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## Numerical investigation on Marangoni convection of binary fluids in a closed microcavity

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### HIGHLIGHTS

- For simple fluids, thermocapillary stresses drive the liquid away from hot regions.
- For binary fluids, the thermal performance is improved by solutocapillary effect.
- For self-rewetting fluids, both the heat and mass transfer are enhanced.
- The non-condensable gas could negatively affecting the heat transfer.

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### ABSTRACT

Phase change can dramatically alter the interfacial temperature, resulting in surface tension gradients and consequently causing Marangoni convection. The numerical investigation on Marangoni convection of binary fluids in a closed microcavity is accomplished in this paper by using the volume of fluid (VOF) model with source terms added by user defined functions (UDF) due to mass transfer, with detailed velocity and temperature fields. For simple fluid, surface tension decreases with increasing temperature, resulting in thermal Marangoni convection that can drive the liquid leave from hot regions and leading to film dryout. For binary fluids, however, the Marangoni convection could also be caused by concentration gradients, resulting in greatly promoted backflow of the fluid. In particular, for self-rewetting fluids which have unique surface tension characteristics that increase with increasing temperature above a critical value, the Marangoni flow can drive the liquid flow towards hot regions, avoiding film dryout. The influence of non-condensable gas is also considered by providing detailed velocity fields near the contact region and it proves that non-condensable gas can negatively affect the heat and mass transfer.

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### 1. Introduction

Micro heat pipes have been widely used in cooling microelectronics, high-power microwave, radar systems, etc., in microgravity and space craft thermal control environments due to its high heat transfer performance and great benefit of energy saving by utilizing latent heat of phase change without external power. Although the applications of micro heat pipes are becoming increasingly common, the nature of liquid evaporation and gas condensation in a micro heat pipe and the Marangoni effects caused by temperature and concentration gradients need to be investigated in detail. Many

theoretical and experimental studies on micro heat pipes have been conducted since the concept of micro heat pipe was proposed by Cotter [1] in 1984. These investigations show that surface tension, wettability and solid–liquid interactions are the primary factors that govern the behavior of various interfaces, especially the liquid–vapor interfaces [2–8]. Therefore the understanding of the interfacial characteristics in a micro heat pipe, and essentially in any heat transfer device, is crucial for improving the heat performance and its industrial applications.

The nonisothermal flow in a micro heat pipe is usually driven by pressure change due to changes of capillary and intermolecular forces along the length of a heat pipe [9]. During the fluid flow, liquid evaporates in the hot region and vapor flows back towards the cold region. These phase change processes can dramatically alter the interfacial temperature, resulting in surface tension

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**Nomenclature**

$E$	apparent energy with the zero defined at 298.15 K (J kg <sup>-1</sup> )
$F_{vol}$	the interface-induced volumetric force (N m <sup>-3</sup> )
$g$	gravity acceleration, m s <sup>-2</sup>
$h_{LH}$	latent heat at 298.15 K (J kg <sup>-1</sup> )
$k$	thermal conductivity (W m <sup>-1</sup> K <sup>-1</sup> )
$p$	pressure (Pa)
$Q$	source term due to heat transfer (W m <sup>-3</sup> )
$S$	source term due to mass transfer (kg s <sup>-1</sup> m <sup>-3</sup> )
$D_{i,m}$	diffusion coefficient for $i$ th species in the mixture (m <sup>2</sup> s <sup>-1</sup> )
$J_i$	diffusion of $i$ th species (kg s <sup>-1</sup> m <sup>-1</sup> )
$Y_i$	mass fraction of $i$ th species
$h_i$	enthalpy of $i$ th species (J kg <sup>-1</sup> )
$T$	temperature (K)
$t$	time (s)

$\vec{v}$	velocity vector (m s <sup>-1</sup> )
$v$	velocity (m s <sup>-1</sup> )

**Greek Symbols**

$\alpha_l$	volume fraction of liquid phase
$\alpha_v$	volume fraction of vapor phase
$\mu$	viscosity (kg m <sup>-1</sup> s <sup>-1</sup> )
$\rho$	density (kg m <sup>-3</sup> )

**Subscripts**

$c$	cold wall
$h$	hot wall
$l$	liquid
$v$	vapor
$i$	$i$ th species
sat	saturation

gradients and consequently thermal Marangoni convection. For simple fluids, surface tension decreases with increasing temperature, resulting in thermocapillary stresses that can drive the liquid leave from hot regions, leading to film dryout [10]. For binary fluids, however, surface tension gradients along a liquid–vapor interface can also be caused by concentration gradients in the nonisothermal flow. In particular, dilute aqueous solutions of alcohols with a high number of carbon atoms, namely self-wetting fluids [11–15], have unique surface tension characteristics that increase with increasing temperature above a critical value. Therefore the Marangoni flow drives the liquid flow towards hot regions, avoiding film dryout for a number of binary fluids.

