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THE STUDY ON FLOW PATTERNS OF CONDENSATION OF SUPERHEATED VAPOR IN NANOCHANNELS

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ABSTRACT

The model of two phases of liquid and vapor flow and vapor condensation under the condition of exerted force was established in parallel nanochannel. Fluid was water molecular and the solid walls are composed of Pt atoms. The process of vapor condensation in nanochannel wall was simulated by molecular dynamic simulation. The different flow patterns of the condensation process of superheated water vapor, which mainly were annular flow, injection flow, slug flow, bubble flow and shrinking bubble flow, were observed under different conditions. For low pressure of water vapor, a new flow pattern which was named as fluctuation flow appeared during condensation process. The simulation results agreed very well with the experimental results provided by references.

Keywords condensation; molecular dynamic simulation; nanochannel; flow pattern

INTRODUCTION

There are many differences between microchannel flow patterns and conventional scale flow patterns. For example, stratified flow doesn't happen in microchannel, and so do slug flow and annular flow. However current experimental researches show that different researchers got different flow patterns[1-2]. Now there are almost not any mechanism researches on these and most researches are based on experiments [3-5]. This paper tries to investigate the variation of flow patterns during the condensation process by molecular dynamics simulation and give some explanations for the transition mechanics of different flow patterns.

Constrained by the computer's calculation capacity, the simulated nanochannel is very short and the number of the simulated molecules is small number of particles. The simulation method with the boundary condition of constant wall temperature was used to observe the different flow patterns during the condensation process. We hope to achieve the similar results as experiments on this by the simulation.

SIMULATION DETAILS

Schematic of model flow and condensation through nanochannel is shown in Fig.1. Poiseuille flow of the superheated water vapor and the condensation of the superheated vapor happen in a nanochannel bounded by two solid walls. The superheated vapor flows along the nanochannel in the x-axis direction driven by an external force applied on the system and the condensation process happens when vapor gets close to the cold wall. The solid wall is composed of platinum atoms. The length of channel in the x-axis direction named as Lx is equal to 29.023σ (about 8.8nm) and the length of channel in the y-axis direction named as Ly is half of the Lx. The width of the channel named as Lz are Lx/8, Lx/6, Lx/4, Lx/2,2Lx /3 respectively. The system is

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periodic in the x and y directions. The initial particle number of superheated water vapor is composed of 864 water molecules. The walls, which are fixed, lie in the x–y plane and are separated in the z direction. Each solid wall is made up of six layers of platinum atoms arranged as a face-centered-cubic crystal lattice and the surface of the lattices contacts with the water molecular. The walls are composed of 2048 Pt atoms.

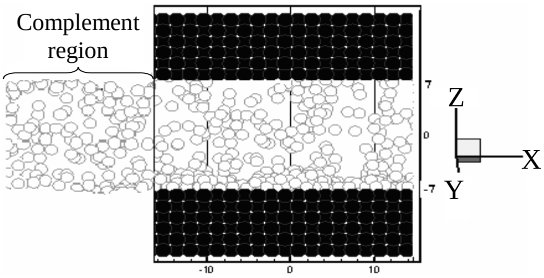

Fig.1 Schematic of model flow and condensation through nanochannel

The well-known L-J potential function is used to consider the interaction between the fluid particles and the interaction between the fluid and wall particles [6]:

$$\phi(r_{ij}) = 4\varepsilon\left[(\sigma / r_{ij})^{12} - (\sigma / r_{ij})^{6}\right] \qquad (1)$$

Here the length parameter $\sigma = 0.303nm$, the energy parameter $\varepsilon = 8.6981\times10^{-21} J$ and molecular mass $m = 2.9986\times10^{-26} kg$ for water. The parameters of the platinum atoms in solid walls are as follows: $\sigma = 0.277nm$, $\varepsilon = 0.4786\times10^{-21} J$, $m = 32.3943\times10^{-26} kg$.

