Transient numerical simulation and research of hydrogen condensation characteristics in a thermosyphon

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Abstract. A transient numerical investigation is performed to study the hydrogen condensation characteristics which are needed in the design and optimization of the heat-exchangers in large scale hydrogen liquefaction system. A two-dimensional numerical model of a thermosyphon has been implemented in ANSYS-FLUENT and the properties database of hydrogen are replaced with REFPROP. The volume of fluid (VOF) multiphase model is adopted to reconstruct the vapor-liquid interface, and the mass transfer and heat generation are modeled by introducing source terms to governing equations. In addition, the surface tension and contact angle are also taken into account. The simulation results, mainly the condensing heat transfer coefficient and temperature difference across the condensate film, are consistent with the public experiment data and new mass transfer time relaxation parameters for condensation are proposed. This study can provide some advice in the design of cryogenic fluid liquefaction system.

1. Introduction
Liquid hydrogen has been widely used as cryogenic propellant for space missions and coolant for superconductors. Cryogenic heat exchangers using cold helium as refrigerant are proper devices to condense hydrogen. To design an efficient heat exchanger, it is necessary to acquire the basic relationship between the film heat-transfer coefficient and temperature difference across the liquid film. With a small latent heat, least molecular weight and nonlinear isobaric specific heat capacity ($c_p$), the condensation of hydrogen shows some extraordinary characteristics with ambient-temperature fluids[1], leading to many existing correlations being invalid for hydrogen.

There are massive experimental and numerical work on the condensation of water and some refrigerants, but few experiment researches are carried on hydrogen[2-4] and different results are obtained. Drayer[2] and Ewald[3] found the film heat-transfer coefficients obtained from experiments were lower than those predicted by Nusselt's theory. However, Ohira[4] performed the experiment in a thermosyphon and found the heat-transfer coefficients mostly met well with predications of Nusselt's theory with the difference limited to within ±20%.

Thermosyphon is an excellent passive thermal transport device that utilizes the latent heat of working fluid to transfer large amounts of heat and has considerable thermal conductivities. Thermosyphon is wickless heat pipe and has three sections: condenser, evaporator and adiabatic section. The circulation of working fluid in a thermosyphon is maintained by phase change and driven by free convection and gravity. FLUENT is a kind of widely used CFD software, which is adopted by...
many researchers to simulate the phase change with the assist of the VOF multiphase model. Here, FLUENT is used to simulate vapor-liquid phase change of hydrogen with 2D axisymmetric model of a thermosyphon to analyse the principle reasons of the low condensing heat-transfer coefficient.

2. Physical Model

2.1. Multiphase Flow Model

The VOF multiphase flow model is adopted to model the vapor-liquid two-phase flow. In the VOF model, fluids are immiscible and only a single set of momentum equations is solved. In the vapor-liquid two-phase flow, \( \alpha_l \) and \( \alpha_v \) are namely volume fraction of liquid and vapor, who must sum to unity. That is, any empty volume is not allowed in the fluid domain. For instance, the computational grid is empty or full of the liquid when \( \alpha_l \) reaches the minimum value of zero or the maximum value of unit, and contains phase interface with \( \alpha_l \) between 0 and 1. By solving continuity equation for the volume fraction of vapor or liquid, the vapor-liquid interface is tracked.

2.2. Phase Change Model

Lee[5] assumes that mass is transferred at an isobaric and quasi thermo-equilibrium state, and introduces following expressions to calculate the mass transferred from liquid to vapor (evaporation) and from vapor to liquid (condensation):

\[
J_{lv} = r_e \alpha_l \rho_l \frac{T - T_{sat}}{T_{sat}} (T \geq T_{sat})
\]

\[
J_{vl} = r_c (1 - \alpha_l) \rho_v \frac{T_{sat} - T}{T_{sat}} (T < T_{sat})
\]

