Original Article

Molecular dynamics study of liquid sodium film evaporation and condensation by Lennard-Jones potential

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Abstract
Deeply understanding the phase change of thin liquid sodium film inside wick pore is very important for further studying high-temperature sodium heat pipe’s heat transfer. For the first time, the evaporation and condensation of thin liquid sodium film are investigated by the Lennard-Jones potential of molecular dynamics. Based on the startup and normal operation of the sodium heat pipe, three different cases are simulated. First, the equilibrium is achieved and the Mass Accommodation Coefficients of the three cases are 0.3886, 0.2119, 0.2615 respectively. Secondly, the non-equilibrium is built. The change of liquid film thickness, the number of gas atoms, the net evaporation flux \(J_{\text{net}}\), the heat transfer coefficient \(h\) at the liquid-gas interface are acquired. Results indicate that the magnitude of the \(J_{\text{net}}\) and the \(h\) increase with the basic equilibrium temperature. In 520–600 K (the startup of the heat pipe), the \(h\) has approached 5–6 W m\(^{-2}\) K\(^{-1}\) while liquid film thickness is in 11–13 nm. The fact shows that during the initial startup of the sodium heat pipe, the thermal resistance at the liquid-gas interface can’t be negligible. This work is the complement and extension for macroscopic investigation of heat transfer inside sodium heat pipe. It can provide a reference for further numerical simulation and optimal design of the sodium heat pipe in the future.

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1. Introduction

With high thermal conductivity, boiling point, low melt point, great capacity, the liquid alkali metal (sodium, potassium, lithium, etc.) could be adopted as the working fluid in many high-temperature and high heat flux energy transportation systems [1,2]. The liquid alkali metal working fluid could be directly used as the coolant in some advanced nuclear energy systems such as the sodium-cooled fast reactor [3–5]. More frequently, liquid alkali metal could be employed as the working fluid of high-temperature heat pipes utilizing its evaporation and condensation characteristics [6,7]. As shown in Fig. 1(a), a high-temperature alkali metal heat pipe consists of the working fluid (alkali metal), a wick structure, end caps, the pipe wall. It is divided into the evaporator section, the adiabatic section, the condenser section. When the heat is transferred into the evaporator section and conducted through the pipe wall and the wick structure, the alkali metal melts to be liquid state. It evaporates gradually. The vapor is driven through the adiabatic section and condenses in the condenser section. And the heat is released during the condensation. With the capillary pressure, the liquid alkali metal returns to the evaporator section through the wick structure and repeats the next circulation. Through the phase change and circulation of the working fluid, the high-temperature alkali metal heat pipe could achieve passive heat transportation effectively and has been widely used in the aerospace [8], energy conversion system such as heat pipe cooled reactor, point-focus concentrated-solar-power system, etc. [9–11].

As shown in Fig. 1(b), in the operation of the high-temperature alkali metal heat pipe, the liquid metal recedes into the wick structure pore and the extended meniscus exists. The phase change happens at the liquid-gas interface of the extended meniscus inside the wick pore [12]. From the wall of the wick structure (Fig. 1(c)), the extended meniscus can be typically divided into three regions: non-evaporating region, the nanoscale thin liquid film, and an intrinsic meniscus region. Due to low thermal resistance and high
heat transfer rate in the thin liquid film, it is a major contributor to the overall heat transfer of the extended meniscus [13]. This region resembles the boundary conditions of the whole extended meniscus [14]. It’s essential to deeply understand the phase-change mechanism of this nanoscale thin liquid film for the further investigation of the heat transfer inside the high-temperature alkali metal heat pipe. It is the complement and extension of the macroscopic experiments. It is also the reference and foundation of the numerical simulation of the heat pipe under the inevitable tendency of multi-scale and multi-physics field coupling computation [15–19].

The related research works include simulation and experiments. For experiments, it’s very difficult to directly observe the phase change of thin liquid film in detail because of the microscale of the wick structure and the high temperature operation conditions [20,21]. For simulation, the CFD model can be hardly constructed to simulate the phase change of thin liquid film of the meniscus inside a microscopic wick structure. The related works are rare [20,22,23]. Whether the conclusion and the results of these works could be applied in the actual operation of the alkali metal heat pipe still need to be validated in the future.

