On the treatment of strong evaporation and condensation flows of a vapor at the fluid dynamic level – Fluid dynamic formulation for phase change problems –

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Abstract. The formulation at the ordinary fluid dynamic level to deal with flow problems, transient to steady, due to phase change processes is proposed. The problems of this kind have to be dealt with based on the kinetic equations because the nonequilibrium nature of the Knudsen layer, which is always existent in the close vicinity of the interface, is the cause for the phase-change processes to occur at the interface. In the continuum limit, however, the nonequilibrium region is extremely small in its thickness and the flow field may well be described by the Navier-Stokes equations. The problem arising, then, is that what kind of boundary conditions for the fluid dynamic quantities are to be applied at the interface. It is the kinetic theory analysis that can give the answer. For problems with weak phase-change processes involved, the appropriate conditions for the fluid dynamic quantities at the interface are available in terms of the *simple analytical expressions* connecting the velocity of the vapor and the jumps in its pressure and tempetarure at the interface. For stronger processes, on the other hand, the corresponding conditions are not existent in the form of analytical expressions; the only one available is in a tabulated form connecting numerically the fluid dynamic quantities concerned. These conditions, however, are valid only for the *steady states of the flow fields* and, therefore, they are not applicable, strictly speaking, to transient flow fields. This *steadiness* of the conditions poses great difficulty on the treatment of phase-change problems, especially when one is concerned with transient to steady flows. However, the difficulty has recently been cleared out by the adaptation of the analytical solutions of the well-known Riemann problem in compressible gas dynamics in the immediate vicinity of the interface. With this adaptation, various transient to steady problems with phase-change processes involved can be treated adequately at the fluid dynamic level, namely, by the compressible Navier-Stokes equations subject to the above mentioned conditions as the boundary conditions at the interface. In this paper, the fluid dynamic formulation for phase-change problems is put forward first and its validity will be shown from the comparison of the results with those of the kinetic equation.

INTRODUCTION

Various flow problems due to evaporation and condensation processes, whether they are transient or steady, are not only of theoretical interest but also of practical importance because they have wide application in engineering, especially in mass, heat and energy transfer systems in aero-space engineering which require accurate and detailed information of the flow fields. The problems of this kind, as is well known, 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 interface. It is this nonequilibrium region that is responsible for the phase-change processes to occur at the interface and its existence, therefore, can never be neglected in any circumstances even in flow fields of the continuum limit. Naturally, the analysis for such problems must necessarily be based on the kinetic equations. In the continuum limit, however, the nonequilibrium region is extremely small in its thickness and the flow field may well be described by the (compressible) Navier-Stokes equations. The problem arising, then, is that what kind of boundary conditions for the fluid dynamic quantities are to be applied at the interface. The answer must be given from the kinetic theory analysis. For problems with weak phase-change processes involved, the appropriate conditions for the fluid dynamic quantities at the interface are available now in terms of *simple analytical expressions* connecting the velocity of the vapor and the jumps in its pressure and tempetarure at the interface. They are the macroscopic conditions holding at the interface, which have been obtained earlier from the kinetic theory analyses in general terms (see e.g., Sone & Onishi [1] for the linearized case and Onishi & Sone [2] for the weakly nonlinear case). For stronger processes, on the other hand, the corresponding conditions are not available in the form of analytical expressions and

they can only be provided from the numerical solutions to the kinetic equations. Actually, they are tabulated from a large number of numerical solutions to specific problems such as half-space and two-surface problems of evaporation and condensation (see e.g., the tables by Aoki & Sone [3] and aslo the tables in our laboratory, which are obtainable on request). In both of these weak and strong cases, however, the conditions are valid only for the *steady states of the flow fields* and, therefore, they are not, strictly speaking, applicable to transient flow fields. This *steadiness* of the conditions poses great difficulty on the treatment of phase-change problems at the fluid dynamic level, especially when one is concerned with transient flows and the transition to their steady states. However, it has recently been found that the difficulty is surmountable with the adaptation of the analytical solutions of the well-known Riemann problem in compressible gas dynamics in the immediate vicinity of the interface. With this, various transient to steady problems with phase-change processes involved can be treated adequately at the fluid dynamic level, in other words, by the compressible Navier-Stokes equations as the governing equations subject to the appropriate boundary conditions with the Riemann solutions adapted. In this paper, the fluid dynamic formulation for phase-change problems is put forward first and, then, its validity will be shown from the comparison of the results for specific problems such as half-surface and two-surface problems of evaporation and condensation with those calculated based on the kinetic equation, the Boltzmann equation of BGK type [4].