In the above equations, \( r \) (unit of \( s^{-1} \)) is the mass transfer time relaxation parameter and plays a key role in the Lee model, where \( r_e \) and \( r_c \) determine transient evaporation and condensation rate respectively. Researchers have not come to an agreement on the value of \( r \). One of the most widely employed values is 100[6], but Wang[7] finds when \( r \) equals to 110, the vapor pressure in steady state is equal to the saturated pressure. A small \( r \) can cause a significant deviation between the interfacial temperature and the saturation temperature, and extremely large values cause numerical convergence problems. In theory, the \( r \) value for evaporation and condensation should be different from each other and relate to the properties of fluids. In the attempt to broaden the range of \( r_c \), divergence is found when \( r_c \) exceeds 1000, and condensation is too week to observe when \( r_c \) is too small. To evaluate the effect of \( r_c \), five cases with different \( r_c \) by setting 100 as default value for \( r_e \) in this research are listed in the table 1.

| case | 1 | 2 | 3 | 4 | 5 |
|------|---|---|---|---|---|
| \( r_c \) (s\(^{-1}\)) | 0.5r_e | 85 | r_e | 110 | 2r_e |

2.3. Surface Tension and Contact Angle

The surface tension force results from the attraction between molecules, whose direction towards the inside of the liquid film. The surface tension can contract the liquid surface and enhance the pressure inside of liquid. In two-phase separating regions, the surface tension plays an important role to decrease interface area to minimize the free energy[8]. As a kind of force, surface tension is modified in the continuum surface force(CSF) model to add to the momentum equation as source term. Contact angle is the angle between the wall and the tangent to the interface at the condensing wall and negatively related to surface energy of the interface, which is a significant parameter in the CSF Model. Good measured contact angle by dipping rod in liquid hydrogen for different materials was
presented in [9], where one could found the contact angle for samples were all zero. Bland[10] infers that liquid hydrogen exhibits a zero contact angle on all surfaces and has confirmed the contact angle for OFHC copper is zero by experiment.

3. Numerical Analysis

3.1. Geometry and Mesh
Geometry of the thermosyphon is shown in figure 1 and the dimensions refer to the literature [4]. Parameters of L1, L2, L3, L4 are respectively 70 mm, 40 mm, 70 mm, 70 mm. The inner diameter of the condenser and evaporator are namely 15 mm and 150 mm. The material of the wall is OFHC copper and the thickness is 1 mm. The 2D axisymmetric mesh is generated in ICEM CFD and the mesh of the near-wall regions are fined. Mesh independence is done with five different number of cells (108935, 162168, 203261, 223125, 262853) by comparing the heat flux of the condenser wall of the first 10s, as shown in the figure 2. As can be seen, the flux keeps constant when the cell number exceed 203261. The mesh with 22315 cells is selected in the simulation.

![Figure 1. Geometry of thermosyphon.](image)

3.2. Calculation Conditions
Material properties are mainly adopted from REFPROP database at reference conditions(22.9 K, 199.5 kPa). The viscosity, thermal conductivity, $c_p$, surface tension and density are fitted into polynomial functions of temperature. Latent heat is 432 kJ/kg, and standard state enthalpy is the product of the molecular weight and latent heat.

![Figure 2. Mesh independence test.](image)

![Figure 3. Heat fluxes of the condenser wall.](image)

