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One-dimensional numerical simulations of heat transfer on the piston effect

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One-dimensional numerical simulations of heat transfer on the piston effect

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Abstract. Strong singularities in thermodynamic and transport properties appear in near-critical fluids, which give birth to the piston effect. In the present study, the piston effect is investigated numerically in a one-dimensional cavity filled with near-critical CO₂, being heated at one side while the other side keeps at initial temperature. The thermodynamics model, which ignores velocity field and assumes uniform pressure field, is numerically solved by explicit finite difference method. The results are presented and discussed from two aspects. In the first part, the results show typical evolutions of temperature and density fields. The variations of temperature, density and pressure are results of competitions and eventual equilibrium between the heating piston effect and the cooling piston effect. In the second part, the results indicate influences of the critical proximity on the equilibrium. Results show that with the increase of critical proximity, piston effect gets weaker, equilibrium time gets longer, and equilibrium temperature becomes smaller.

1. Introduction

Strong singularities in thermodynamic and transport properties appear in near-critical fluids. Specifically, the isothermal compressibility, the isobaric expansion coefficient and specific heat capacity at constant pressure diverge while thermal diffusivity tends to zero [1]. As the result, theoretically, the process of heat transfer extremely slows down under zero gravity, namely critical slowing down, leading to a substantial increase in relaxation time of temperature field. However, in 1985, in an experiment measuring specific heat capacity at constant volume of supercritical SF₆ under microgravity environment, researchers actually observed a critical speeding up. Because the phenomenon was exactly contrary to their expectation, many researches started to pay great attention to studying it [2].

Early studies mainly focused on explanations, theoretical analyses and experimental verifications of the abnormal phenomenon. In 1990, three groups put forward their explanations based on different approaches independently. Ounce et al. proposed a theoretical model based on thermodynamics theories [3]. Bourke et al. raised a numerical model based on thermodynamics theories [4]. Napoli et al. named the phenomenon the piston effect (PE), and presented the process of PE more directly through numerical simulation [5]. Afterwards, Napoli and Carlos, based on the abnormal physical properties, studied through matched asymptotic descriptions techniques [6]. Then they put forward the decoupling of temperature and density relaxations, and solved physical process of PE based on a one-dimensional partial heated model theoretically: after the wall of a sealed container filled with supercritical fluid being heated, an extremely thin thermal boundary layer forms near the heated



boundary. Supercritical fluid has relatively higher thermal expansion coefficient and compressibility. As the result, thermal boundary layer expands and compresses the bulk fluid. By this means, energy is transferred from the boundary layer to the bulk fluid quickly through pressure wave, leading to a rapid temperature rise in the bulk fluid. As for experimental studies, researchers mainly measured temperature variations with thermistors or measured density variations with interferometers in early experiments, in order to verify the existence of PE and the decoupling of temperature and density relaxations. In 2006, Miura et al. made the first experimental observation of thermos-acoustic waves with ultra-sensitive interferometers [7]. Then Shen and Zhang [8] carried on a series of numerical simulations, studying the influences of thermal boundary conditions and initial conditions on thermos-acoustic waves. Besides, they also studied the propagation and reflection of thermos-acoustic waves.

In this paper, one-dimensional numerical simulations are performed by using thermodynamics model. The PE in a one-dimensional sealed cavity being heated at one side while the other side keeps at initial temperature is studied. Such a physical model results in the coexistence of heating piston effect and cooling piston effect. The competitions of the two kinds of PE is revealed by analyzing the evolutions of temperature and density fields. In addition, the influences of critical proximities on their interactions are discussed.

2. Physical model and governing equations

2.1. Physical model

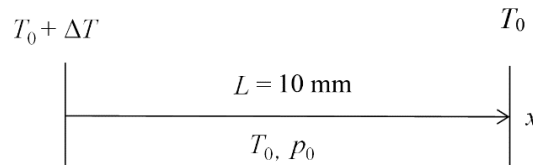


Figure 1. The physical model.

As shown in Fig.1, the physical model is a one-dimensional sealed cavity filled with CO_2 of which the length is $L = 10 \text{ mm}$. Its initial temperature and pressure are T_0 and p_0 respectively. Left wall temperature suddenly rises by ΔT at initial time while the other side keeps at initial temperature T_0 . In order to exclude the influences of natural convection, the gravity is ignored. In this paper, the initial conditions are chosen along the critical isochore ($\rho = \rho_c$), and the initial temperature is determined through the dimensionless reduced temperature ε , given by

$$\varepsilon = \frac{T - T_c}{T_c}$$

In this paper, the parameter ε measures the proximities to the critical point. The critical parameters of CO_2 are $p_c = 7.38 \text{ MPa}$, $T_c = 31 \text{ }^\circ\text{C}$, $\rho_c = 468.6 \text{ kg m}^{-3}$, with p_c , T_c and ρ_c the critical pressure, temperature and density, respectively. The physical properties of CO_2 are obtained from NIST database [9].

