

Numerical Investigation of Transient Steam Condensation in a Steam-Hydrogen-Air Mixture under Thermosolutal Convection

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1. Introduction

Natural convection is a buoyancy-driven flow generated by density variations within a fluid subjected to gravity. In conventional thermal natural convection, these density variations arise primarily from temperature differences, with warmer, lighter fluid tending to rise and colder, denser fluid tending to descend [1,2]. Such buoyancy-driven circulation provides an important passive mechanism for heat transport in enclosed systems [2]. When thermal effects dominate the density variation, the resulting flow can be described primarily in terms of temperature-induced buoyancy [1].

The thermal-hydraulic environment of a nuclear reactor containment during a severe accident is considerably more complex. Steam released from the reactor coolant system can coexist with the air initially present in the containment, while hydrogen may be generated through high-temperature oxidation of zirconium-based fuel cladding by steam [3]. The containment atmosphere consequently becomes a multicomponent steam-hydrogen-air mixture. In such a gas mixture, density depends not only on temperature and pressure but also on the mixture molecular weight, which varies with species composition. This effect is particularly important because hydrogen is substantially lighter than both steam and air. Consequently, appreciable changes in hydrogen, steam, and air concentrations can generate significant composition-induced density variations, making a conventional thermal-only buoyancy treatment insufficient.

Under such conditions, the flow is more appropriately described as thermosolutal, or double-diffusive, natural convection. In pure thermal convection, buoyancy originates primarily from temperature-induced density differences. In thermosolutal convection, however, density variations

arise simultaneously from temperature and species-concentration gradients. The corresponding thermal and solutal buoyancy contributions may either reinforce or oppose one another, depending on the temperature and concentration distributions. Furthermore, heat and species diffuse at different rates, allowing the thermal and concentration boundary layers to evolve differently. The relative importance of the two buoyancy mechanisms is commonly characterized by the buoyancy ratio, while the ratio of thermal to mass diffusivity is represented by the Lewis number [4].

Steam condensation further strengthens this coupling. When a steam-air-hydrogen mixture contacts a sufficiently cold condenser surface, steam is selectively removed from the gas phase, whereas the non-condensable gases remain. Their accumulation near the condenser introduces an additional mass-transfer resistance that restricts steam transport toward the condensing surface and reduces condensation heat transfer [5,6]. At the same time, selective steam removal changes the local gas composition and mixture molecular weight. Consequently, the gas adjacent to the condenser experiences both temperature-induced and composition-induced density variations. Depending on the hydrogen to noncondensable gases ratio of the remaining non-condensable mixture, the thermal and solutal buoyancy contributions may therefore reinforce or oppose each other.

The present study numerically investigates the transient condensation of steam on a vertical condenser tube in a closed vessel containing a steam-hydrogen-air mixture. Gas density is evaluated using the full ideal-gas mixture relation, thereby accounting for both thermal and compositional effects on buoyancy. Particular attention is given to the transient evolution of the condensation heat-transfer coefficient as steam is progressively depleted and the non-

condensable fraction becomes enriched. The numerical implementation of thermosolutal natural convection is validated against the double-diffusive cavity benchmark reported by Koufi et al. [4], which considers opposing temperature and concentration gradients in a mixture-filled enclosure.

2. Numerical Model

Fig. 1 illustrates the geometry of the two-dimensional axisymmetric vessel of 1.5m diameter and 3.5m height. The vertical condenser of 19mm diameter and 1m length is mounted on the axis and held at fixed subcooling.

All the other boundaries are kept adiabatic and impermeable, so the only mass leaving the domain is the condensate forming on the subcooled vertical condenser. The vessel is initially filled with a ternary gas mixture of steam, hydrogen, and air, uniform at 0.4 MPa pressure, with a condenser wall subcooling of 50 K.