In order to calculate the interaction between the platinum atoms and the water moleculars, Lorentz-Berthelot mixing law is used [7]:

$$\sigma_{ap} = (\sigma_{ar} + \sigma_{pt})/2.0 \qquad (2)$$

$$\varepsilon_{ap} = \sqrt{\varepsilon_{ar} \times \varepsilon_{pt}} \qquad (3)$$

The fluid molecules have been assumed to be constituted of quantities of spherical molecules, so Newton's second law can be used to describe the molecular motion in the system. The motion equations are solved by the leap-frog algorithm. In order to attain effective computer simulations, the non-dimensional units were used: the unit of length is the molecular diameter σ ; the unit of the molecule mass is m; the unit of energy (strength of interaction in the L-J potential) is e; the unit of time is set to $\sigma\sqrt{m/\varepsilon}$; the unit of density is $m\sigma^{-3}$). The cut-off radius, beyond which the intermolecular interaction can be neglected, is 3.5 and a non-dimensional time step is 0.005 in this paper.

In order to keep the condensation process sustained and to be stable, it is necessary to add fluid molecules into the vapor space according to the density variation of the space during the condensation process. In the entrance of the nanochannel, there is a certain supplemental region and the vapor in this region is always in superheated state with the temperature of 300℃. The density of vapor space was calculated per 1,000 steps. If that value was less than the initial vapor density, it indicates that some particles have condensed on the walls and particles are needed to add into the vapor space during the condensation. Particles are obtained randomly from the complement region and stayed randomly in the inlet of the nanochannel. It is worthy to note that the size of the vapor space is decreased in the condensation process. The vapor space must be determined correctly according to the state of condensation.

A condensation process under the condition of pressure being 3.7177MPa was studied firstly.

In order to study the effects of channel width on the formation of flow patterns, the external force is set to dimensionless 2.0(about 51pN), the vapor temperature is 300℃ and the pressure of the vapor is 3.7177MPa. The corresponding saturation temperature of this pressure is about 245℃.As long as the wall temperature is below 245℃, the condensation process will begin. Under the conditions of five kinds of channel width and four kinds of wall temperature, flow patterns are simulated when the nanochannel width is Lx/8, Lx/6, Lx/4, Lx/2,2Lx /3 and the wall temperature is 150℃, 100℃, 50℃, 20℃, respectively.

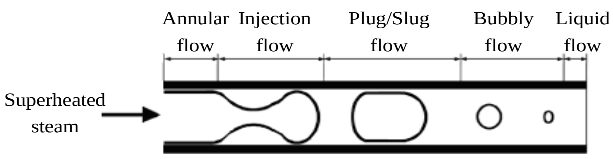

Fig.2 Different flow patterns at different times in microchannel

Under the conditions of the different channel widths and wall temperatures, the results show that the sequence of different flow patterns is consistent always. They are annular flow，injection flow, slug flow, bubble flow and shrinking bubble flow successively, as shown in the Fig.2 and the simulation results match well with the experimental results in

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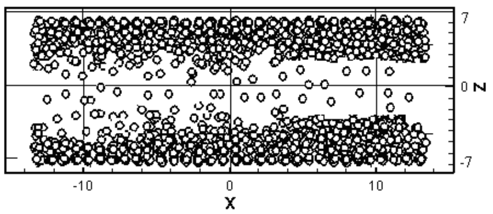
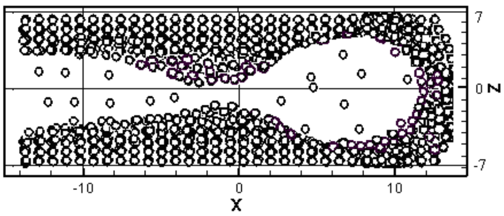
reference [1]. The channel width and wall temperature changes, the transition location between different flow patterns will change. The simulation results also show that the number of the flow patterns is related to the external force acting on the fluid. A larger force leads to fewer kinds of flow patterns and a smaller one leads to more kinds of flow patterns. As shown in the table 1, bigger external force means the fluid has more kinetic energy and the rapid fluid flow in the channel leads to the insufficient condensation, thus the appearing probability of the flow patterns such as the bubbly flow and shrinking bubble flow that need full condensation is lowered naturally. Different flow patterns under the condition of different external force and the temperature of 300℃ are shown in the table 1.