FORMULATION AT FLUID DYNAMIC LEVEL

Consider a two-phase flow system of a vapor and its condensed phases with smooth and arbitrary geometrical shapes. Initially, the vapor and its condensed phases are in complete equilibrium at a temperature T_0. Let the pressure and density of the vapor at this initial state be denoted by P_0 and ρ_0, respectively. Suppose that, at time $t = 0$, the temperature of at least one of the condensed phases is suddenly changed, say, from T_0 to T_W. This leads to the onset of the phase change process at the condensed phase, giving then rise to a transient motion of the vapor producing various nonlinear waves in the flow field, a shock wave accompanied by a contact region (sometimes expansion waves involved) when $T_W > T_0$ and a fan of expansion waves when $T_W < T_0$. We put forward here the appropriate formulation for problems of this kind in order to be able to deal with transient to steady motions of the vapor at the ordinary fluid dynamic level. This formulation, which may be called the *fluid dynamic formulation*, consists of the (compressible) Navier-Stokes equations as the governing equations for motions of the gas phase and the macroscopic conditions valid at the interfaces derived from the kinetic theory analysis as the boundary conditions.

Navier-Stokes equations

The system of the Navier-Stokes equations as the governing equations describing the motions of a gas phase may be written in the form

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho u_i \\ \rho(e+\frac{1}{2}u^2) \end{bmatrix} + \frac{\partial}{\partial x_j}\begin{bmatrix} \rho u_j \\ \rho u_i u_j + P\delta_{ij} - \tau_{ij} \\ \rho u_j(h+\frac{1}{2}u^2) - u_i\tau_{ij} + q_j \end{bmatrix} = 0 \tag{1}$$

$$\left.\begin{aligned} &P = \rho RT, \qquad h = \gamma e = \frac{\gamma}{\gamma-1}RT \qquad \left(\gamma \equiv \frac{c_p}{c_v}\right) \\ &\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\frac{\partial u_l}{\partial x_l}\delta_{ij}, \qquad q_i = -\lambda\frac{\partial T}{\partial x_i} \qquad \left(\frac{\mu}{\mu_0} = \frac{T}{T_0}, \quad \frac{\lambda}{\lambda_0} = \frac{T}{T_0}\right) \end{aligned}\right\} \tag{2}$$

where t is the time; x_i is the rectangular coordinate system; ρ, u_i, P and T are, respectively, the density, the velocity vector, the pressure and the temperature of the gas; τ_{ij} is the viscous stress tensor and δ_{ij} is the Kronecker delta; q_i is the heat flux vector; e and h are the specific internal energy and enthalpy, respectively, R and γ being the gas constant per unit mass and the specific heat ratio ($\gamma = 5/3$ for monatomic gas molecules assumed here). c_p and c_v are, respectively, the specific heats at constant pressure and constant volume. μ and λ are the viscosity and the thermal conductivity of the gas, respectively, and they are here assumed to be proportional to the local temperature T. Note that the quantities with suffix 0 such as μ_0 and λ_0 are the corresponding quantities at a certain reference state, say, at the initial uniform state.

Initial and Boundary conditions

The initial conditions, say at time $t = 0$, may be specified, for example, as

$$u_i = 0, \qquad P = P_0, \qquad T = T_0 \tag{3}$$

everywhere in the flow field. These conditions correspond to a stationary uniform state of the gas, which may be quite common. Of course, the conditions do not have to be uniform, they may be the functions of space coordinates.

The boundary conditions at the phase boundary, on the other hand, should be specified as follows:

1) for *weak phase change processes*: the boundary conditions are given in terms of the analytical expressions as

$$\left.\begin{aligned} & u_i t_i = 0 \\ & \frac{P - P_W}{P_W} = C_4^* \frac{u_i n_i}{(2RT_W)^{1/2}} \qquad (C_4^* = -2.132039) \\ & \frac{T - T_W}{T_W} = d_4^* \frac{u_i n_i}{(2RT_W)^{1/2}} \qquad (d_4^* = -0.446749) \end{aligned}\right\} \quad \text{at} \quad x_i = x_{iW} \tag{4}$$

where x_{iW} is the position vector of the boundary surface. t_i and n_i are a unit tangential vector and the unit outward normal vector on the surface. T_W is the temperature of the boundary surface itself and P_W is its unique function. Actually P_W has been taken as the saturated vapor pressure at T_W, which is given by the Clapeyron-Clausius relation as

$$\frac{P_W}{P_0} = \exp\left\{-\Gamma\left(\frac{T_0}{T_W} - 1\right)\right\}, \qquad \Gamma \equiv \frac{h_L}{RT_0} \tag{5}$$

h_L being the latent heat of vaporization per unit mass. Expression (4) are the macroscopic conditions holding at the phase boundary having been given earlier by Onishi & Sone [2] from their weakly nonlinear asymptotic analysis for general motions of a vapor based on the Boltzmann equation of BGK type [4].