Theoretical and experimental investigations on heat and mass transfer in micro heat pipes have been conducted to obtain the fundamental understanding of transport processes. Most of these studies focus on the heat transport in micro heat pipes with different structures, such as trapezoidal, triangulator V-shaped cross section [16–18]. Few models consider the surface tension and hence the Marangoni effect on phase change of binary fluids or self-wetting fluids [11–15]. Very few studies the detail of liquid evaporation and gas condensation in the micro heat pipes, e.g., the liquid and vapor phase velocity fields [19–21]. Since simulation of the Marangoni convection of binary fluids in arbitrary geometries has rarely been reported in the literature and closed microcavity is perhaps the simplest model for revealing the mechanisms, we investigate numerically the effect of Marangoni convection on phase change of several binary fluids in a closed microcavity with square cross section by providing detailed velocity and temperature fields, with consideration of the influence of non-condensable gases on heat and mass transfer. The purpose of this paper is for a better understanding of the transport processes and designing of micro heat pipes, thus a further investigation on a real micro heat pipe can be performed based on this study.

## 2. Numerical model

### 2.1. Governing equation

The numerical investigation on flow of binary fluids in a closed microcavity is accomplished by using the volume of fluid (VOF) model in FLUENT software package, with source terms added by user defined functions (UDF) due to mass transfer in multiphase flows. In the VOF model, the tracking of the interface(s) between

the phases is accomplished by the solution of a continuity equation for the volume fraction of one (or more) of the phases. For the liquid and vapor phases, these equations are:

$$\frac{\partial \alpha_l}{\partial t} + \nabla \cdot (\vec{v} \alpha_l) = \frac{S}{\rho_l} \quad (1)$$

$$\frac{\partial \alpha_v}{\partial t} + \nabla \cdot (\vec{v} \alpha_v) = \frac{S}{\rho_v} \quad (2)$$

where  $\alpha_l$  is volume fraction of liquid phase and  $\alpha_v$  is volume fraction of vapor phase. Volume fractions of all phases sum to unity,

$$\alpha_l + \alpha_v = 1 \quad (3)$$

The volume fraction equation is solved through implicit time discretization. The continuity, momentum and energy equations are, respectively,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S \quad (4)$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot [\mu (\nabla \vec{v} + \nabla \vec{v}^T)] + \rho \vec{g} + F_{vol} \quad (5)$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [\vec{v} (\rho E + p)] = \nabla \cdot (k \nabla T) + Q \quad (6)$$

where  $\rho$  is the density (kg m<sup>-3</sup>),  $\vec{v}$  velocity vector (m s<sup>-1</sup>),  $t$  time (s),  $p$  pressure (Pa),  $\mu$  viscosity (kg m<sup>-1</sup> s<sup>-1</sup>),  $F_{vol}$  interface-induced volumetric force (N m<sup>-3</sup>),  $E$  apparent energy (J kg<sup>-1</sup>),  $k$  thermal conductivity (W m<sup>-1</sup> K<sup>-1</sup>), and  $S$  is the source term (kg s<sup>-1</sup> m<sup>-3</sup>) due to mass transfer and can be described as [22,23]

$$S = r_l \alpha_l \rho_l (T_l - T_{sat}) / T_{sat}, \quad T_l \geq T_{sat} \quad (7)$$

$$S = r_v \alpha_v \rho_v (T_l - T_{sat}) / T_{sat}, \quad T_l \leq T_{sat} \quad (8)$$

The interfacial temperature is assumed at the saturation temperature,  $T_{sat}$ . For this purpose, the coefficients  $r_l$  and  $r_v$  are hereby specified at 100 s<sup>-1</sup> in order to numerically maintain the interface temperature within  $T_{sat} \pm 1$  K.

The heat transfer is simply determined from the mass rate of evaporation or condensation, in addition to the conduction and

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