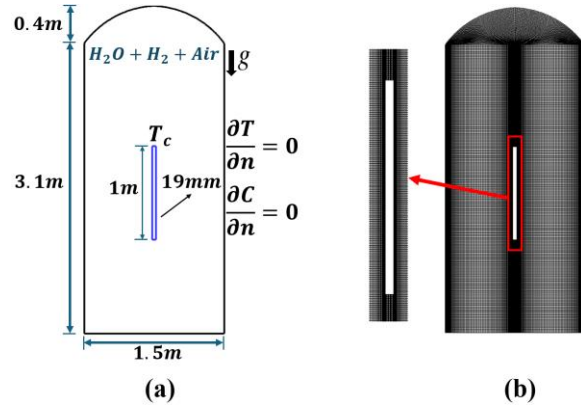


Fig. 1. Computational domain and mesh: (a) vessel geometry and boundary conditions, and (b) locally refined mesh in the vicinity of the vertical condenser tube.

2.1 Governing Equations

The mixture is treated as a compressible ideal gas, so the two-dimensional, ideal-gas, transient formulation is governed by the following governing equations accounting for conservation of mass, momentum, and energy. Additionally, the species conservation equation is added for the ternary gas mixture.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \quad (1)$$

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \Delta \cdot \vec{\tau} + \rho \vec{g} \quad (2)$$

$$\frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\vec{v} (\rho E + p)) = \nabla \cdot \left((k_{eff} \nabla T) - \sum_i^j h_i J_i \right) + S_h \quad (3)$$

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

SST k- ω model, resolved to the wall, is used for turbulence modeling.

To retain the differing mobilities of hydrogen and air through steam, the Fuller correlation combined with the Wilke mixing rule for the ternary gas mixture is used to evaluate the binary diffusivities.

2.2 Wall Condensation Model

Figure 2 illustrates the condensation process in the presence of non-condensable gases. Because only the vapor undergoes condensation, the net mass flux of the non-condensable species across the gas-liquid interface is zero. Consequently, the total interfacial mass flux is equal to the vapor mass flux. The transport of vapor toward the interface is modeled by accounting for both convective and diffusive contributions.

$$\dot{m}'' = \frac{\rho D_{v,m}}{1 - Y_{v,i}} \frac{\partial Y_v}{\partial n} \bigg|_i \quad (5)$$

The volumetric source terms are evaluated in the wall-adjacent computational cell of volume V_c bounded by a condenser-wall face of area as:

$$S_m = \dot{m}'' \frac{A_f}{V_c}, \quad S_v = Y_v S_m, \quad S_h = h_{fg} S_m \quad (6)$$

Where h_{fg} denotes the latent heat of vaporization of steam. The interfacial composition is determined from local thermodynamic equilibrium. When condensate-film resistance is neglected, the interfacial steam mass fraction is calculated as:

$$Y_{v,i} = \frac{M_v p_v(T_{w,i})}{[M_v p_v(T_{w,i}) + M_{nc}(p - p_v)(T_{w,i})]} \quad (7)$$

if $p_v(T_{w,i}) \geq p_{vs}(T_{w,i})$

Where $p_v(T_{w,i})$ is the local vapor partial pressure evaluated at the wall temperature and $p_{vs}(T_{w,i})$ is the corresponding saturation vapor pressure. Thus, condensation occurs only when the local vapor partial pressure exceeds the saturation pressure at the condenser surface.

Buoyancy is modeled using a thermosolutal formulation, in which the thermal and compositional contributions to the density variation are retained separately. This treatment is particularly important for steam-air-hydrogen mixtures because the non-condensable species have substantially different molecular weights, allowing concentration gradients to either reinforce or oppose the thermally induced buoyancy.

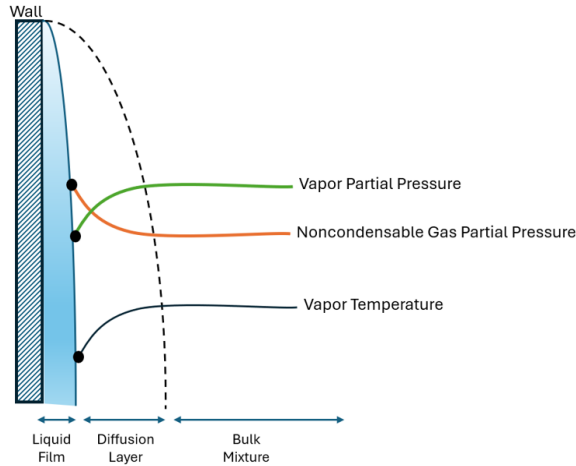


Fig. 2. Steam condensation in the presence of non-condensable gases

The condensation heat-transfer coefficient (CHTC) is evaluated from the area-averaged condensation heat flux and the temperature difference between the bulk gas and the condenser wall:

$$CHTC = \frac{q_{ave}}{T_{bulk} - T_c} \quad (8)$$

Where q_{ave} is the area-averaged heat flux over the condenser surface and T_c is the condenser-wall temperature. This definition is used to quantify the instantaneous condensation heat-transfer performance during the transient vapor-depletion process.

2.2 Model Validation

The numerical model was validated against two independent benchmark cases, as shown in Fig. 3. First, the double-diffusive natural-convection results of Koufi et al. [4] were reproduced for different buoyancy ratios, with good agreement obtained for the local Nusselt number distributions. The model was assessed against the TOSQAN steady-state 1 data reported by Dehbi et al. [7], where the predicted axial vapor mole-fraction profile closely follows the reference data. These comparisons confirm the model's ability to capture both thermosolutal convection and steam condensation in the presence of non-condensable gases.

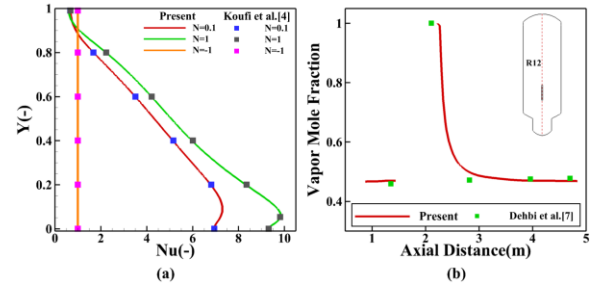


Fig. 3. Validation of the present numerical model against (a) the double-diffusive natural-convection benchmark of Koufi et al. [4] and (b) the axial steam mole-fraction measurements from the TOSQAN steady-state 1 [7].

3. Results and Discussions

Figure 4 shows the temperature and hydrogen distributions for $X_{Hyd/Non} = 0.7$ and 0.3 . Although the thermal boundary conditions are unchanged, substantially different flow-induced stratification develops as the hydrogen to noncondensable gases ratio is varied. For $X_{Hyd/Non} = 0.7$, the cooled region originating from the condenser extends predominantly upward, resulting in a lower-temperature upper region. Hydrogen is also preferentially transported toward the upper part of the vessel. In contrast, for $X_{Hyd/Non} = 0.3$, the cooled gas is transported downward, and a colder lower region develops, accompanied by an accumulation of hydrogen in the lower part of the vessel.

This reversal originates from the competition between thermal and solutal buoyancy. Cooling adjacent to the condenser increases the local gas density and therefore produces a downward thermal-buoyancy contribution.

Condensation, however, simultaneously removes steam and enriches the remaining gas in non-condensable species. When the non-condensable mixture is hydrogen-rich, the associated reduction in the local mixture molecular weight generates an upward solutal-buoyancy contribution that can overcome the downward thermal effect. The resulting circulation therefore transports the cooled, hydrogen-enriched gas upward. For the air-rich mixture, steam removal produces a comparatively heavier near-wall mixture, so the compositional contribution acts in the