2) for *strong phase change processes*: no analytical expressions are available as the boundary conditions for the fluid dynamic quantities and, therefore, we must content ourselves with their numerical relations, which are expressed as

$$u_i t_i = 0, \quad \frac{P}{P_W} = F_1\left(\frac{u_i n_i}{c}\right), \quad \frac{T}{T_W} = F_2\left(\frac{u_i n_i}{c}\right) \qquad \text{(at the surface with evaporation process taking place)} \tag{6}$$

$$u_i t_i = 0, \quad \frac{P}{P_W} = G\left(\frac{u_i n_i}{c}, \frac{T}{T_W}\right) \qquad \text{(at the surface with condensation process taking place)} \tag{7}$$

where c is the local sound speed of the vapor defined by $c = (\gamma RT)^{1/2}$. The functions F_1, F_2 and G are the ones given numerically, the original tables for which may be found in Aoki & Sone [3]. However, the tables we have used here are the slightly more refined ones, in which a number of numerical data newly calculated in our laboratory has been added (these data may be obtained from Onishi on request).

It is noted here again that the conditions for weak cases and stronger cases stated here are for the *conditions at the steady states of the flow fields*. Therefore, they are not applicable, strictly speaking, to transient flow problems as they stand; they have to be adapted by the solutions of the Riemann problem in the immediate vicinity of the phase boundary as already mentioned in the Introduction. A brief explanation of this adaptation will be made here.

For simplicity, suppose that a one-dimensional transient flow of a vapor would be prevailing in the whole flow region ($-\infty < x < \infty$) in the absence of the condensed phase. Within this flow field, let the plane condensed phase with its temperature T_W be introduced and occupy the negative half-space ($x < 0$) with its interface at the origin ($x = 0$) of the coordinate. The flow field ($x > 0$), now labeled by region (1), may then be disturbed, in general. However, is there any possibility to be able to introduce the condensed phase in the flow field without causing any appreciable disturbances on it ? The answer would be the insertion of a certain *fictitious inner region* between the phase boundary at $x = 0$ and the point at $x = \Delta x$ of the transient flow field, Δx being, for example, the mesh size of the space coordinate in the numerical scheme. The fictitious flow field may connect appropriately the transient flow field of region (1) and the conditions specified at the phase boundary. These conditions are none other than the macroscopic conditions provided by the kinetic theory analysis, analytical or numerical. This fictitious flow field may, in general, involve a shock wave followed by a contact region and possibly a fan of expansion waves (see Fig. 1) and may be considered to be given by the solution of the well-known Riemann problem for which the analytical expressions are

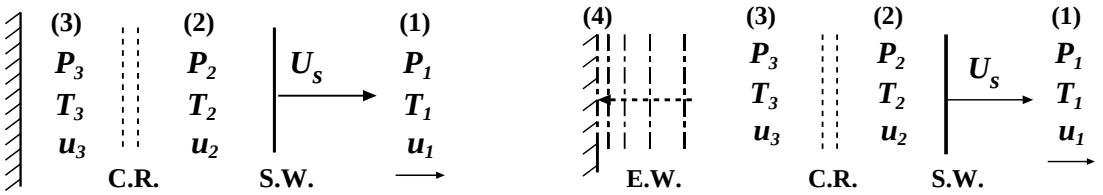

FIGURE 1. A schematic view of a flow field within a fictitious inner region inserted conceptually between the edge of the actual transient flow region (1), say at $x = \Delta x$, and the phase boundary at $x = 0$. The fictitious region consists, in general, of a shock wave (S.W.) with its propagation speed U_s, a contact region (C.R.) following the shock wave and a fan of expansion waves (E.W.). **left:** subsonic evaporation case (no expansion waves). **right:** supersonic evaporation but sonic at the interface; in this case the leftward-traveling expansion waves are swept backward with their front wave being on the interface, the region (4) becoming degenerate to a surface on the interface.

available (see e.g., Liepmann & Roshko[5]). If this fictitious flow region is physically possible, then the relevant fluid dynamic quantities (P_3, u_3, T_3) for subsonic case and (P_4, u_4, T_4) for supersonic case may well satisfy the so-called appropriate boundary conditions for evaporation and condensation given in Eq. (4) or in the corresponding numerical tables mentioned before, depending on the strength of the phase change process occurring at the phase boundary.