Table.1 Different flow patterns under the condition of different external force at 300℃

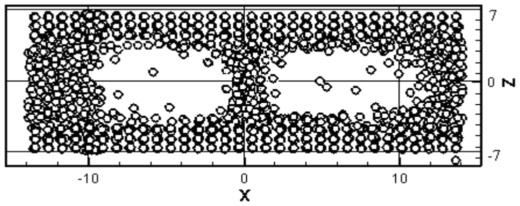
External force	Flow patterns (Tvapor=300℃ p=3.7177MPa)
2.0（51pN）	Annular flow; Injection flow; Slug flow; Bubble flow; Shrinking bubble flow (Fig.4(a)—Fig.4(e))
4.0(102pN)	Annular flow ; Injection flow; Slug flow; Bubble flow;
6.0(153pN)	Annular flow ; Injection flow; Slug flow; Bubble flow;
8.0(204pN)	Annular flow ; Injection flow;
10.0(255pN)	Annular flow



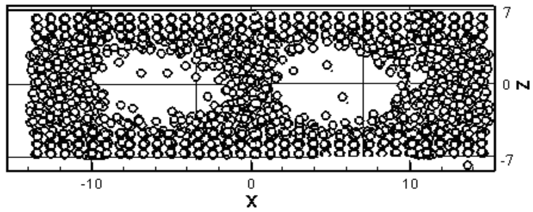
(a) Annular flow (after 30000steps)



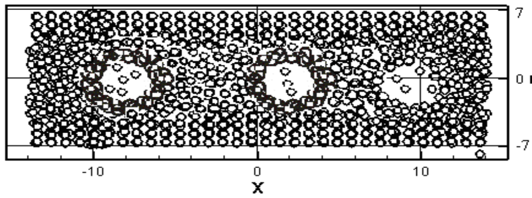
(b) Injection flow (after 40000steps)



(c) Slug flow (after 50000steps)



(d) Bubble flow (after 70000steps)



(e) Shrinking bubble flow (after 90000steps)

Fig.3 Different flow patterns during the condensation process at a high pressure

THE TRANSITION OF FLOW PATTERNS

In order to obtain a clear observation of various flow patterns for further research, the external force must be set properly. If the external force is excessively large, a full condensation of water vapor cannot appear in simulated regions. After several simulated experiments, it is found that the external force set to 2.0 is the relatively ideal simulated condition.

(a) Change from injection flow to slug flow

It is the condensation in the vertical direction that leads to the conversion of the injection flow into slug flow. Thus, the conversion is largely influenced by the channel width and the wall temperature. The effects of channel width and wall temperature on transition from injection flow to slug flow are shown as Fig.4. It is shown that the wider the channel is, the longer time will be needed to finish the transition. Under the condition of lower wall temperature (20℃-50℃), the transition time varies linearly with the channel width. On the contrary, if the wall temperature becomes higher (100℃-150℃), there will be two different results. As to the comparatively narrow channel, the transition time varies linearly with the channel width. In the wider channel, the

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relationship between the channel width and the transition time is non-linear. There are two explanations for this phenomenon. Firstly, due to the impact of thermal resistance of liquid film, the condensation rate will slow down for the higher temperature condition. In the narrower channel, the liquid gets together before the action of the thermal resistance of the liquid film. Because of the thermal resistance, the system needs more time to finish the transition process. In this situation, there exists linear relationship between the transition time and the channel width. Secondly, wall temperature is another factor that influences the transition time. If the wall temperature is lower, the condensation speed is faster. Even in the wider channel, the liquid bridge can be completed in a short time under the condition of lower temperature and the transition time still varies linearly with the channel width. The channel width and the wall temperature are the two factors that influence the conversion of injection flow into slug flow. The higher the wall temperature is, the longer the will be needed. The wider the channel is, the longer the time will be needed in the transition process.

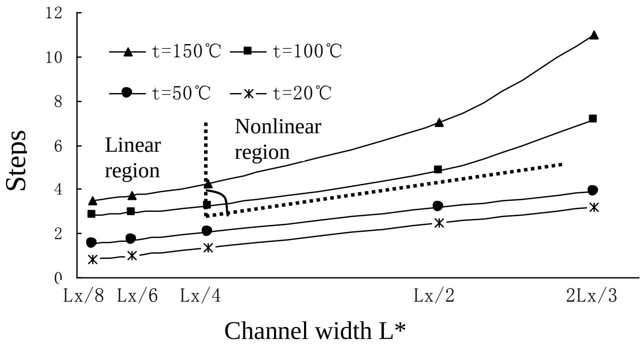

Fig.4 Effects of channel width and wall temperature on transition time from injection flow to slug flow

(b) Change from the Slug flow to the bubble-flow

It is the influence of the movement of vapor in the horizontal direction that leads to the conversion of slug flow into bubble flow. The main reason for this conversion is that the vapors first combine and then separate from each other.