Due to the above difficulties, it’s necessary to adopt an effective tool to study this process. Molecular dynamics (MD) simulation is always a powerful tool to study evaporation and condensation of the thin liquid film [24,25]. Hu and Sun [26] studied the effect of nanostructures on the heat transfer coefficient of an evaporating meniscus in water film and nucleate boiling through MD simulation. It was revealed that the heat transfer coefficient would increase with the thickness of the water film before arriving at the critical thickness. The critical thickness would increase with the roughness of the nanostructure. Liang et al. [27] studied the steady-state evaporation and condensation of fluid Ar in a nanochannel to achieve the validity of the exact Schrage relationship in the accurate predictions of the rates of the associated processes. Chen et al. [28] studied the effects of liquid film thickness and simulation box geometry on the phase transition of fluid Ar through MD simulation. It was found that the explosive boiling and bubble nucleation phenomena respectively happened in the simulation boxes with different lengths under the substrate temperature of 150 K. Many other studies had also been done, whereas the objects were mostly water, argon, and some organic molecules [14,29–37]. The MD simulation of evaporation and condensation about liquid metal atoms is rare and old. Only Bhansali et al. [38] studied an evaporating sodium droplet in 1998. They only obtained some thermal properties such as density and vapor pressure.

In this paper, based on the specific sodium heat pipe inside the (Passive Residual Heat Removal System) of MSR (Molten Salt Reactor) [39], MD simulation software LAMMPS [40] is employed to investigate the evaporation and condensation of thin liquid sodium film during the startup and normal operation conditions. Through equilibrium simulation, MACs of three cases are determined. Based on equilibrium simulation, non-equilibrium simulation is conducted. In the non-equilibrium simulation, the thickness of the liquid film is observed, net evaporation mass flux and heat transfer coefficient at the liquid–gas interface are obtained. In section 2, the model and methods are described. In section 3, results from MD simulation are shown and discussed. Finally, the conclusions are given.

2. Model and methods

The MD simulation is different from some traditional methods of the thermohydraulic area. It is novel and abstract for some inherent cognizance. Generally, it is processed in a virtual simulation box. The followings are some simplifications and assumptions:

(1) The related MD simulation mainly adopted water and argon as the working fluid. In this paper, the working fluid is the liquid sodium. And the inherent limitation of metal atoms’ electronic effect exists in MD simulation. Our work is only an initial exploration and the first attempt to the nanoscale phase change mechanism inside sodium heat pipe by molecular dynamics method. Hence, the above effect is neglected in our work.

(2) The liquid sodium is assumed as the Lennard-Jones fluid, hence the Lennard-Jones potential is employed to calculate the atoms’ interaction. Due to the short-range oscillatory behavior inside liquid sodium, the Lennard-Jones potential may have its limitations in modeling sodium [33]. In this paper, the Lennard-Jones potential is chosen because of its commonality in modeling microscopic evaporation and the lack of mature potential of sodium atoms’ evaporation. The specific validation can be seen in section 2.2.

(3) According to the process mode of many related works, the thin liquid sodium film region of the meniscus is abstracted as a nanoscale liquid film and put on the solid wall. Gold, copper, and platinum are common solid wall materials in related MD simulations. Based on the actual conditions of the sodium heat pipe, the gold wall is chosen.

2.1. The configurations of the simulation system

As shown in Fig. 2, the simulation system is a box with the size of $8.4 \times 8.4 \times 58.2$ nm$^3$. Periodic boundary conditions are applied in $x$ and $y$ directions. Fixed boundary conditions are applied in $z$ directions. In the box, 9 layers of gold atoms are constructed to form each of the two solid walls. Different layers match with different
functions. From outside to inside, the first layer of gold atoms is set as a fixed wall to keep the volume of the system constant; the bottom inside eight layers are set as the heat source; the upper inside eight layers are set as the heat sink. The liquid sodium film is put on each of the two solid walls.