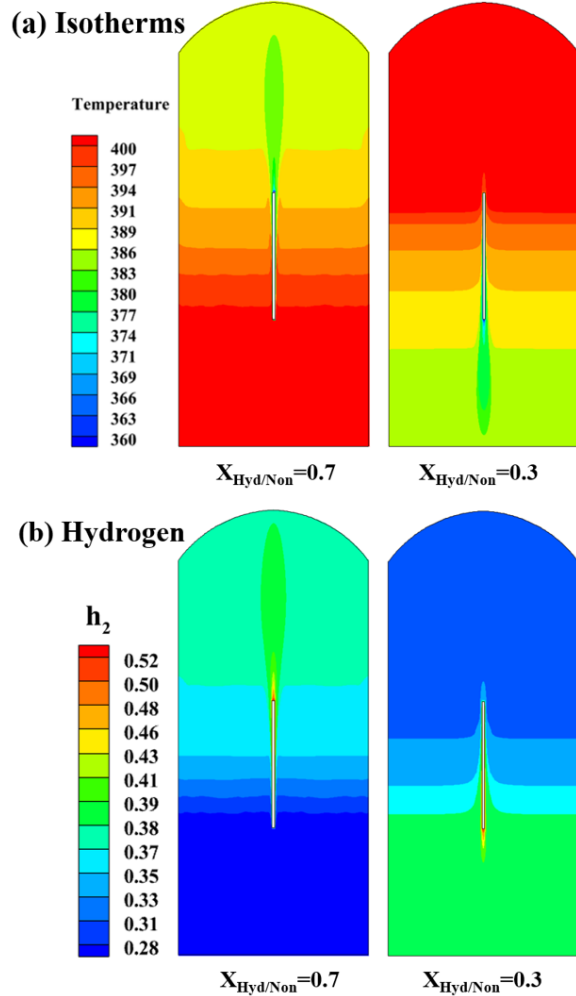


Fig. 4. Distributions of (a) temperature and (b) hydrogen mole fraction for $X_{H_{yd}/Non} = 0.7$ and 0.3

same direction as the thermal buoyancy and promotes downward transport. The circulation direction is therefore governed by the combined thermosolutal density response rather than by temperature alone.

The vertical profiles in Fig. 5 quantify the stratification observed in Fig. 4. For $X_{H_{yd}/Non} = 0.3$, the lower part of the vessel remains colder, whereas the temperature increases toward the upper region. The hydrogen concentration shows the opposite vertical tendency, with preferential accumulation in the lower part of the vessel. This distribution is consistent with the downward transport generated when thermal and solutal buoyancy act in the same direction.

For $X_{H_{yd}/Non} = 0.7$, the profiles are reversed. The upper region becomes colder while simultaneously exhibiting a substantially higher hydrogen concentration. Although cooling alone would tend to increase local density, strong hydrogen enrichment lowers the mixture molecular weight sufficiently to maintain the lighter gas in the upper region. The simultaneous reversal of the temperature and hydrogen profiles therefore demonstrates that solutal buoyancy can overcome the conventional thermally induced circulation.

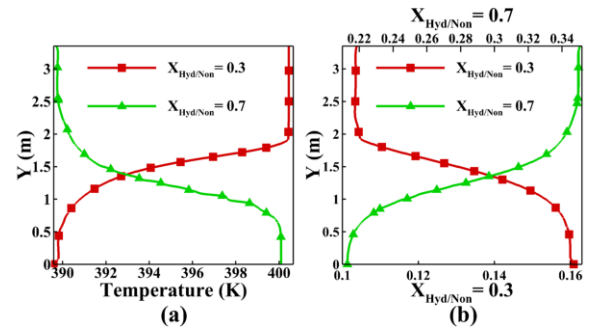


Fig. 5. Vertical profiles of (a) temperature and (b) hydrogen mole fraction for $X_{H_{yd}/Non} = 0.7$ and 0.3

Figure 6 shows the temporal evolution of the area-averaged condensation heat-transfer coefficient together with the vapor and hydrogen mole fractions for $X_{H_{yd}/Non} = 0.7$. The CHTC decreases sharply during the early stage of condensation and subsequently declines more gradually. During the same period, the vapor mole fraction continuously decreases, while the hydrogen mole fraction increases as steam is selectively removed from the gas mixture.