The next problem is to determine this fictitious flow field for a given actual transient flow field with (P_1, T_1, u_1) so that the fluid dynamic quantities, say P_3, T_3 and u_3 for subsonic evaporation case, can satisfy the imposed relations [such as Eq. (4) with (P, T, u) there replaced by (P_3, T_3, u_3)]. This is easily accomplished by utilizing the analytical solution for the Riemann problem. For this, let the Mach number of the fictitious shock wave be $M_s \equiv (U_s - u_1)/c_1$, U_s and c_1 being, respectively, the propagation speed of the shock wave and the sound speed at temperature T_1 in region (1). From the Rankine-Hugoniot relations across the shock wave (S.W.) and the conditions across the contact region (C.R.), we have

$$\frac{P_3}{P_1} = \frac{P_2}{P_1} = 1 + \frac{2\gamma}{\gamma+1}\left(M_s^2 - 1\right), \qquad \frac{u_3}{c_1} = \frac{u_2}{c_1} = \frac{2}{\gamma+1}\left(M_s - \frac{1}{M_s}\right) + \frac{u_1}{c_1} \qquad \text{with} \qquad M_s \equiv \frac{U_s - u_1}{c_1} \tag{8}$$

With P_3 and u_3 satisfying Eq. (8) for $M_s \geq 1$, if (P_3, T_3, u_3) can satisfy the imposed conditions such as Eq. (4) or the relations in the corresponding numerical tables, the appropriate boundary conditions at the interface ($x = 0$) for the actual flow field may be given as

$$P(0) = P_3, \qquad T(0) = T_3, \qquad u(0) = u_3 \tag{9}$$

From the discussion similar to the above, the appropriate boundary conditions for supersonic transient evaporation cases may become

$$P(0) = P_4, \qquad T(0) = T_4, \qquad u(0) = u_4 \tag{10}$$

where $P_4/P_W = 0.2075$, $T_4/T_W = 0.6434$ and $u_4/c_4 = 1.0$ (see Aoki & Sone [3] for these numerical values).

The condensation cases, on the other hand, the fictitious inner region consists only of a fan of rightward-traveling expansion waves (see Fig. 2) for subsonic condensations and no inner region for supersonic cases. For subsonic cases,

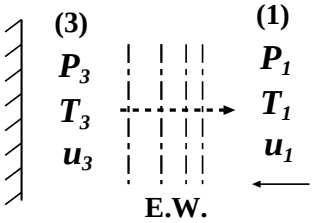

FIGURE 2. A schematic view of a flow field within a *fictitious inner region* inserted conceptually between the actual flow region (1) ($u_1 < 0$) and the phase boundary at $x = 0$. The expansion waves (E.W.) are rightward-traveling waves in this case.

from the isentropic relations and the Riemann invariant (J^-), we have

$$\frac{P_3}{P_1} = \left(\frac{c_3}{c_1}\right)^{\frac{2\gamma}{\gamma-1}} = \left(\frac{T_3}{T_1}\right)^{\frac{\gamma}{\gamma-1}} \qquad \text{and} \qquad u_1 - \frac{2}{\gamma-1}c_1 = u_3 - \frac{2}{\gamma-1}c_3 \tag{11}$$

then

$$\frac{P_3}{P_1} = \left(\frac{c_3}{c_1}\right)^{\frac{2\gamma}{\gamma-1}} = \left(\frac{T_3}{T_1}\right)^{\frac{\gamma}{\gamma-1}} = \left\{1 - \frac{\gamma-1}{2}\left(\frac{u_1}{c_1} - \frac{u_3}{c_1}\right)\right\}^{\frac{2\gamma}{\gamma-1}} \tag{12}$$

If the above (P_3, T_3, u_3) can satisfy the imposed conditions, the appropriate boundary conditions at the interface for the actual flow field may be given as

$$P(0) = P_3, \qquad T(0) = T_3, \qquad u(0) = u_3 \tag{13}$$

For supersonic condensation cases, no fictitious inner region is needed and directly we have an inequality relation

$$\frac{P(0)}{P_W} \geq F_b\left[\frac{u(0)}{c(0)}, \frac{T(0)}{T_W}\right] \qquad \text{for} \qquad \frac{|u(0)|}{c(0)} > 1$$

given by Aoki & Sone [3]. In this case, unfortunately, the setting of the appropriate boundary conditions is left unresolved.