2.2. The potential and validation

As mentioned above, the Lennard-Jones potential is used in the simulation. Its description is as follows:

\[
\phi_{ij} = 4\epsilon \left\{ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^{6} \right\}
\]  

(1)

In Eq. (1), \( r \) is the distance between two atoms; \( \sigma \) is the distance where no interaction exists between two atoms; \( \epsilon \) is the depth of the potential well. The parameters \([38,41]\) are listed in Table 1.

The validation of MD simulation lies in whether the potential could reflect the physical properties of the subject. They include the microscopic Lennard-Jones fluid properties and some macroscopic thermal physical properties. For this purpose, three models are built in our previous work \([50]\). The first is 8.4 \( \times \) 8.4 \( \times \) 20 nm\(^3\) and consists of a single liquid sodium droplet (Fig. 3(a)). The second is 8.4 \( \times \) 8.4 \( \times \) 80 nm\(^3\) and consists of a liquid film and bottom gold wall (Fig. 3(b)). The third is 2.0 \( \times \) 2.0 \( \times \) 2.0 nm\(^3\) and consists of a piece of solid sodium (Fig. 3(c)). They are used to obtain the saturated pressure, the liquid density, and the melting point.

As shown in Fig. 4, the saturated pressure agrees well with the data from the NIST \([42,43]\). The potential could reproduce the behaviors of the Lennard-Jones fluid. Compared with the experiment data \([44]\), the discrepancy of liquid density and melting point are 2.04%-13.3%, 0.8% respectively (Figs. 5 and 6). Based on these results, the potential has its reasonability in the simulation.

2.2. The potential and validation

2.3. The simulation procedure

According to the initial design of the sodium heat pipe in PRHRS of MSR, the startup phase is in 600–760 K while the normal operation is in 800–1000 K \([7,39]\). As shown in Table 2, three cases are simulated based on the above background. The former two cases are aimed at the startup while the last is aimed at the normal operation. The specific process of simulation includes four steps:

(1) The initial simulation system is energy minimized to a stable state.
(2) The NVT ensemble is conducted to achieve equilibrium states at 600 K, 700 K, 800 K via Nose-Hoover thermostat for 6 ns.
(3) To get data of equilibrium states, the NVE ensemble is used to retain equilibrium states of four cases for 1 ns.
(4) Based on the equilibrium simulation, the NVT ensemble is changed into the NVE ensemble for sodium atoms. Meanwhile, the bottom wall is increased 120 K and the upper wall is decreased 80 K in the NVT ensemble. Through these two settings, the whole system goes into the non-equilibrium simulation, which is run for 20 ns.

The simulation time step size is set as 1 fs for all cases. MATLAB is used to post-process information (kinetic energy, potential, the position of each atom, density along the z-direction, etc.) from LAMMPS and OVITO \([45]\) is used to achieve visualization of the phase change process of sodium film.

2.4. Numerical model

From the microscopic view, the property of mass transportation at the liquid-gas interface could be described by net evaporation flux (or the evaporation rate), \( J_{\text{net}} \). It is the difference between evaporation and condensation. In this paper, the Schrage relationship is used to get \( J_{\text{net}} \).

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### Table 1

The Lennard-Jones parameters used in the MD simulations (The Lorentz-Berthelot mixing rule \([30]\) is employed to calculate parameters for Na–Au interactions).

<table>
<thead>
<tr>
<th></th>
<th>Na–Na</th>
<th>Au–Au</th>
<th>Na–Au</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \epsilon ) (eV)</td>
<td>0.051528</td>
<td>0.1509</td>
<td>0.44128</td>
</tr>
<tr>
<td>( \sigma ) (Angstrom)</td>
<td>3.24</td>
<td>2.9385</td>
<td>2.637</td>
</tr>
</tbody>
</table>
\[
J_{\text{net}} = \frac{\alpha}{2} - \sqrt{\frac{M}{2\pi R}} \left( \frac{P_l}{\sqrt{T_l}} - \frac{P_v}{\sqrt{T_v}} \right)
\]  