The conversion between this two flow patterns take place in the horizontal direction. It is not the channel width and the wall temperature but the external force in the horizontal direction that influences the conversion process. The results of the simulation proved our hypothesis. The time of conversion doesn't obviously vary with the changes of the channel width and the wall temperature. That is shown as Fig.5. This indicates that the channel width and the wall temperature are not the main factors, which influence this kind of conversion. Fig.6 presents the relationship between the transition time and the external force on this kind of conversion. It is shown that the transition time varies with the force, which shows that the force in the horizontal direction is the main factor that influences the conversion of slug flow into bubble flow.

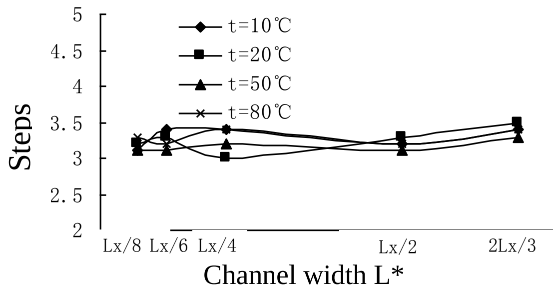

Fig.5 Effects of channel width and wall temperature on transition time from slug flow to bubble flow

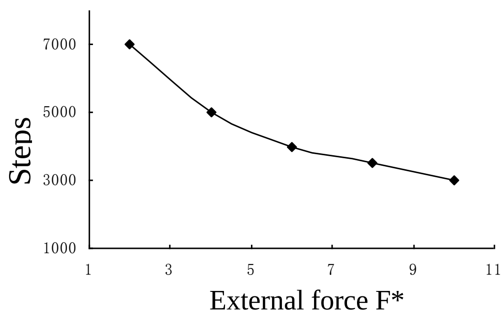

Fig.6 Effects of external force on transition time from slug flow to bubble flow when the channel width is Lx/6

PARAMETER STATISTICS IN THE VAPOR CONDENSATION PROCESS

(a) The velocity profile the condensation process

The profile of fluid velocity in nanochannel is compiled during the vapor condensation process under the conditions of constant temperature 300℃, wall temperature 20℃ and the external force 2.0. When the condensation occurs, the fluid exists as the superheated vapor and the velocity profile, which is shown as Fig.7, is quadratic. As the condensation process goes on, the water vapor gradually condensates on the wall surface and the liquid drops become bigger. Then the velocity profile deviates from the standard quadratic curve.

The viscous of liquid is higher than that of vapor at the same shearing force, which results in small changes in the velocity gradient. So the velocity profile in the vapor-liquid

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interface will be discontinuous. With the further condensation, the channel is fulfilled with liquid water and the velocity profile becomes the quadratic curve again. However, due to the difference in specific heat capacity，the average velocity in liquid phase is obviously smaller than the average velocity in vapor phase. Liquid has a higher heat capacity and contains more heat energy. According to the energy conservation law, more thermal energy will lead to less kinetic energy which can help to explain the fact that the velocity in liquid phase is smaller than in vapor phase.

