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Thermomechanical effects in supercritical binary fluids

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ABSTRACT

Thermomechanical effects, i.e., Piston effect (PE), Soret effect (SE), and Dufour effect (DE), occur in supercritical binary fluids when subjected to boundary thermal perturbation due to the diverging compressibility, vanishing thermal diffusivity and mass diffusion. We numerically study those effects in a 1-D slab with a size of 10 mm by solving a complete set of governing equations, which are derived considering the supercritical hydrodynamics, mass transfer and energy conservation simultaneously. The characteristics of these thermomechanical effects in the supercritical binary fluid and liquid binary fluid on different timescales (acoustic and diffusion timescales) are clarified, respectively. Because of the existence of the strong PE in the supercritical binary fluid, the fluid bulk is heated up uniformly, and the SE appears on both sides simultaneously. The direction of mass diffusion is determined by the relative magnitude between concentration gradient and temperature gradient, i.e., gradient ratio γ, and there is a balance gradient ratio γ_b in each specific binary fluid under a certain condition. The DE is verified by comparing the results of binary fluid and the corresponding pseudo-pure fluid with the same thermo-physical properties. The DE is considerable in supercritical binary fluid, but negligibly small in liquid ethanol/water binary fluid because of the weak SE. These thermomechanical effects in different binary fluids (including supercritical, liquid and gaseous ones) mainly differ in the relative magnitudes and the traveling speed of thermoacoustic wave.

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1. Introduction

Binary fluid is deeply involved in industries, such as air (regarded as the binary fluid of nitrogen and oxygen) separation and refrigerant mixture, and it is a hot and complex research topic in the fields of fluid dynamics and heat transfer. Because of the interactions between different components, there are unique characteristics in heat and mass transfer of the binary fluid system. In the phase change heat transfer, e.g., evaporation/boiling and condensation, the mass transfer in the concentration boundary layers weakens the heat transfer coefficient compared with that of the pure fluids of the components [1]. There have been an abundance of studies on heat transfer characteristics of the binary fluid at the liquid or gaseous state; however, not many results are for the supercritical state. When the temperature and pressure of a fluid both exceed their respective critical values (T_c and P_c), it reaches the supercritical state, where there is no apparent difference between the liquid state and gaseous state. The supercritical fluid is characterized by a large density, large specific heat and small

viscosity. These unusual properties of supercritical fluid make it widely used in the industrial applications, such as superconducting magnet cooling and transcritical CO_2 automobile air-conditioning. Different fluids show similar characteristics on thermo-physical properties at supercritical state: diverging compressibility and ultra-small thermal diffusivity. The dramatic variations of the thermo-physical properties give rise to a particular thermo-fluidic phenomenon: the fluid bulk is heated up uniformly by the thermoacoustic wave induced by the thermal perturbation. This phenomenon is termed as Piston effect (PE) as the expanding thermal boundary layer acts like a piston. Since it was first observed in a microgravity experiment with supercritical SF_6 in 1985 [2], many theoretical, experimental and numerical studies were conducted on PE to understand its mechanism [3–5]. However, almost all the researchers considered this effect in pure fluids, and the propagation of thermal perturbation in the supercritical binary fluid is not fully understood, yet.

The PE was successfully observed by Nakano and Shiraishi [6] in supercritical artificial air (binary mixture of nitrogen and oxygen with the molar fraction of 0.79 and 0.21, respectively) by means of two-exposure holographic interferometry [7]. Later on, the PE was numerically studied in the same fluid by a 1-D physical model

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Nomenclature

c	concentration of the component, –		x	coordinate, m
c_P, c_v	specific heat capacity, J kg^{-1} K^{-1}		Δx	grid size, m
D_m	mass diffusion coefficient, m^2 s^{-1}			
D_T	thermal diffusion coefficient, m^2 s^{-1} K^{-1}		*Greek symbols*	
H	parameter in Eq. (16)		α_T	isothermal compressibility, Pa^{-1}
J	mass flux, kg m^{-2} s^{-1}		β	thermal expansivity, K^{-1}
k_T	thermal diffusion ratio, –		γ	gradient ratio, K^{-1}
l	length of slab, m		γ_b	balance gradient ratio, K^{-1}
P	pressure, MPa		ρ	density, kg m^{-3}
Q	heat, W		η	kinetic viscosity, Pa s
q	heat flux, W m^{-2}		μ	chemical potential, J kg^{-1}
r	ratio of specific heat capacities, c_P/c_v, –		κ	thermal conductivity, W m^{-1} K^{-1}
S_T	Soret coefficient, K^{-1}		σ'_{ij}	viscous stress tensor, Pa
T	temperature, K		δ_{ij}	unit tensor
ΔT	temperature rise, K			
t	time, s		*Subscripts*	
t_a	acoustic time, s		0	initial parameter
Δt	time step, s		c	critical parameter
u	velocity at x coordinate, m s^{-1}		i, j, k	tensor
V	velocity vector, m s^{-1}			
v_s	local sonic speed, m s^{-1}			

[8], in which the PE was also investigated. These studies testified the existence of PE in the supercritical binary fluid, but the difference and similarity between the PEs in binary fluid and pure fluid need further discussion.

