s)^2 + \xi_y^2 + \xi_z^2] \end{array} \right] f^s d\xi_x d\xi_y d\xi_z \quad (3)$$

$$F_e^s = \frac{N^s}{(2\pi R_s T^s)^{3/2}} \exp \left\{ -\frac{(\xi_x - u^s)^2 + \xi_y^2 + \xi_z^2}{2R_s T^s} \right\} \quad (4)$$

$$F_e^{st} = \frac{N^s}{(2\pi R_s T^{st})^{3/2}} \exp \left\{ -\frac{(\xi_x - u^{st})^2 + \xi_y^2 + \xi_z^2}{2R_s T^{st}} \right\} \quad (5)$$

$$u^{st} = u^{ts} = \mu_s u^s + \mu_t u^t, \quad T^{st} = T^s + 2\mu_s \mu_t (T^t - T^s) + \frac{m_s}{3k} \mu_t^2 (u^t - u^s)^2, \quad \mu_s = \frac{m_s}{m_s + m_t} \quad (6)$$

where s appearing as superscript and subscript refers to *A* or *B* and t refers to *B* or *A*. (ξ_x, ξ_y, ξ_z) is the molecular velocity vector; f^s , N^s , u^s , T^s and $P^s (= N^s k T^s)$ are, respectively, the distribution function, the number density, the mean flow velocity, the temperature and the partial pressure of s -component gas; F_e^s and F_e^{st} are the local Maxwellian distributions for molecules of s -component gas characterized by the macroscopic quantities (N^s, u^s, T^s)

and (N^s, u^{st}, T^{st}) , respectively; m_s is the molecular mass of s-gas; $R_s = k/m_s$ is the gas constant per unit mass, k being the Boltzmann constant. $N^s \kappa_{ss}$ and $N^l \kappa_{sl}$ represent the number of collisions per unit time of a molecule of s-gas due to the self and cross collisions, respectively, thus $N^s \kappa_{ss} + N^l \kappa_{sl}$ being the average collision frequency for a molecule of s-gas irrespective of its collision partners. The collision frequencies are related to the transport coefficients of the mixture and its component gases and, hence, κ_{ss} and κ_{sl} ($= \kappa_{ls}$), which are assumed to be constant and of the same order of magnitude, can be evaluated from these coefficients at some equilibrium reference state (see e.g., Hamel [4]), say at infinity, as

$$\left. \begin{aligned} \eta^M &= \frac{P_0^A}{N_0^A \kappa_{AA} + N_0^B \kappa_{AB}} + \frac{P_0^B}{N_0^A \kappa_{AB} + N_0^B \kappa_{BB}}, & \eta^s &= \frac{P_0^s}{N_0^s \kappa_{ss}}, & \lambda^s &= \frac{5}{2} R_s \eta^s \\ D_{AB} &= \frac{(m_A + m_B) k T_0}{m_A m_B N_0 \kappa_{AB}} & (N_0 &= N_0^A + N_0^B) \end{aligned} \right\} \quad (7)$$

where η^M and D_{AB} are the viscosity and the diffusion coefficients of the mixture, respectively, η^s and λ^s being the viscosity and thermal conductivity of s-gas.

Once the distribution function f^s is obtained, the normal stress τ_{xx}^s , the energy flux E^s of s-gas can be calculated from

$$\left. \begin{aligned} \tau_{xx}^s &= -m_s \iiint (\xi_x - u^s)^2 f^s d\xi_x d\xi_y d\xi_z \\ E^s &= \frac{1}{2} m_s \iiint \xi_x (\xi_x^2 + \xi_y^2 + \xi_z^2) f^s d\xi_x d\xi_y d\xi_z \end{aligned} \right\} \quad (8)$$

Now, as the initial conditions for the present problem, we have

$$\left. \begin{aligned} \tilde{T} &= T_0 & \text{for } -D \leq x \leq 0 \\ f^s &= \frac{N_0^s}{(2\pi R_s T_0)^{3/2}} \exp\left\{-\frac{\xi_x^2 + \xi_y^2 + \xi_z^2}{2R_s T_0}\right\} & \text{for } x > 0 \end{aligned} \right\} \quad (9)$$

for the temperature of the condensed phase and for the distribution function of the component s-gas, respectively. As to the boundary conditions, we have on the edge of the condensed phase