CHARACTERISTIC PARAMETERS

Let the length scale and the velocity scale of the problems under consideration be L and U_0, respectively. The time scale τ_0, then, may be taken as $\tau_0 = L/U_0$. With these scales together with the fluid dynamic quantities at a certain reference state, say, at the initial state, the system of the governing Navier-Stokes equations, the initial and the boundary conditions is appropriately nondimensionalized and, hence, the behavior of a flow field may then be characterized by

$$\frac{T_W}{T_0}, \qquad \Gamma \equiv \frac{h_L}{RT_0} \quad \left(\text{or} \quad \frac{P_W}{P_0}\right), \qquad Ma \equiv \frac{U_0}{c_0}, \qquad Re \equiv \frac{\rho_0 U_0 L}{\mu_0}, \qquad Pr \equiv \frac{c_p \mu_0}{\lambda_0} = \frac{\gamma}{\gamma-1}\frac{R\mu_0}{\lambda_0} \tag{14}$$

where c_0, one of the candidates of the velocity scale, is the sound speed at the reference state defined by $c_0 \equiv (\gamma RT_0)^{1/2}$ and c_p is the specific heat at constant pressure. The nondimensional parameters Ma, Re and Pr are the flow Mach number, the Reynolds number and the Prandtl number at the reference state, respectively. In addition, if we introduce the Knudsen number $Kn \equiv l_0/L$, l_0 being the mean free path of the gas molecules at the reference state defined by $l_0 = (\mu_0/P_0)(8RT_0/\pi)^{1/2}$, there exists a relation among the parameters Ma, Re and Kn as $Re \sim Ma/Kn$. Specifically, for the Boltzmann equation of BGK type [4], the relation becomes $Re = (8\gamma/\pi)^{1/2}(Ma/Kn)$.

RESULTS AND DISCUSSION

Various flow problems with simple geometries such as half-space problems and two-surface problems with plane, cylindrical and spherical geometries, have been treated based on the *fluid dynamic formulation* with a simple Mac-Cormack scheme applied. The problems themselves are well known and the explanation of the flow fields will not be given here but only the results in order to show the validity of this new governing system at the fluid dynamic level. Owing to the limited space, only the results for condensation cases (more complex than the evaporation cases) onto a spherical condensed phase are shown in Fig. 3, where the dotted lines indicate the corresponding results based on the kinetic theory formulation. Good overall agreement, not only qulitative but also quantitative, can be seen between the results based on the two governing systems. The quantitative difference, which is perceived in the close vicinity of the condensed phase and may be attributable to the existence of the Knudsen layer, must be allowed in the fluid dynamic formulation because this formulation does not take full account of the existence of the Knudsen layer but only its effects through the boundary conditions which are the reflections of its existence. Figure 4 shows, on the other hand, the results without the adaptation of the Riemann solutions incorporated just for reference, from which one can see the zigzag distributions at early stages of the flow field. The smaller the temperature ratio T_W/T_0 of the condensed phase, i.e., the stronger the condensation process, this zigzag behavior prevails into the flow field and the calculation does not proceed any more.