Boundary conditions are referred to the literature [4], in which when the temperature difference across the liquid film is 2.9 K, the condensation heat flux is 4200 Wm$^{-2}$ on the condenser wall. The outer wall of the condenser has constant temperature of 20 K and evaporator is given a constant heat flux of 865.3 Wm$^{-2}$. The other outer faces are adiabatic and all the inner walls are non-slip. Vapor and liquid are defined as the primary and secondary phase respectively. To reach convergence quickly, the initial temperature patched for liquid and vapour are namely 22.7 K and 23.2 K. Gravitational acceleration of 9.81 ms$^{-2}$ is applied in the negative axial direction. The filling ratio is the ratio of initial
liquid volume per total volume of evaporation section, which affects the performance of thermosyphon significantly. 50%, the widely adopted value for filling ratio by many researchers[11; 12], is chosen by patching 1.2 liters of normal liquid hydrogen in the shadow region of figure 1. A time step of 0.0003s is chosen in the transient simulation. PISO scheme is used for pressure-velocity coupling, which performs additional neighbor correction and skewness correction. First order upwind scheme is adopted to discretize the momentum and energy equations. Geo-Reconstruct and PRESTO discretization are respectively performed for the volume fraction and pressure interpolation scheme. Geo-Reconstruct is the most accurate interface tracking method which is recommended for most transient calculations with VOF model. In the present study, the simulation is considered converged when the scaled residual of the mass and velocity components is less than $10^{-4}$. Laminar model is selected because Reynolds number does not exceed 237 in the experiment[4].

4. Results and Analysis

4.1. Results
Simulations reach steady state after around 120s. Condensation heat fluxes of each second for the 5 cases are recorded as shown in the figure 3. To get the vapor-side temperature of the film, temperature of five points on the axis, whose $z$(mm) value are respectively 114, 102, 90, 78 and 66, are monitored and averaged. In the five cases, the vapor-side temperatures all reach the saturated temperature of 22.9 K in the steady state. As can be seen, heat fluxes in the case 2 mostly approach to the target value of 4200 Wm$^{-2}$, that is, 85 is the optimum value for $r_c$.

4.2. Phenomena Analysis

4.2.1. Condensation Film. Three sections of condenser in case 3 at 7s are amplified in figure 4. The condensate on the vertical wall of section (a), (b) and (c) are namely thin, laminar and wavy film, which meets well with the description in literature[8]. Because the top wall strengthens the condensation, there generates a block of liquid in the corner, which should be paid attention to the installation of the thermometers measuring the saturated gas temperature in experiment. For the five cases, condensation heat fluxes become larger and film becomes much thicker when $r_c$ is increased.

4.2.2. Condensation Droplet. Figure 5 amplifies the section (d) of figure 4, recording the process of the appearance, expansion and drop of a droplet. The appearance of droplet is the result of sudden change of the diameter, and the characteristics in dropping down may correspond to the force conditions. Before the droplet separating from the wall, the droplet is in equilibrium of forces. With the continuous condensate flowing down, the droplet leaves the wall under the action of gravity. After the separation, the surface tension force drives the droplet to tight up to the axis and gravity drives the droplet down. Because of the droplet, film thickness keeps changing in the condensation process, which leading the condensation heat fluxes fluctuates continually, as show in the figure 3. The droplet can be considered as disturbance to the liquid film which could improve the performance. Since $r_c$...
affects the amount of condensation, a bigger \( r_c \) can thicken the liquid and reduce the time between two droplets, which has both negative and positive effects on condensation from this sense.

Figure 5. Contours of liquid droplet.

5. Conclusion
A transient simulation is performed to study the hydrogen condensation characteristics with a 2D axisymmetric numerical model of a thermosyphon in FLUENT. The simulation results show good agreement with the experiment data, which confirms that Lee model is also applicable for thermosyphon using hydrogen as working fluid. The effect of mass time relaxation parameter is investigated in the study and there exists a proper range and an optimum value for \( r_c \). A bigger \( r_c \) can reduce the time to reach steady state, but also lead to a thicker film. For this study, optimum value for \( r_c \) is 85 when setting \( r_e \) as 100. The condensate on the vertical wall in order of height are namely thin, laminar and wavy film, which meets well with theory. The appearance of the droplet is due to the sudden change of diameter of the thermosyphon, and the development and drop are due the force conditions. The droplet influences the refreshment of the film, whose effect on the heat-transfer coefficient needs more study. The study can benefit the design of cryogenic fluid liquefaction system.

Acknowledge
This work was supported by the fund of Key Laboratory of Cryogenics, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences [CRYOQN201711].

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