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Numerical Investigation on the Effect of Container Geometry on Water Evaporation in Pure Vapor at Low Pressures

SiBo Wan [1], YouRong Li [1*]
1 School of Energy and Power Engineering, Chongqing University, Chongqing 400044, China
(*Corresponding Author: liyourong@cqu.edu.cn)

ABSTRACT

To explore the effect of different container geometry and interface curvature on water evaporation at low pressure, a two-side mathematical model is established, and a series of numerical simulations are carried out. According to the calculation results, the surface curvature has distinct effects on the development of thermocapillary convection, and thus affects the flow and temperature distribution in the liquid phase. The difference in the dominant convection will lead to the difference in the energy transmission mode. In addition to thermal conduction, the roles of thermocapillary convection and buoyancy flow should be considered.

Keywords: evaporation, thermocapillary convection, buoyancy flow, energy transfer

1. INTRODUCTION

Water evaporation is a natural phenomenon with a wide range of industrial, medicinal, and agricultural applications, its research has important value in seawater desalination, printing, self-assembly of colloidal particles, thermal management of electronic equipment, DNA chip manufacturing, etc. With the continuous deepening of research, discoveries have led to the expansion of the application of evaporation, such as the use of water evaporation to generate electricity, which is promising progress in clean energy technology.

Liquid evaporation involves the complex coupling between heat transfer and convection of fluid, and the interface phenomenon is inevitably intertwined with heat transfer. In the past, the research in this field mainly focused on the evaporation of water droplets into the air at atmospheric conditions, the mechanism of low-pressure evaporation has not received much attention. However, it is necessary to study this evaporation mechanism, not only because evaporation at low pressures is of great significance in some advanced applications (such as vacuum flash evaporation cooling) [1], but when the pressure is reduced, other mechanisms, including Marangoni convection and buoyancy convection, are also playing a role. The different control mechanisms lead to different characteristics of interface phenomena and fluid flow during evaporation.

In 1999, Fang and Ward [2] carried out a series of experiments on the evaporation of water in a funnel at low pressures and measured the temperature on both sides of the gas-liquid interface through thermocouples. They found that the temperature jump occurred at the evaporation interface, and the temperature at the vapor side is always higher than that of the liquid phase. The direction of the temperature jump is opposite to that predicted by the kinetic theory, and the value is also one order of magnitude different. After that, the research on evaporation at low pressures gradually began to enrich, and the theoretical research on evaporation flux also gradually developed. Ward and Fang [3] proposed SRT expression without fitting any empirical coefficient based on a series of experimental measurements, and Bedeaux and Kjelstrup [4] derived the expression of mass and heat flux based on the NET (non-equilibrium thermodynamic theory), simulation based on MD (molecular dynamics) and DFT (density functional theory) is becoming the basic method to explore the phase transition process. In addition, there is some controversy about the role of the internal flow of liquid in evaporation. Some studies [5] believe that thermocapillary convection can promote evaporation, the energy balance equation at the interface can only be satisfied when both thermal conduction and thermocapillary convection are taken into account. However, some experimental and simulation results [6]

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show that the effect of thermocapillary convection on evaporation can be almost ignored.

Since the evaporation process is affected by the internal flow of the fluid, the geometric configuration of the container and the curvature of the free surface will cause differences in convection and interface characteristics. To clarify the impact of flow instability on the energy transfer at the interface, a two-side mathematical model is established in this work to simulate the evaporation process of water at low pressures with different geometric structures and interface curvature.

2. MODEL AND METHOD

2.1 Physical model

The schematic view of the physical model is illustrated in Fig. 1. The entire device can be simplified to a two-dimensional axisymmetric problem due to the axial asymmetry of the cylindrical pool and the funnel. All elements of the experimental system are shown, including liquid, vapor, solids, and vacuum chamber wall.