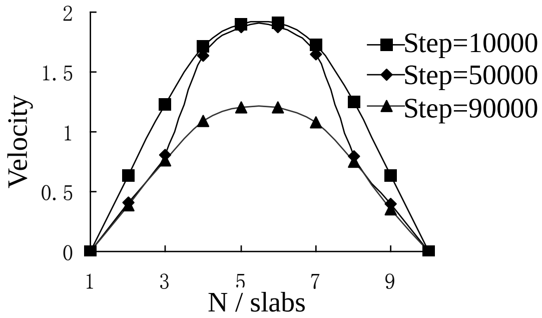


Fig.7 The velocity profile

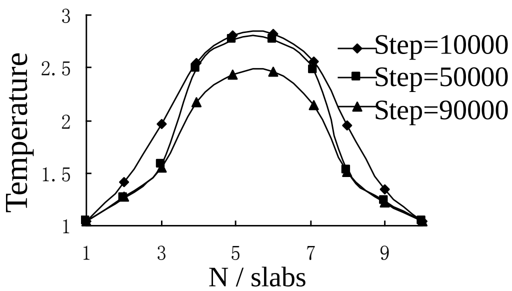


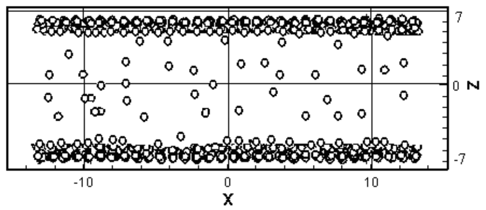
Fig.8 The temperature profile

(b)The temperature profile during the condensation process

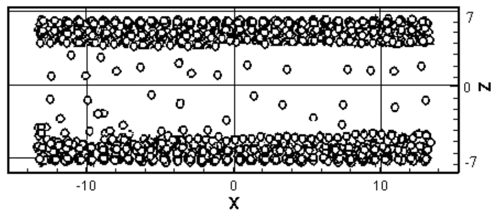
Fig.8 shows that the temperature profile and the velocity profile have a similar trend in a large degree. In the coexistence of vapor and liquid, an inflection point appears on the temperature profile which stands for the liquid-vapor interface. The difference of heat conductive factors of vapor and liquid can explain this phenomenon. Due to the higher thermal conductivity in liquid phase, the heat can transfer fully among the layers which results in a smaller temperature differences among the layers. On the contrary, the temperature difference is larger in vapor phase, so there is a discontinuously inflection point on the temperature profile which stands for the liquid-vapor interface.

VAPOR CONDENSATION UNDER LOW-PRESSURE CONDITION

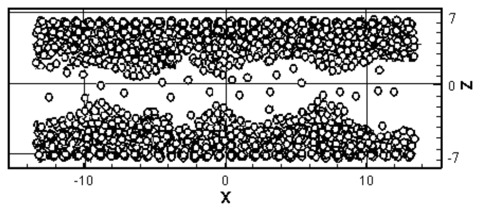
The process of vapor condensation was simulated under the low pressure of 0.3833MPa in order to get a comprehensive study on the conversion of flow patterns during the condensation process. Initial temperature of water vapor is still set to 300℃. In order to compare the simulation results under low pressure with one under high pressure, the simulation system is the same in size. The initial number of the vapor particles is 108 in the simulation system. The density of the vapor maintains 80kg/m^3 during the simulation course.



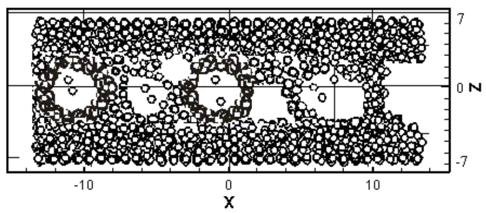
(a) 30000 steps



(b)50000 steps



(c)100000 steps



(d)180000 steps

Fig.9 The condensation process at low pressure

When the pressure of water vapor is 0.3833MPa, the corresponding saturation temperature is 142℃. The wall temperature is 20℃. As shown in the Fig.9, a new flow pattern—fluctuation flow emerges. The pattern will change from annular flow to fluctuation flow and finally into bubble

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flow. However, injection flow and slug flow will not appear and the bubble flow comes from fluctuation flow directly. The formation mechanism of the bubble flow here is very different with that under high pressure where the bubble flow emerges because of the formation of the minute bubbles that comes from the pursuing and aggregation of the bubbles in the flow direction.

CONCLUSIONS

1. Molecular dynamics simulation was successfully used to simulate the flow pattern conversion during the process of the condensation of water vapor.
2. The results show that during the conversion process, flow patterns orderly change from annular flow to injection flow, slug flow, bubble flow and finally shrinking bubble flow under high vapor pressure. The simulation results are in good agreement with the results in references on experimental researches.
3. Under low pressure of water vapor, a new flow pattern−fluctuation flow appears during condensation process.
4. Under high pressure of the water vapor, it is the condensation in the vertical direction that causes the conversion of injection flow into slug flow. The aggregation of bubble in the horizontal direction leads to the conversion of slug flow into bubble flow.

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