When a binary fluid system in equilibrium is subjected to a temperature perturbation, the migration of components occurs because of the differences in mass diffusion properties and chemical potential, leading to concentration changes at different locations. This phenomenon is known as Soret effect (SE) [9]. The mass diffusions driven by the concentration gradient and temperature gradient will reach equilibrium and such equilibrium is determined by the thermal diffusion coefficient D_T (Note the thermal diffusion coefficient here is a mass transport property driven by uneven temperature field, and it differs from the thermal diffusivity, i.e., $\kappa/(\rho c_p)$) and mass diffusion coefficient D_m. The relative ratio between the two coefficients is defined as Soret coefficient S_T, and it is deduced from the concentration balance between the mass diffusions driven by concentration gradient $\partial c/\partial x_i$ and temperature gradient $\partial T/\partial x_i$. The mass flux in a binary system without considerable pressure gradient can be written as [10]

$$J_i = -\rho D_m \frac{\partial c}{\partial x_i} - \rho D_T c_0 (1 - c_0) \frac{\partial T}{\partial x_i} \tag{1}$$

where c_0 is the initial molar fraction of the reference component. When the binary system reaches steady state, we have $J_i = 0$, implying

$$\frac{\partial c}{\partial x_i} = -\frac{D_T}{D_m} c_0 (1 - c_0) \frac{\partial T}{\partial x_i} \tag{2}$$

Then the Soret coefficient is defined as follows with the dimension of K^{-1}.

$$S_T = \frac{D_T}{D_m} \tag{3}$$

There have already been researches focusing on supercritical binary fluid. Okong'o and Bellan [11] numerically studied the transitional mixing behavior of a supercritical heptane/nitrogen binary layer, and Nakano and Maeda [12] experimentally studied the mass transfer in supercritical nitrogen/oxygen binary fluid. However, the studies on SE mainly focused on the fluids at liquid or gaseous state, such as gas mixtures, liquid mixtures and solutions [9,13,14], and the main methodologies to measure S_T for different mixtures [10,15,16] and to investigate the influence of SE on the system stability [17,18]. According to the pervious results, S_T relates to both chemical and thermo-physical properties, and the sign of S_T may even vary with the change of state and the composition [12,16,19]. Therefore, the characteristics of SE at liquid or gaseous state cannot be extrapolated to the supercritical state.

Under the effects of temperature and concentration gradients, the mass diffusion process is associated with heat transfer, and such phenomenon is Dufour effect (DE), namely the heat flux transported with the mass diffusion. DE is negligibly slight in the process with strong heat and mass transfer [20], but in the case with relatively mildly changing boundary conditions or slow convection, the DE would apparently enhance the heat transfer [21]. Alam and Rahman [22] investigated SE and DE in free and forced convection of gaseous binary fluid in a porous medium, indicating that the flow and temperature fields were appreciably affected by these two effects.

According to the above content, we can infer that the SE and DE highly depend on the temperature distribution in the fluid. But the response of a binary fluid in equilibrium to thermal perturbation at supercritical state is much different from that at the state far from the supercritical region (far-critical state, i.e., gas or liquid state). The fluid bulk is evenly heated up due to the PE at supercritical state; however, the fluid bulk at far-critical state is gradually and unilaterally heated by the thermal perturbation through conduction or convection. Consequently, the temperature distribution (temperature gradient) in the fluid at supercritical state is completely different from that at far-critical state, resulting in particular characteristics of SE and DE, which will be discussed in the present study.

The PE and SE at supercritical binary fluid have been observed and numerically verified in mixtures of nitrogen and oxygen [6,8], but there was almost no further discussion on their detailed thermal and fluid dynamics and the interactions between them. Raspo et al. [23] investigated the SE under the influence of the PE in binary mixtures of supercritical carbon dioxide and naphthalene. But naphthalene was in solid state under the studied conditions, thus the binary system consisted of supercritical fluid