$$\tilde{T} = T_c \quad \text{at } x = -D. \quad (10)$$

At infinity ($x \rightarrow \infty$), the condition for the distribution function f^s of the component gas remains to be the same as that given by Eq. (10) but for $\xi_x < 0$. However, at the interface surface of the condensed phase ($x = 0$), we have

$$\left. \begin{aligned} \tilde{T} &= T_W \\ f^A &= \frac{\tilde{N}_W^A}{(2\pi R_A T_W)^{3/2}} \exp\left\{-\frac{\xi_x^2 + \xi_y^2 + \xi_z^2}{2R_A T_W}\right\} & \text{for } \xi_x > 0 \\ \tilde{N}_W^A &= \alpha_c N_W^A + (1 - \alpha_c) N_D^A & (0 \leq \alpha_c \leq 1) \\ N_W^A &= \frac{P_W^A}{k T_W}, & \frac{P_W^A}{P_0^A} &= \exp\left\{-\Gamma \left(\frac{T_0}{T_W} - 1\right)\right\} & \left(\Gamma \equiv \frac{h_L}{R_A T_0}\right) \\ N_D^A &= -\frac{2\sqrt{\pi}}{(2R_A T_W)^{1/2}} \iiint_{\xi_x < 0} \xi_x f^A d\xi_x d\xi_y d\xi_z \\ f^B &= \frac{N_W^B}{(2\pi R_B T_W)^{3/2}} \exp\left\{-\frac{\xi_x^2 + \xi_y^2 + \xi_z^2}{2R_B T_W}\right\} & \text{for } \xi_x > 0 \\ N_W^B &= -\frac{2\sqrt{\pi}}{(2R_B T_W)^{1/2}} \iiint_{\xi_x < 0} \xi_x f^B d\xi_x d\xi_y d\xi_z \\ -\lambda_c \frac{\partial \tilde{T}}{\partial x} &= E^A + E^B + \rho^A u^A (h_L - c_p^A T^A) \end{aligned} \right\} \quad (11)$$

where \tilde{N}_W^A and N_W^B represent the number densities of the molecules of A-gas and B-gas, respectively, leaving the interface surface after the interaction with it. T_W is the temperature of the interface surface of the condensed phase and is a function of time to be determined as a part of the solution. λ_c is the thermal conductivity of the condensed phase. h_L is the latent heat of vaporization per unit mass of the condensable gas and c_p^A is its specific heat at constant pressure. The parameter α_c represents a fraction of the molecules of condensable A-gas emitted from the interface with an equilibrium number density N_W^A , whereas $1 - \alpha_c$ represents the remaining fraction of the molecules reflected from the interface as if they were noncondensable gas molecules. It is a parameter associated with a certain kind of the imperfectness of the interface first introduced by Wortberg and his co-workers [5] in their experimental and approximate analytical studies on this kind of problems, and here it is called the *imperfectness* parameter. N_W^A is an equilibrium number density, which is a unique function of T_W , and is given here as the saturated vapor number density corresponding to T_W given by the Clapeyron-Clausius relation (see e.g., Landau and Lifshitz [6]). P_W^A is the saturated vapor pressure corresponding to T_W just as P_0^A is to T_0 . Γ is a non-dimensional parameter, which is here called the latent heat parameter. The other quantity N_D^A , which is the number density for molecules of A-gas reflected from the interface as if they were noncondensable gas molecules, is determined by the condition of *no net mass flow* across the interface. N_W^B is also determined by the condition of *no net mass flow* of the molecules of the noncondensable B-gas across the interface. N_D^A and N_W^B are both unknown quantities to be obtained as part of the solution.

Now, let us introduce here the length scale L and time scale τ_0^A for the present problem defined, respectively, by

$$L \equiv \frac{\sqrt{\pi}}{2} l_0^A \quad \text{and} \quad \tau_0^A \equiv \frac{L}{(2R_A T_0)^{1/2}} = \frac{l_0^A}{(8R_A T_0/\pi)^{1/2}} \quad \text{with} \quad l_0^A = \frac{(8R_A T_0/\pi)^{1/2}}{N_0^A \kappa_{AA} + N_0^B \kappa_{AB}} \quad (12)$$

where l_0^A is the mean free path of the molecules of the condensable A-gas at the initial state and, therefore, τ_0^A represents their mean collision time. With these scales, the appropriate nondimensionalization of the set of the governing equations, initial and boundary conditions gives us the following parameters which characterize the motions of the mixture and its component gases:

$$\frac{T_c}{T_0}, \quad \frac{D}{L}, \quad \frac{\lambda_c}{\lambda_0^A}, \quad \frac{\kappa_c}{\kappa_0^A}, \quad \Gamma, \quad \frac{N_0^B}{N_0^A}, \quad \frac{m_B}{m_A}, \quad \frac{\kappa_{AB}}{\kappa_{AA}}, \quad \frac{\kappa_{BB}}{\kappa_{AA}}, \quad \alpha_c \quad (13)$$

where λ_0^A and κ_0^A are the thermal conductivity and the thermal diffusivity of the condensable gas at the initial state, respectively, κ_0^A being defined by $\kappa_0^A \equiv \lambda_0^A / (\rho_0^A c_p^A)$. The specification of the above parameters gives the flow field as functions of t/τ_0^A and x/L .

In order to make the numerical analysis of the present problem easier, the following new functions

$$\left[\begin{array}{c} g^s \\ G^s \\ G^{st} \end{array} \right] \equiv \iint \left[\begin{array}{c} f^s \\ F_e^s \\ F_e^{st} \end{array} \right] d\xi_y d\xi_z \quad \text{and} \quad \left[\begin{array}{c} h^s \\ H^s \\ H^{st} \end{array} \right] \equiv \iint (\xi_y^2 + \xi_z^2) \left[\begin{array}{c} f^s \\ F_e^s \\ F_e^{st} \end{array} \right] d\xi_y d\xi_z \quad (14)$$

have also been introduced here (see e.g., Chu [7]). Rewriting the original equations with these new variables, we then obtain the simultaneous equations for the four unknown functions (g^A, h^A, g^B, h^B) of three independent variables (t, x, ξ_x) instead of having two unknown functions (f^A, f^B) of five independent variables ($t, x, \xi_x, \xi_y, \xi_z$).

RESULTS AND DISCUSSION

Actual calculations have been carried out based on a simple difference scheme for more than 20 cases, setting $D/L = 20.0$ and $\kappa_{AA} = \kappa_{AB} = \kappa_{BB}$, for simplicity. Several of these cases will be discussed here. For this discussion, the fluid dynamic quantities of the mixture P, N, ρ, E, u and T , which are defined by

$$P = P^A + P^B, \quad N = N^A + N^B, \quad \rho = \rho^A + \rho^B, \quad E = E^A + E^B, \quad u = \frac{\rho^A}{\rho} u^A + \frac{\rho^B}{\rho} u^B, \quad T = \frac{N^A}{N} T^A + \frac{N^B}{N} T^B \quad (15)$$

are also introduced. The corresponding quantities with suffix 0 represent the values at the initial state (hereafter, the same applies to the other quantities). c_0^s is the sound speed of s-gas at the initial state defined by $c_0^s \equiv (\gamma R_s T_0)^{1/2}$.

Incidentally, the corresponding sound speed of the mixture c_0 is $c_0 \equiv (\gamma RT_0)^{1/2} = c_0^A (R/R_A)^{1/2}$, R being the gas constant per unit mass of the mixture given by $R \equiv (\rho_0^A/\rho_0)R_A + (\rho_0^B/\rho_0)R_B$.

One of the typical transient flow fields due to evaporation process at the interface surface is shown in Fig. 1 in terms of the temperature distributions and in Fig. 2 in terms of the pressures of the mixture and its component gases. Figure 1 shows how the jump in temperature occurring at the interface varies with time and how the temperature distribution is being formed in the flow field owing to the propagation of the produced shock wave followed by the contact region. Specifically, the right figure shows the transition of a shock wave with time and at about $t/\tau_0^A = 2000$ the shock wave almost fully establishes itself, although the rear portion of it, which is still curved, is being augmented gradually by the continuous overtaking of the compression waves produced at the interface (cf. Onishi and Yamada [2]). The magnitude of the temperature jumps first increases from zero and then approaches a constant value