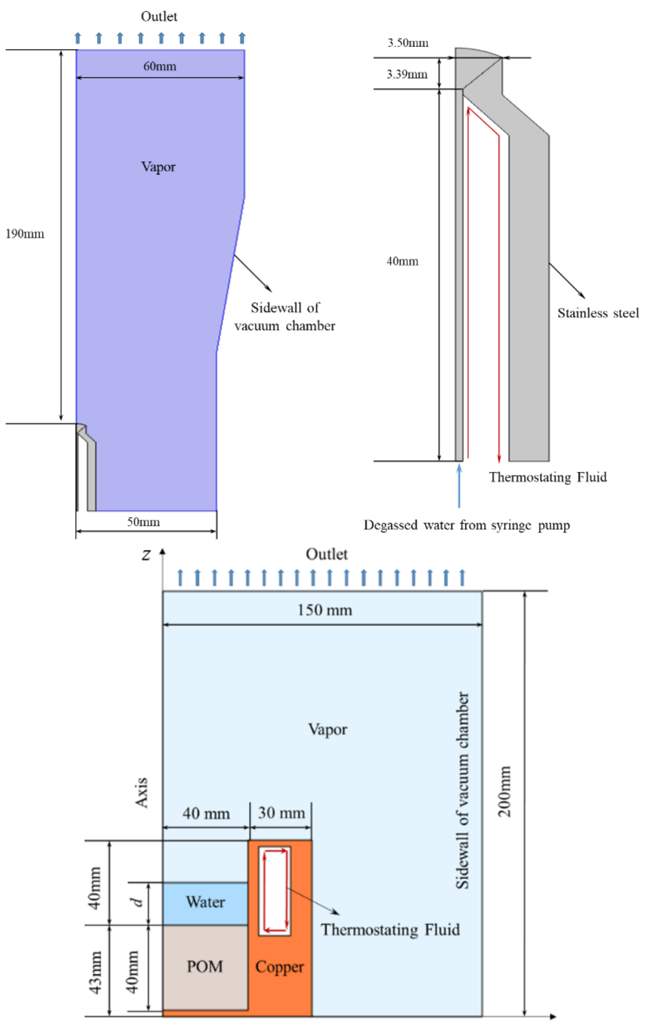


Fig. 1. Schematic of the physical system. Upper: Ward and Duan [7]; Below: Zhang et al.[8]

2.2 Mathematical model

For the mathematical model, the liquid phase and vapor phase are considered incompressible and compressible respectively. To simplify the model, several assumptions are introduced: (1) The density of the liquid is considered as a function of temperature only, while the density of vapor follows the ideal gas equation of state; (2) The Marangoni effect is taken into account and the surface tension is a linear function of temperature; (3) The temperature jump at the liquid-vapor interface is considered. The no-slip boundary conditions are adopted for all solid walls, and the sidewall of the vacuum chamber is set as the thermal insulation boundary condition. The SRT expression is applied to the liquid-vapor interface to calculate the mass flux of evaporation.

2.3 Sumerical validation

The mathematical model is solved by the finite element method. Considering the balance of calculation efficiency and accuracy, in the finite element formulation, the second-order Lagrange element is chosen for velocity components while the pressure field used Lagrange linear shape elements to discretize. The average mass flux calculated by the mathematical model is compared with experimental results, as shown in Fig. 2. The great agreement between the simulation results and the experimental measurements shows the correctness of the mathematical model.

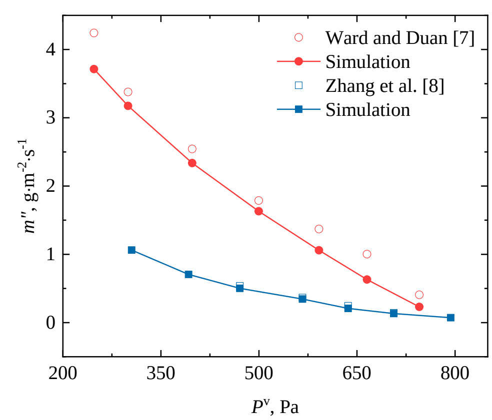


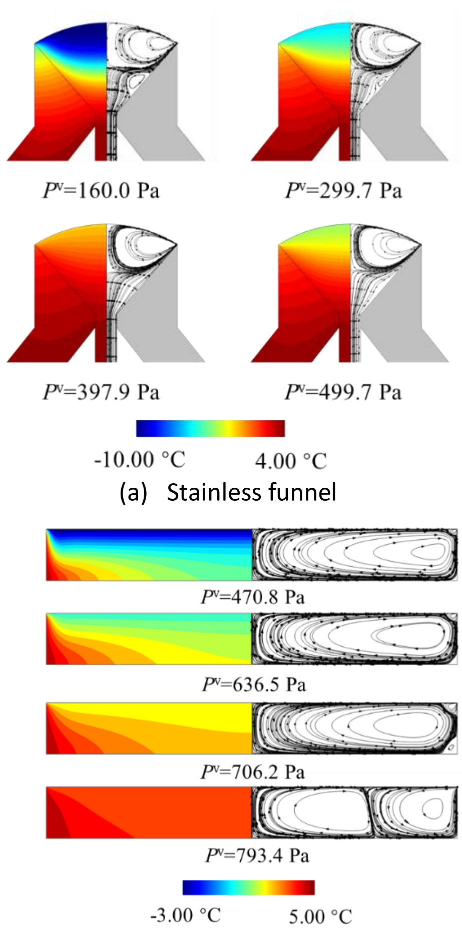
Fig. 2. Comparison of the evaporation mass flux with experimental results