2.2. Governing equations

Boukari *et al.* [4] put forward a thermodynamics model to describe the PE under zero gravity in a single-phase supercritical fluid in a sealed container. They ignored the velocity field in the fluid, and assumed that the pressure in the whole domain is uniform. This model has a relatively simple form and is convenient for programming and calculating. Therefore, it is widely accepted by researchers [10-12]. The energy equation for a one-phase fluid is given by

$$\rho c_p \frac{DT}{Dt} = \nabla \cdot (\lambda \nabla T) + T \beta_p \frac{Dp}{Dt} + \Phi \quad (1)$$

with ρ the density, p the pressure, T the temperature, λ the thermal conductivity, β_p the isobaric expansion coefficient, Φ the viscosity dissipation term. When ignoring velocity and applying a uniform pressure field, a further reduced equation can be derived as following:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + T \beta_p \frac{\partial p}{\partial t} \quad (2)$$

The equation of state is the linearized equation of state, expressed as

$$\rho = \rho_0 + \rho [\alpha_T (p - p_0) - \beta_p (T - T_0)] \quad (3)$$

Equations (2) and (3) are not close, so it's necessary to derive a pressure equation from mass conservation equation, which is given by [4]

$$p = p_0 + \frac{\int_V \rho \beta_p (T - T_0) dV}{\int_V \rho \alpha_T dV} \quad (4)$$

The equations stated above can be solved by discretization and iterative processes. Then we obtained the developments of temperature, pressure and density fields under the PE.

3. Numerical method

In this paper, the governing equations (2), (3) and (4) are solved by explicit finite difference method. Generally speaking, there are two kinds of finite difference methods, the explicit one and implicit one. Each has their own advantages [13]: explicit method is relatively easier to construct process and program, though its selection of time step is restricted by stability conditions, when grid size is pretty small, the time step should be small enough to have numerical stability; as for implicit method, there is no restriction for time step to guarantee numerical stability. However, programing and constructing are relatively more complex, and it will take more time for every single time step. For these reasons, explicit method is mainly used to solve unsteady situation, it is better for solving exact solution over time; implicit method is widely employed in solving stationary problems, its accuracy of process over time is not very important. This is an unsteady problem in essence, considering the high demand for accuracy, so it is proper to use explicit finite difference method in this study. As for discretization methods, taking computational accuracy and time consuming into account, the time derivative term in Eq. (4) is discretized with first-order forward difference scheme, and the spatial derivative terms are discretized with second-order central difference scheme. In addition, the grid size selected is $\Delta x = 0.01$ mm, and time step is $\Delta t = 0.001$ s or 0.005 s. This selection guarantees stability conditions of explicit method. Figure 2 gives the algorithm flowchart we used in simulations.

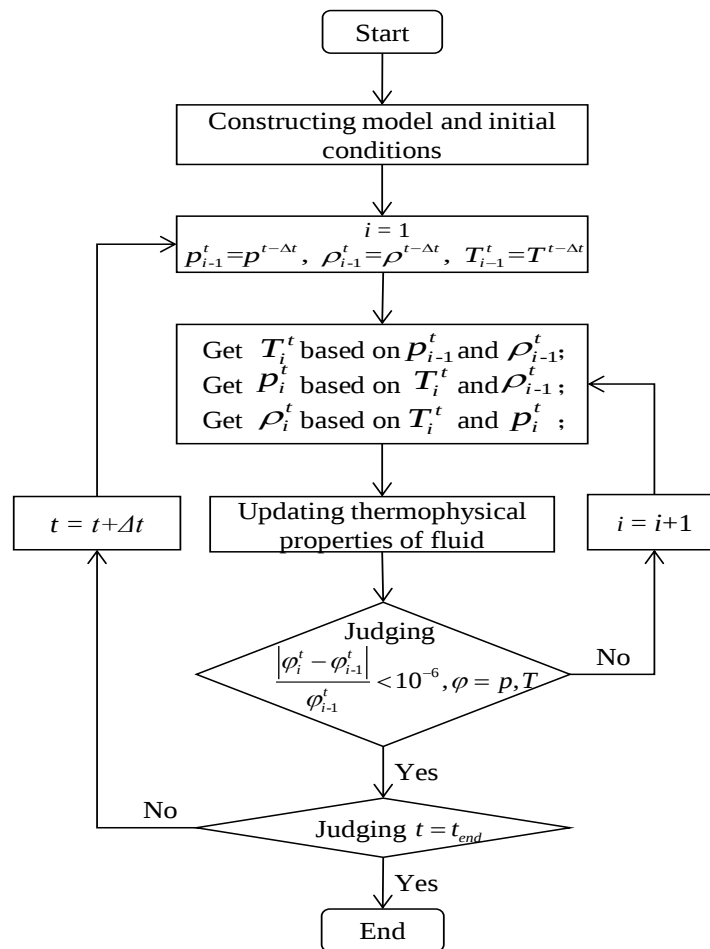


Figure 2. Algorithm flowchart in simulations.