(2)

where \( M \) is the molar mass; \( R \) is the universal gas constant; \( \alpha \) is the MAC; \( T_v \) and \( T_f \) are the vapor temperature and liquid film temperature; \( P_v \) and \( P_l \) are the saturated pressure of \( T_v \) and \( T_f \). The system is divided into small layers (0.01 Å) along the z-direction. The density and temperature of each layer, the position of each atom could be obtained (section 2.3). According to the variation of the density distribution, the liquid-gas interface, the liquid zone, gas zone, and the atoms’ phase (liquid or gas) could be determined. By summing and averaging the related layer’s temperature, the \( T_v, T_f \) could be obtained. Based on \( T_v, T_f \) and Fig. 4, the \( P_v, P_l \) could be acquired.

Using statistic methods from Liang et al. [27,46,47], MAC is determined in the equilibrium of every case. As shown in Fig. 7, gas atoms generally happen three behaviors [14,32] at the liquid-gas interface (the position of \((\rho_l+\rho_v)/2 \) in Fig. 8): some gas atoms condensate into the liquid and become liquid atoms; some would be reflected directly by the interface; others would first happen condensation, then evaporate from liquid and become gas atoms again. In Fig. 9, a virtual plane is set above the liquid-gas interface. The distance between this plane and interface is set as 3.5\( \sigma_{Na-Na} \) (the cutoff used in the simulation). Using Eq. (3) to Eq. (5), the average normal velocity, \( u_m \), and the characteristic time \( \Delta t \) is obtained. In the range of \( \Delta t \), the ratio of atoms getting out of the virtual plane is seen as the ratio of atoms happening the latter two behaviors, thus the MAC (\( \alpha \)) could be obtained through Eq. (6). The \( \Delta ts \) of the three cases are 12.2 ps, 11.3 ps, 10.6 ps.

\[
d = 3.5\sigma_{Na-Na}
\]  

(3)
This paper focuses on the thin liquid sodium conduction caused by interfacial atoms’ collision is very weak. And of the three cases are 0.021, 0.014, 0.007 respectively. The heat caused by atoms evaporation and condensation as well as the heat conduction contained by Eq. (7):

\[
\Delta e_{i\nu} = \left( u_i + P_{i\nu} + \frac{1}{2} M_{i\nu} v_{i\nu}^2 \right) - \left( u_i + P_{i\nu} + \frac{1}{2} M_{i\nu} v_{i\nu}^2 \right)
\]

\[
h = \frac{q}{T_{i\nu} - T_V}
\]

In Eq. (9), \(u_i\) and \(u_i\) are the internal energy of the liquid and vapor, \(v_{i\nu}\) and \(v_{i\nu}\) are the specific volume of the liquid and vapor, and the kinetic energy terms, \(1/2M_{i\nu}v_{i\nu}^2\) are related to the bulk motion of fluid and they are neglected in this paper. Therefore, \(\Delta e_{i\nu}\) is the difference of the latent heat between vapor and liquid.

3. Results and discussion

3.1. Equilibrium simulation

The equilibrium states of the three cases are shown in Fig. 10. The MACs of four cases are 0.3886, 0.2119, 0.2615. As shown in Fig. 11, the distribution of temperature and potential of bottom liquid film and its near vapor zone of three cases are obtained. The temperature distribution reflects the strength of the atoms’ kinetic energy. The absolute value of atoms’ potential reflects the strength of the atoms’ interaction. The negative potential represents the attractive interaction of atoms. In Fig. 11, the liquid atoms’ kinetic energy increases with the equilibrium temperature. They can overcome the attractive interaction of surrounding atoms and become gas atoms more easily. The absolute value of the potential of the liquid film is decreasing from case 1 to case 3. The attractive interaction is weakening. Meanwhile, increasing equilibrium temperature also intensifies the reflection at the interface (The ratio of reflected gas atoms of four cases are 0.2462, 0.4187, 0.4379). The above three factors make the decline of the MAC from case 1 to case 2. In detail, the MAC in case 3 is larger than the MAC in case 2. In case 3, the attractive interaction of the wall (−0.7−0.6 eV) dominates with the decrement of initial liquid film thickness (~1.5 nm). The liquid atoms evaporate difficultly and the MAC increases slightly.