3. RESULTS AND DISCUSSION

3.1 The flow and temperature distribution

The temperature distribution and flow field in the liquid are shown in Fig. 3 when water evaporates from two different containers. The heating temperature is consistent with the experiment, T_h=4 and 5 ℃ respectively. It can be found that the development of Marangoni convection is affected by the curvature of the interface, and buoyancy convection plays an important role in the velocity distribution. When water evaporates in the funnel, the intense temperature gradient at the triple point induces thermocapillary convection. Due to the convex evaporation surface, thermocapillary flow fully develops along the liquid-vapor interface, occupies almost half of the funnel, and becomes the main convection inside the liquid. Since the thermal conductivity of the stainless steel side wall is much greater than that of water, the isotherm is found to be parabolic according to the temperature distribution, which means that the temperature of the liquid near the sidewall is higher than the water temperature near the center of the cavity on the same horizontal line. Therefore, the dense fluid flows downward along the funnel rim when the pressure is low enough. At the same time, due to the effect of buoyancy, the falling fluid will return and form a clockwise buoyancy convection vortex. With the increase of pressure, the temperature difference between the free surface and the sidewall decreases, and the buoyancy effect weakens, making the buoyancy vortex near the edge of the funnel gradually decrease and then disappear.

For the evaporation of water in the cylindrical pool, no matter whether the evaporation envelope is concave or planar, the thermocapillary convection only exists in the corner near the triple point, and the buoyancy convection almost occupies the entire container, squeezing and suppressing the development of the thermocapillary convection in the corner along the interface to the centerline. As the pressure rise, a small buoyancy vortex is generated between the side wall and the bottom of the pool, which is because of the existence of a water layer with maximum density. When the pressure increases to 800 Pa, the interface cooling effect is weakened, and the driving force of buoyancy convection is insufficient, hence the Marangoni convection and buoyancy convection occupy half of the container respectively.



(b) Cylindrical pool

Fig. 3. Flow and temperature distribution in the liquid phase at different pressures

3.2 *The uniform-temperature layer*

According to the axial temperature distribution shown in Fig. 4, when water evaporates in a stainless steel funnel, a thin layer with nearly uniform temperature appears below the liquid-vapor interface when the pressure is low enough. Within this water

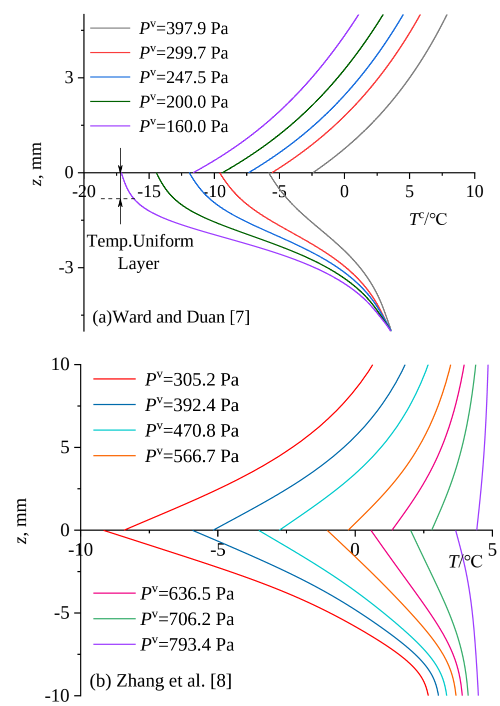


Fig. 4. The axial distribution of temperature near the liquid-vapor interface at centerline

layer, the temperature gradient is very small. This phenomenon is first discovered by Ward and Duan [7], they put forward the concept of a uniform-temperature layer, but they did not have a clear definition of it. For quantitative analysis, we define the thickness of the uniform-temperature layer as $\delta = z[T_i]-z[T_i-\gamma(T_h-T_i)]$, where $z[T_i]$ is the height of the interface, and the value of γ is 0.03. Therefore, $z[T_i-\gamma(T_h-T_i)$ denotes the vertical position that the temperature changes between the interface temperature and the throat temperature of the funnel is less than 3%.