4. Results and discussions

4.1. Typical evolutions of temperature and density fields

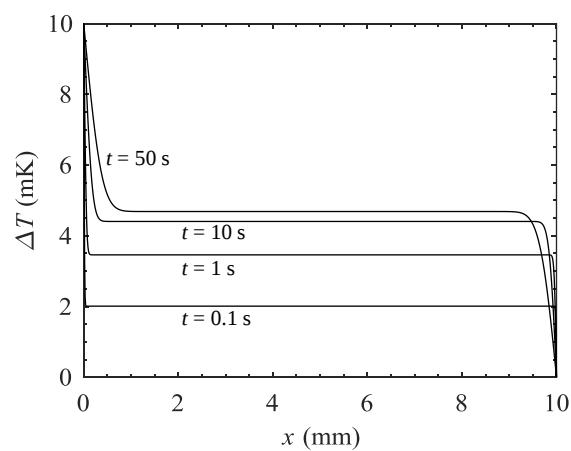


Figure 3. Spatial distributions of temperature at different time ($\varepsilon = 0.001$).

Figure 3 plots spatial distributions of temperature at different time for $\varepsilon = 0.001$. After the temperature at the left wall rises suddenly, heat diffuses into the fluid. A hot boundary layer (HBL) then appears near the left wall. Due to the diverging compressibility of near-critical CO_2 , the HBL expands strongly and activates the *heating piston effect* (HPE), leading to a rapid, homogenous rise of bulk temperature. Besides, due to the right boundary keeping at initial temperature, the loss of heat results in the formation of temperature gradients, namely that a cold boundary layer (CBL) forms near the right boundary. Similarly, the contraction of the CBL causes the *cooling piston effect* (CPE), leading to a rapid, homogenous drop in bulk temperature. Therefore, the variations of bulk temperature in Fig.3 are results of competitions between the HPE and the CPE, where the horizontal part of the lines represents the bulk fluid. One should also bear in mind that since the CPE is a result of the HPE, the former is always weaker than the latter. Obviously, during 0.1 s to 50 s, the boundary layers develop gradually, bulk temperature becomes higher, but the rate of increase in bulk temperature drops gradually. The reason is that initially, the HPE is strong while the CPE is weak. However, as time goes by, bulk temperature gets higher. The HPE gradually becomes weak while the CPE gets strong. We can conclude that the deceleration in the change of bulk temperature results from the equilibrium between the HPE and the CPE. To study such an equilibrium, we could define the equilibrium time as the moment when the rise of bulk temperature per unit time (0.01 s) is smaller than 0.1% of the amount the bulk temperature rises during the first 0.01s. It should be noted that the term *equilibrium* used here doesn't refer to the thermal equilibrium of the whole system, but represents the balance between the HPE and the CPE.

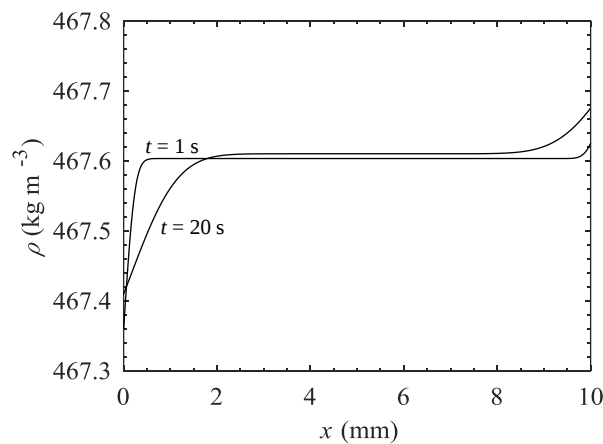


Figure 4. Spatial distributions of density at different time ($\varepsilon = 0.05$).

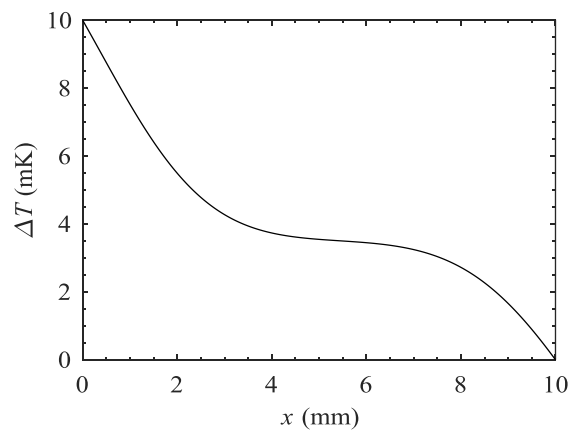


Figure 5. Temperature field at late time ($\varepsilon = 0.05$, $t = 100$ s).