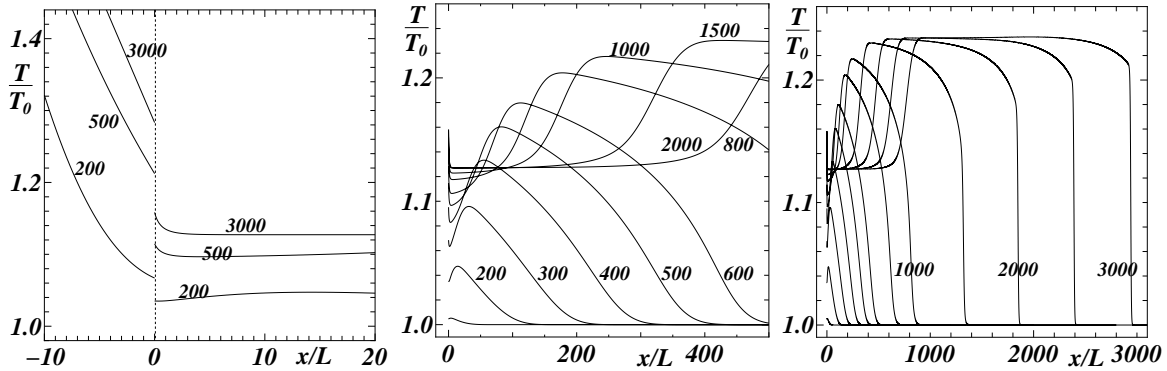


FIGURE 1. Transient distributions of the temperature of the mixture due to the evaporation process at the interface at $x = 0$. $T_c/T_0 = 2.0$, $D/L = 20.0$, $\lambda_c/\lambda_0^A = 50.0$, $\kappa_c/\kappa_0^A = 0.5$, $\Gamma = 5.0$, $N_0^B/N_0^A = 0.01$, $m_B/m_A = 2$, $\kappa_{AA} = \kappa_{AB} = \kappa_{BB}$ and $\alpha_c = 1.0$. The numbers in the figures indicate the time t/τ_0^A . Note that the scales of abscissa of the three figures are different. $T/T_0|_{x=0} = 1.0349$ at $t/\tau_0^A = 200$; $T/T_0|_{x=0} = 1.1146$ at $t/\tau_0^A = 500$; $T/T_0|_{x=0} = 1.1519$ at $t/\tau_0^A = 1000$; $T/T_0|_{x=0} = 1.1584$ at $t/\tau_0^A = 3000$.

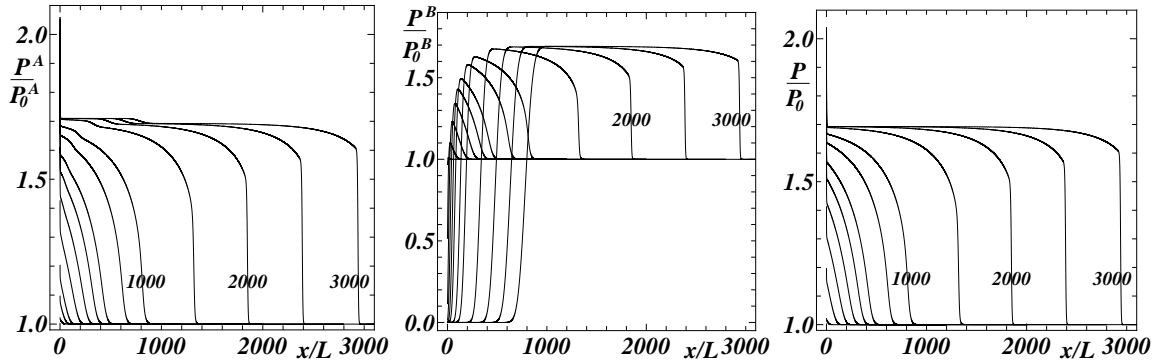


FIGURE 2. Transient distributions of the pressures of the mixture and its component gases due to the evaporation process at the interface at $x = 0$. $T_c/T_0 = 2.0$, $D/L = 20.0$, $\lambda_c/\lambda_0^A = 50.0$, $\kappa_c/\kappa_0^A = 0.5$, $\Gamma = 5.0$, $N_0^B/N_0^A = 0.01$, $m_B/m_A = 2$, $\kappa_{AA} = \kappa_{AB} = \kappa_{BB}$ and $\alpha_c = 1.0$. The numbers in the figures indicate the time t/τ_0^A . $P^A/P_0^A|_{x=0} = 2.0599$, $P^B/P_0^B|_{x=0} \cong 0.0$, $P/P_0|_{x=0} = 2.0395$ at $t/\tau_0^A = 3000$.