The distribution of the uniform-temperature layer thickness δ along the interface is shown in Fig. 5, and its profile along the horizontal direction is parabolic. With the decrease in pressure, the thickness of the uniform-temperature layer thickens at the centerline but remains almost constant near the sidewall. The thin layer is not found in the process of water evaporation in the cylindrical pool, the fluid temperature increases almost linearly with the depth of the liquid layer below the evaporation surface. The key factor causing this difference is thermocapillary convection, which fully develops at the convex surface. Below the Marangoni convection vortex, the vertical direction of the liquid flow is opposite. The mixing of the two contrary flows is the most important reason for the formation of the uniform-temperature layer. However, at the planar or concave free surface, the thermocapillary convection only exists in the corner near the triple point and fails to produce sufficient mixing with the buoyancy convection below, resulting in the absence of the uniform-temperature layer.

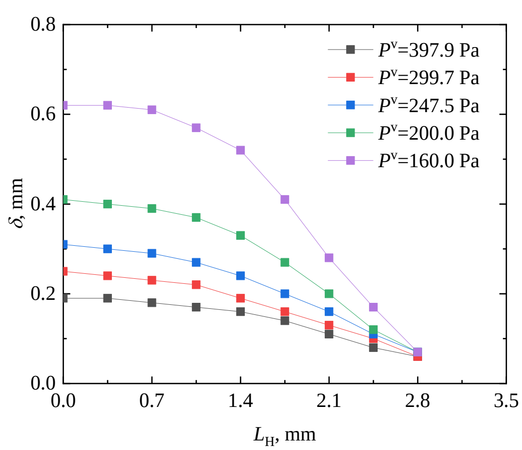


Fig. 5. Distribution of uniform-temperature layer thickness along the horizontal position

3.3 The energy transfer mode

The study of the energy transfer mechanism in the evaporation process is a significant factor to reveal the essence of evaporation. Thermal conduction undoubtedly plays a decisive role in energy transfer, but the contribution of different convection to evaporation also needs to be paid attention to. Through the energy balance of the liquid-vapor interface, the contribution of different heat transfer modes to evaporation is calculated, as shown in Fig. 6. It can be found that when the heating element is located on the liquid side, the heat flux of the vapor phase can be almost ignored, but the energy transfer mode in the liquid phase is different. When water evaporates in the stainless steel funnel, there is only Marangoni convection occupies the surface, and thermal conduction is the main body of heat transfer. However, with the decrease of pressure, the contribution of thermocapillary convection gradually becomes non-negligible, and even becomes an important part of energy supply.