In the numerical simulation of the sodium heat pipe, the evaporation rate is the key parameter for the interfacial characteristics of heat and mass transfer. It is calculated by the Schrage relationship. In this relationship, the MAC is very important. It is generally acquired by some experienced values or assumed to be 1 [49]. Although the sodium is assumed as the Lennard-Jones fluid in this work, the above results will provide a new view for its determination with the development of the mature related MD model in the future.

3.2. Non-equilibrium simulation

The non-equilibrium of three cases is carried out based on equilibrium simulation. The equilibrium state of mass and heat transfer is broken and non-equilibrium is introduced by changing the temperature of the bottom wall and upper wall. The non-equilibrium evaporation of three cases is shown in Figs. 12–14. In case 1–2, the variation tendency is obvious: the bottom liquid film thickness decreases, and the upper liquid film thickness increases. In case 3, the evaporation is more intense. The change of liquid film...
and gas atoms is hard to observe until 20 ns. The specific change of liquid film thickness and gas atoms’ number, the $J_{\text{net}}$, and $h$ at the interface are discussed in detail in 3.2.1, 3.2.2, and 3.2.3.

3.2.1. Change of liquid film thickness and the number of gas atoms

In Fig. 15, with the proceeding of the non-equilibrium, the bottom liquid film thickness decreases to 0.6–1 nm and the upper liquid film thickness increases to 13 nm, 12.6 nm, 6 nm respectively.

In Fig. 16, the number of gas atoms is first in 4000–5000, 12668–13852, 18000–19000. It starts to decrease in 10 ns, 6 ns, 14 ns respectively. Finally, it arrives at 1800, 5434, 15028.

3.2.2. Net evaporation flux at the liquid-gas interface

The net evaporation flux, $J_{\text{net}}$ of three cases are shown as in Fig. 17. From case 1 to case 3, the magnitude of $J_{\text{net}}$ becomes larger with the equilibrium temperature. The variation tendency of $J_{\text{net}}$, bottom (the $J_{\text{net}}$ at the bottom interface) and $J_{\text{net}}$, upper (the $J_{\text{net}}$ at the upper interface) are opposite. The $J_{\text{net}}$, bottom grows in 0–20 ns.
while the $J_{\text{net, upper}}$ decreases. Especially in the last period of the former two cases, the $J_{\text{net, upper}}$ approaches to $10^{-4}$-$10^{-3}$ magnitude, which means the mass transfer of this region has been near equilibrium.

The distribution of temperature and potential of bottom liquid film and near vapor zone of case 1, case 3 are shown in Fig. 18, Fig. 19. Essentially, the transition from liquid atoms to gas atoms is the process that the liquid atoms overcome the attractive
interaction of surrounding atoms and finally leave the liquid film and become gas atoms. Although the temperature of the bottom wall is increasing in 0–10 ns of case 1 (Fig. 18(b)), the temperature of the bottom liquid film hasn’t grown markedly. The liquid atoms’ kinetic energy is still small. And the attractive interaction hasn’t decreased largely. In this period, evaporation happens slightly. With the proceeding of non-equilibrium, the liquid atoms get enough kinetic energy and the attractive interaction of liquid atoms has reduced. As a result, the evaporation becomes intense and the $J_{\text{net, bottom}}$ begins to increase in case 1. The basic equilibrium built in case 1 is weaker than the latter two cases. The liquid atoms’ kinetic energy is less than the latter two cases even the non-equilibrium has been constructed. When the atoms leaving the bottom liquid film get to the upper interface, the surplus kinetic energy is small. Meanwhile, due to the influence of the upper cold wall and attraction from the upper liquid film, these atoms can be easily condensed. The $J_{\text{net, upper}}$ is gradually decreasing to $10^{-4}$ magnitude and the mass transfer at this interface is approaching equilibrium. For case 2, the basic equilibrium temperature and the atoms’ kinetic energy are both higher than case 1. When the non-equilibrium is introduced, the thin liquid film evaporates easily and the $J_{\text{net, bottom}}$ increases obviously in the initial period compared to case 1. The total tendency and inner mechanism of case 2 are the same as case 1 (the distribution of temperature and potential of the related zone during non-equilibrium in case 2 are not shown in this paper because of the space constraints and the above similarity).