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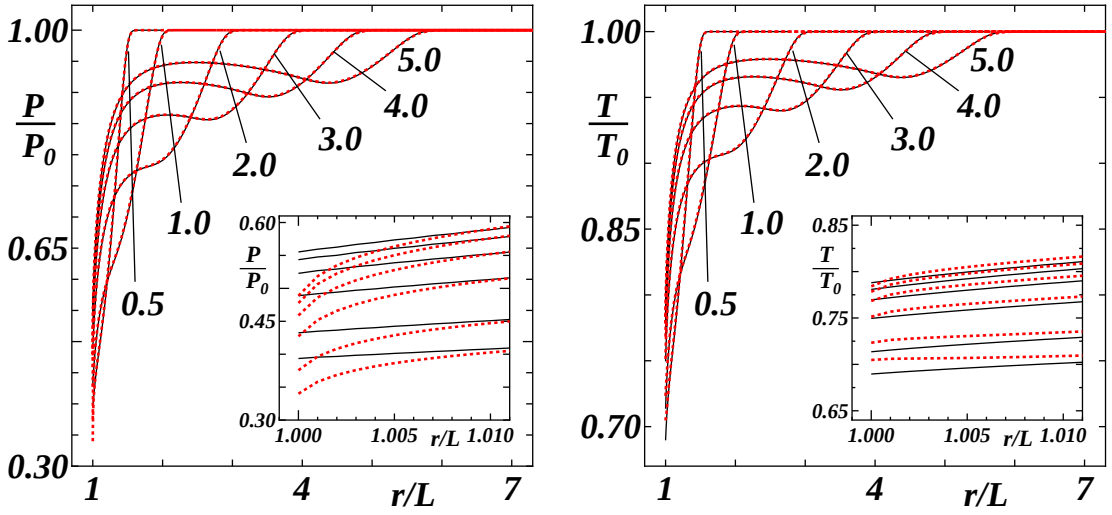

FIGURE 3. Transient pressure and temperature distributions of a vapor around its spherical condensed phase with its radius L. $T_W/T_0 = 0.8$, $\Gamma = 11.0$ ($P_W/P_0 = 0.064$, $\rho_W/\rho_0 = 0.080$), $Re = 412.026$ ($Kn = 0.005$) and $Pr = 1.0$. The numbers in the graphs indicate the time t/τ_0, τ_0 being defined by $\tau_0 \equiv L/(2RT_0)^{1/2}$. **Solid lines**: the present results based on the *fluid dynamic formulation with Riemann solutions applied*. **Dotted lines**: the results by Onishi & Fuchs [6] based on the kinetic equation [4].

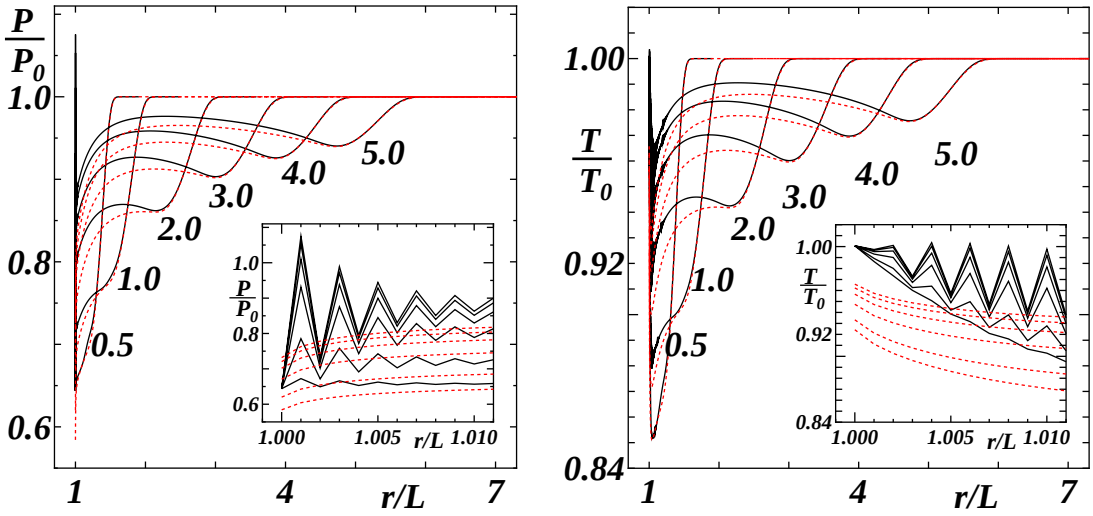

FIGURE 4. Transient pressure and temperature distributions of a vapor around its spherical condensed phase with its radius L. $T_W/T_0 = 0.9$, $\Gamma = 11.0$ ($P_W/P_0 = 0.295$, $\rho_W/\rho_0 = 0.327$), $Re = 412.026$ ($Kn = 0.005$) and $Pr = 1.0$. The numbers in the graphs indicate the time t/τ_0, τ_0 being defined by $\tau_0 \equiv L/(2RT_0)^{1/2}$. **Solid lines**: the results based on the *fluid dynamic formulation with Riemann solutions* ***not*** *applied*. **Dotted lines**: the results by Onishi & Fuchs [6] based on the kinetic equation [4]. Note that the calculation without the Riemann adaptation breaks down when $T_W/T_0 = 0.8$ with the other parameters being the same.

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