with time, which means that the flow field has approached a final state (not a steady state, strictly speaking). In the figures, the steep gradients of the temperatures and pressures can be recognized in a small region ($x/L \sim O(1)$) in the immediate vicinity of the interface. This region is the so-called Knudsen layer, the thickness of which is of the order of the molecular mean free path, and it always manifests itself in the close vicinity of the boundary surface. In the uniform region ($0 < x/L \sim 600$ at $t/\tau_0^A = 3000$), which connects the contact region and the Knudsen layer, the noncondensable gas contained in a small amount initially is almost zero because it is driven almost completely into the contact region owing to the evaporation flow. The roles of the latent heat parameter Γ and the thermal conductivity ratio λ_c/λ_0^A are qualitatively the same in the present mixture case as in the pure-vapor case studied earlier by Onishi and Yamada [2], i.e., the larger the values of Γ , the weaker become the phase change processes and hence smaller

become the mass and energy flows and the larger the thermal conductivity ratio λ_c/λ_0^A , the stronger become the phase change processes (the physical explanation is given there). However, when Γ becomes smaller than a certain definite

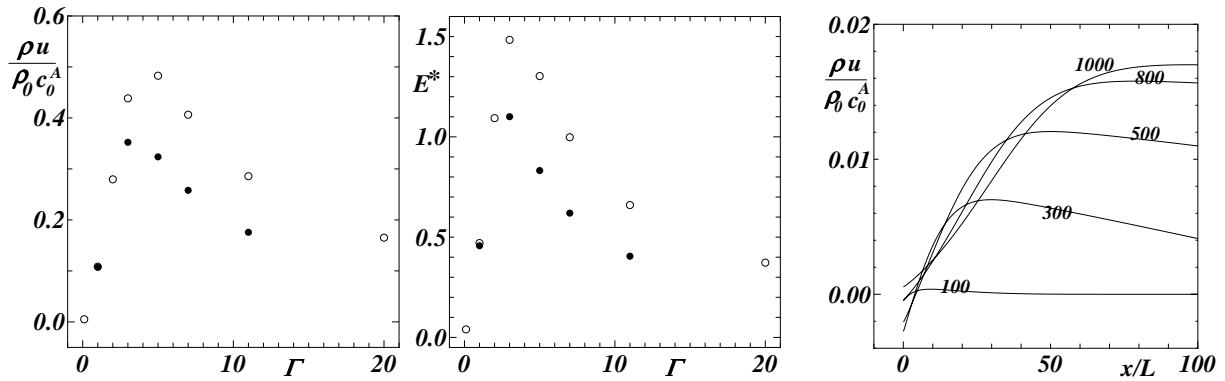


FIGURE 3. The total mass flow $\rho u/\rho_0^A c_0^A$ and energy flow $E^* = E/P_0(2R_A T_0)^{1/2}$ of the mixture at the steady state versus the latent heat parameter Γ . $T_c/T_0 = 2.0$, $D/L = 20.0$, $N_0^B/N_0^A = 0.01$, $m_B/m_A = 2.0$, $\kappa_{AA} = \kappa_{AB} = \kappa_{BB}$ and $\alpha_c = 1.0$. The **white circle**: $\lambda_c/\lambda_0^A = 50.0$, $\kappa_c/\kappa_0^A = 0.50$; The **black circle**: $\lambda_c/\lambda_0^A = 30.0$, $\kappa_c/\kappa_0^A = 0.32$. The existence of the maxima of the mass and energy flows can be expected. The graph on the flush right shows the temporary *negative mass flow*, the parameters for which are the same as in Figs. 1 and 2 except that here $\Gamma = 0.01$. The values of this *negative mass flow* are $\rho u/\rho_0^A c_0^A|_{x=0} = -0.0027$ at $t/\tau_0^A = 300$ and $\rho u/\rho_0^A c_0^A|_{x=0} = -0.0021$ at $t/\tau_0^A = 500$.

value, the mass and energy flows decrease again, which means that there exist their maximum values at a certain value of Γ . This behavior is shown in Fig. 3. This is a striking contrast to what we have studied so far in which the condensed phases have no internal structures at all.

Finally, the *negative mass flow*, another feature of the present problem, manifests itself during a certain period of time when the latent heat parameter Γ becomes extremely small but it disappears soon as time goes on. A typical example of this is shown in the graph on the flush right of Fig. 3. The existence of this *negative mass flow* at the steady state has first been discussed analytically by Sone & Onishi [8]. The explanation is also given in Onishi & Ooshida [9].

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