In case 3, the non-equilibrium is built on the higher equilibrium temperature and it is more intense than the former two cases. In the initial period, the thickness of the bottom liquid film is near 1.5 nm and the potential between liquid atoms has been in $-0.2-0.1$ eV (the absolute value is smaller than case 1 and case 2). The attraction between liquid atoms is weak. Due to the enhancement of the bottom wall’s temperature, the liquid atoms get a large amount of kinetic energy. These two factors make the evaporation more intense and the $J_{\text{net, bottom}}$ increase sharply during this period. With the decrease of bottom liquid film thickness, the attractive interaction from the bottom wall ($-0.6-0.7$ eV) dominates. The bottom film thickness and the $J_{\text{net, bottom}}$ could remain in a range. From Fig. 19, the temperature of the upper liquid film decreases to 700–800 K. This temperature range is higher than case 1, 2. The condensation is hard to happen than in the former two cases. Hence the change amount of thickness of the upper liquid film is not as many as case 1 and case 2.

### 3.2.3. Heat transfer coefficient at the liquid-gas interface

Fig. 20 shows the $h$, heat transfer coefficient at the liquid-gas interface of three cases in non-equilibrium. The total tendency of the $h$ is similar to the $J_{\text{net}}$. In every case, the $h_{\text{bottom}}$ (the $h$ at the bottom interface) increases while the $h_{\text{upper}}$ (the $h$ at the upper interface) decreases. Especially in case 1, the $h_{\text{upper}}$ decreases from 13 ns and finally reaches 5–6 W m$^{-2}$ K$^{-1}$. In the last period of non-equilibrium of case 1, the heat transfer at the upper interface has been weakened and a large thermal resistance has formed.
As mentioned in the 2.3 section, the heat transfer at the liquid-gas interface is achieved by the phase change at the interface. In Fig. 17, the magnitude of the $J_{\text{net}}$ increases from case 1 to case 3. This reflects the improvement of the intensity of the phase change and the increment of the release of the latent heat. The phase change heat transfer at the interface is enhanced from case 1 to case 3. Similarly, the magnitude difference of $J_{\text{net}}$ between the bottom interface and the upper interface also causes the $h_{\text{bottom}}$ to be larger than the $h_{\text{upper}}$ in every case. In the last period of non-equilibrium of case 1, the $J_{\text{net, upper}}$ has been in $10^{-4}$ magnitude and the mass transfer at the upper interface is approaching equilibrium. This fact
Fig. 17. The net evaporation flux during non-equilibrium evaporation in three cases.

Fig. 18. Distribution of temperature and potential of liquid film and its near vapor zone in 0, 10, 20 ns during non-equilibrium evaporation in case 1: (a) the upper liquid film and near vapor zone; (b) the bottom liquid film and near vapor zone.
means that the energy transfer caused by phase change has been weakened extremely. The \( h_{\text{upper}} \) finally approaches a very low magnitude and a large thermal resistance forms. The phenomenon, variation tendency, and mechanism of case 2 are similar to case 1. It is built at a higher equilibrium temperature compared to case 1. The \( J_{\text{net}} \) has a higher magnitude and the phase change is more intense. In the same last period, although the \( h_{\text{upper}} \) decreases as case 1, its magnitude is larger than that in case 1.