In Fig.4, we show profiles of density field at different time for $\varepsilon = 0.05$. Heat diffusion and the two kinds of piston effects cause the variations in temperature, which also results in the change of density. The left HBL and right CBL along with the homogenous bulk fluid (horizontal part of the lines) are clearly observed in Fig.4. Indeed, after the sudden rise of the temperature at the left wall, the HBL expands and its density drops, activating the HPE. As the result, the bulk fluid is compressed and its density increases. Similarly, the contraction of CBL cause the CPE, leading to the decrease in bulk density. Since HPE is always stronger than CBL, the overall effect is compression and the bulk density increases gradually. Obviously, during 1 s to 20 s, the bulk density gets higher.

Figure 5 plots the temperature field at late time for $\varepsilon = 0.05$. It is observed that, as time goes by, the influences of the piston effect disappear, and both of the boundary layers develop through diffusion and merge to each other. Eventually, temperature field should be linear distribution.

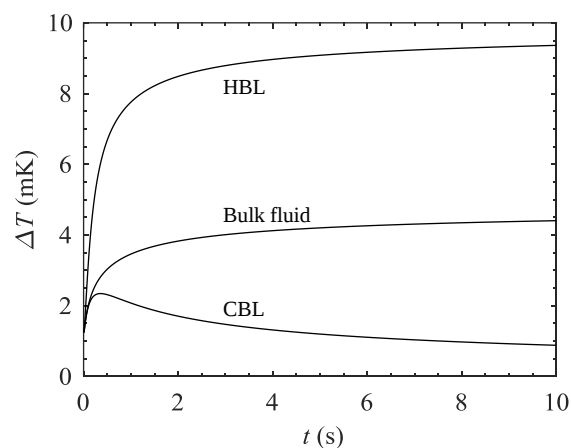


Figure 6. Time evolutions of temperature at different spatial points ($\varepsilon = 0.001$), where the words indicate the locations of the points.

We plot time variations of temperature at three typical spatial points in Fig.6. It shows that, after the sudden rise of the temperature at the left wall, the temperature of the point in the HBL rise rapidly during short time. Then, the HBL expands, activating the HPE. As the result, the temperature of the point in the bulk fluid rises fast and evenly. Meanwhile, the fluid near the right wall first goes through a brief temperature rise due to the HPE, which drops then through heat diffusion. As time goes by, the interaction between HPE and CPE gradually approaches to equilibrium, and the increase rate of bulk temperature decreases.

4.2. Influences of the critical proximity on the equilibrium

Table 1. The measured equilibrium time and temperature for different critical proximities.

Critical Proximity (ε)	Equilibrium Time (s)	Equilibrium Temperature (mK)
0.001	3.24	4.04
0.005	11.9	3.78
0.01	19.5	3.63
0.05	68.5	3.29

Now we discuss the behaviors of equilibrium for different critical proximities. Table 1 gives the measured equilibrium time and temperature for different critical proximities. It is observed that with the increase of critical proximity, piston effect gets weaker, equilibrium time gets longer, and equilibrium temperature becomes lower. The reasons are presented below. The fluid at large critical

proximity has a small compressibility. And since piston effect is closely related to the compressibility of the fluid. So under the same temperature disturbances, the intensity of HPE/CPE decreases with increased critical proximity. Larger the critical proximity, weaker the HPE, and smaller the rise amount of bulk temperature. As the result, the CPE also becomes weak due to the coupling effect of the bulk temperature and critical proximity. Both the HPE and the CPE get weak at large critical proximity, since the temperature disturbances are identical, we can conclude that it takes more time for HPE and CPE approaching to equilibrium. So the phenomenon stated above occurs.

5. Conclusion

In this paper, we conduct a series of explorations into the piston effect in a sealed cavity filled with near-critical CO₂ under zero gravity, with one heated boundary and the other boundary keeping at initial temperature. The results are presented and discussed from two aspects. In the first part, the results show typical evolutions of temperature and density fields, which are indeed the competitions between the heating piston effect and the cooling piston effect. In fact, the sudden rise of temperature activates the HPE, then the HPE triggers the CPE. Initially, the HPE is strong while the CPE is weak. As time goes by, the HPE gradually becomes weak while the CPE gets strong, eventually they approach to an equilibrium. In the second part, the results indicate influences of the critical proximity on the equilibrium. Results show that with the increase of critical proximity, piston effect gets weaker, equilibrium time gets longer, and equilibrium temperature becomes smaller.

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