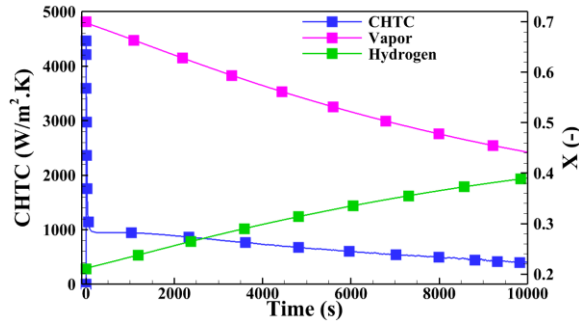


Fig. 6. Transient evolution of CHTC, vapor mole fraction, and hydrogen mole fraction for $X_{Hyd/Non} = 0.7$

The initial high CHTC corresponds to a steam-rich atmosphere and relatively weak non-condensable accumulation near the condenser. As condensation proceeds, vapor depletion and hydrogen enrichment increase the resistance to steam transport toward the cold surface, leading to progressive degradation of the condensation heat-transfer coefficient. In addition, the evolving mixture composition continuously modifies the thermosolutal buoyancy balance and hence the convective transport supplying vapor to the condenser. The transient CHTC is therefore controlled by the coupled evolution of species composition, mass-transfer resistance, and buoyancy-driven circulation.

4. Conclusion

A numerical study was performed to investigate transient steam condensation in a closed vessel containing a steam-hydrogen-air mixture, with particular emphasis on the coupling between thermal and solutal buoyancy. The numerical model was validated against the double-diffusive natural-convection benchmark of Koufi et al. and the TOSQAN steady-state 1. The results show that the non-condensable gas composition strongly influences the direction of buoyancy-driven transport. For the hydrogen-rich mixture, condensation-induced reduction of the local mixture molecular weight generates an upward solutal buoyancy that can overcome the downward thermal contribution, whereas the air-rich mixture promotes downward transport. This competition produces opposite temperature and hydrogen stratification within the vessel. During the transient condensation process,

continuous vapor depletion and hydrogen enrichment increase the resistance to steam transport toward the condenser, resulting in a progressive reduction of the condensation heat-transfer coefficient. These results demonstrate that both thermal and solutal density variations should be considered when evaluating steam condensation in hydrogen-containing containment atmospheres.

REFERENCES

- [1] J. H. Oh, D.-G. Kim, D. H. Kim, S. A. Aodu, and I. S. Park, Influence of Prandtl Number on the Chaos Transition for Pure Natural and Rayleigh–Bénard Convections inside a Rectangular Cavity, *International Communications in Heat and Mass Transfer*, Vol. 155, 107511, 2024.
- [2] S. A. Aodu, D.-G. Kim, G. Choi, and I. S. Park, Numerical Investigation of the Electro-Thermo-Convection Heat Transfer Enhancement in a Square Annulus Involving a Heated Square Block, *International Communications in Heat and Mass Transfer*, Vol. 147, 106984, 2023.
- [3] R. Gharari, H. Kazeminejad, N. Mataji Kojouri, and A. Hedayat, A Review on Hydrogen Generation, Explosion, and Mitigation during Severe Accidents in Light Water Nuclear Reactors, *International Journal of Hydrogen Energy*, Vol. 43, No. 4, pp. 1939-1965, 2018.
- [4] L. Koufi, Y. Cherif, Z. Younsi, and H. Naji, Double-Diffusive Natural Convection in a Mixture-Filled Cavity with Walls' Opposite Temperatures and Concentrations, *Heat Transfer Engineering*, Vol. 40, No. 15, pp. 1268-1285, 2019.
- [5] J. Su, Z. Sun, G. Fan, and M. Ding, Experimental Study of the Effect of Non-Condensable Gases on Steam Condensation over a Vertical Tube External Surface, *Nuclear Engineering and Design*, Vol. 262, pp. 201-208, 2013.
- [6] A. Dehbi, A Generalized Correlation for Steam Condensation Rates in the Presence of Air under Turbulent Free Convection, *International Journal of Heat and Mass Transfer*, Vol. 86, pp. 1-15, 2015.
- [7] A. Dehbi, F. Janasz, and B. Bell, Prediction of Steam Condensation in the Presence of Noncondensable Gases Using a CFD-Based Approach, *Nuclear Engineering and Design*, Vol. 258, pp. 199-210, 2013.