In some periods of non-equilibrium, the \( h_{\text{bottom}} \) fluctuates and some peak values exist. In case 1, the \( h_{\text{bottom}} \) fluctuates in 8 ns and reaches the peak value, 19 kW m\(^{-2}\) K\(^{-1}\). In case 2, the \( h_{\text{bottom}} \) fluctuates three times in 0–7 ns and the peak values are 48, 15, 20 kW m\(^{-2}\) K\(^{-1}\) respectively. In case 3, the frequency and the peak values of the fluctuation increase. Only after this fluctuation, the \( h \) could remain in a stable range. Combining the former sections’ results with the temperature of liquid film, vapor in Table 3, three reasons result in this: first, the change of temperature of the upper wall and bottom wall causes a disturbance. This disturbance’s intensity grows from case 1 to case 3 (0–7 ns in case 2); second, in the initial period of non-equilibrium, the temperature of the wall and the liquid film change earlier than the vapor zone, which causes hysteresis. In some periods, the temperature difference between liquid film and vapor zone is very small (1–7 K) while the \( J_{\text{net}} \) and the latent heat difference have changed, which causes the fluctuation of \( h \) (8 ns in case 1; 1 ns, 3 ns, 9 ns in case 3); third, with the proceeding of non-equilibrium, the amount of energy transfer is improved greatly and the \( h \) fluctuates (5 ns in case 3).

The results indicate that the thermal resistance at the liquid-gas interface should be considered with the thickness of the thin liquid film and the different operation conditions. In 520–600 K of the startup phase, the thickness of the thin liquid film is 11–13 nm, this thermal resistance couldn’t be neglected. In the normal operation phase of the heat pipe (case 3), it can be ignored.

4. Conclusion

In this paper, the molecular dynamics method is adopted to study the mechanism of evaporation and condensation of thin liquid sodium film of the meniscus. The sodium is assumed as the Lennard-Jones fluid in MD simulation. Based on the startup and normal operation of the sodium heat pipe used in PRHRS of MSR, three cases are simulated. The MAC, the variation of liquid film thickness and gas atoms’ number, the \( J_{\text{net}} \), and the \( h \) at the liquid-gas interface are obtained. The results are analyzed and the
microscopic mechanism is revealed. The conclusions are summarized as follows:

1. The MACs of three cases are 0.3886, 0.2119, 0.2615 respectively. With the increment of equilibrium temperature, the liquid atoms will get a good deal of kinetic energy and overcome the attraction to become gas atoms. And the reflection of atoms at the liquid-gas interface will become more intense. The ratio of condensed atoms will decrease.

2. Although the Lennard-Jones model has its limits, the MACs of this work could still give a new view for the parameter determination of simulation of the sodium heat pipe with the development of mature MD model of sodium evaporation in the future.

3. The heat transfer at the liquid-gas interface depends on the intensify of phase change. The variation tendency of the \( h_{\text{net}} \) is similar to the \( h_{\text{net, upper}} \). The heat transfer coefficient \( h_{\text{upper}} \) at the liquid-gas interface of the thin liquid film drops with the thickness. Especially in case 1, the \( h_{\text{net, upper}} \) has approached zero and the mass transfer has been near equilibrium.

Although the Lennard-Jones model has its limits, the MACs of this work could still give a new view for the parameter determination of simulation of the sodium heat pipe with the development of mature MD model of sodium evaporation in the future.

(2) When the non-equilibrium is built on the higher equilibrium temperature, the liquid atoms could get more kinetic energy to become gas atoms. The phase change at the liquid-gas interface could proceed more easily and intensely. The magnitude of the \( J_{\text{net}} \) becomes larger. The loss of kinetic energy of gas atoms, the cold upper wall, and the attraction from the upper liquid film influence the \( J_{\text{net, upper}} \). Especially in case 1, the \( J_{\text{net, upper}} \) has approached zero and the mass transfer has been near equilibrium.

(3) The heat transfer at the liquid-gas interface depends on the intensify of phase change. The variation tendency of the \( h \) is similar to the \( J_{\text{net}} \). The heat transfer coefficient \( h_{\text{upper}} \) at the liquid-gas interface of the thin liquid film drops with the thickness. Especially in 520–600 K of case 1, the \( h_{\text{upper}} \) has approached 5–6 W m\(^{-2}\) K\(^{-1}\) (a very small magnitude) with the 11–13 nm of thin liquid film thickness.

### Declaration of competing interest

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.

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