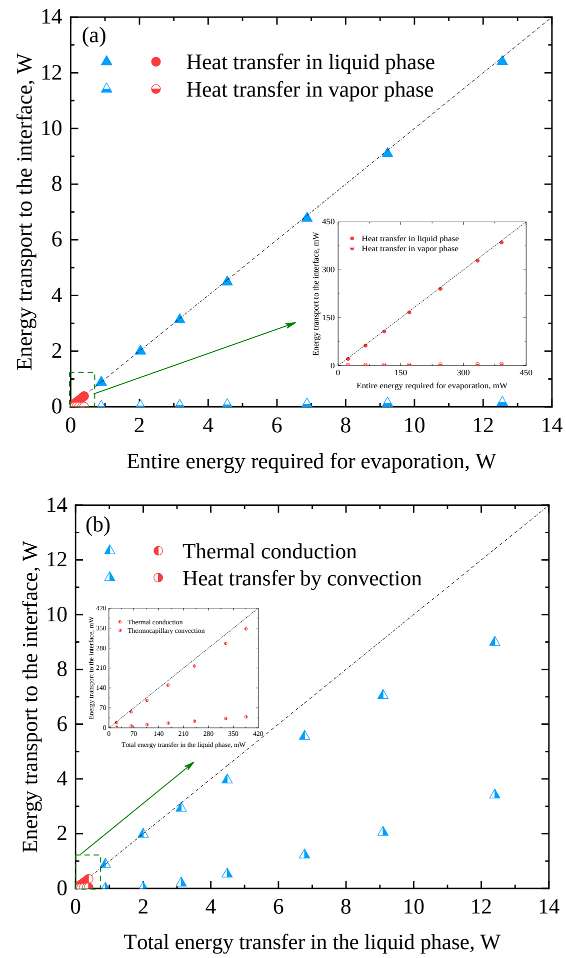
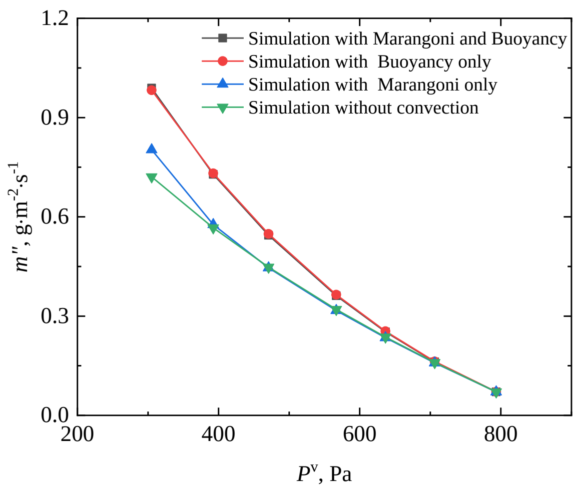
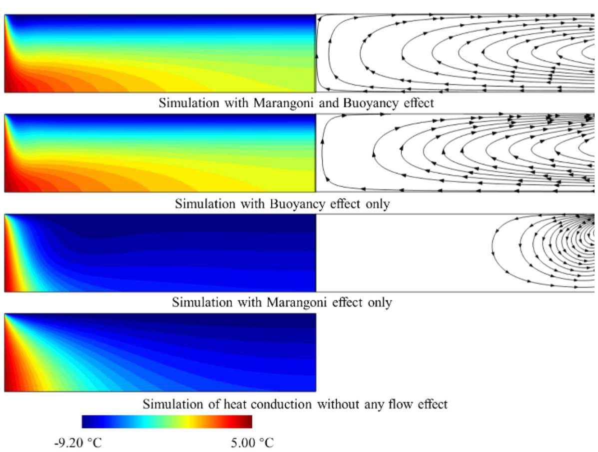


Fig. 6. (a) The energy transferred between the liquid and vapor phases to evaporation interface; (b) The contribution of the thermal conduction and convection for heat transfer in liquid phase at the different pressures. Blue triangle: from Zhang et al. [8]; Red circle: from Ward and Duan [7]

In the process of water evaporation in the cylindrical pool, buoyancy convection replaces thermocapillary convection as the main flow. Through simulation at four working conditions including both buoyancy and Marangoni effect, only Marangoni effect, only buoyancy effect, and without convection, the comparison of mass flux is shown in Fig.7(a). It can be found that the evaporation rate with buoyancy only is almost the same as that with both buoyancy and the Marangoni effect. According to the flow and temperature distribution shown in Fig. 7(b), buoyant convection brings the thermal fluid at the sidewall to the bottom, making the temperature of the entire bottom increase, thereby increasing the evaporation intensity in the central area, while the thermocapillary convection existing in the corners transfers the heat directly from the wall to the evaporation free surface and promotes the evaporation of the triple point. However, if the buoyancy effect is ignored, only thermocapillary convection exists in the



(a) Variation of the average evaporation flux



(b) The flow and thermal fields

Fig. 7. Variation of the average evaporation flux at the interface with pressure at different convection conditions (a) and the flow and thermal fields (b). The green line represents an isotherm with T=4 ℃, where water has the maximum density

liquid pool. At the centerline, the cold fluid at the interface is brought to the bottom of the liquid pool by the flow, which reduces the overall temperature of the central area and weakens evaporation. Therefore, in addition to thermal conduction, buoyancy convection is also an important source of energy for the interface in the cylindrical pool, which is far more important than Marangoni convection.

4. CONCLUSIONS

Based on a series of numerical simulations of water evaporation in different geometric containers, it can be found that the curvature of the liquid-vapor interface will affect the development of thermocapillary convection, thus affecting the temperature distribution and energy transfer in the liquid. The convex surface will promote the development of thermocapillary convection and facilitate its mixing with the flow in the opposite direction below, forming the uniform-temperature layer. On the other hands, the planar or concave surface will inhibit diffusion of thermocapillary convection along the interface towards the centerline, making buoyancy convection become the main convection to maintain evaporation. Besides, the thermal conduction cannot provide all the energy required for evaporation, the contribution of thermocapillary convection and buoyancy flow cannot be ignored.

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DECLARATION OF INTEREST STATEMENT

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. All authors read and approved the final manuscript.

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