Transactions of the Korean Nuclear Society Spring Meeting
Jeju, Korea, May 23-24, 2019

Computational analysis of wall condensation in the presence of non-condensable gas mixture containing a light gas with CUPID

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1. Introduction

Accurate prediction of containment building pressure at safety analysis is essential to guarantee containment integrity in the event of a severe accident [1]. In particular, it was generally agreed that hydrogen stratification and vapor condensation/re-evaporation directly affect containment pressure [2] and therefore, experimental and analytical studies have been carried out with large scale facilities such as PANDA and ThAI [3, 4]. Meanwhile, commercial CFD codes, as well as lumped parameter codes, have been validated and being improved in numerical studies to predict those phenomena more accurately.

In the modeling of the natural convection and condensation/evaporation on the containment wall, user defined models are necessary and in this context, CUPID, KAERI's inhouse code, has an advantage as it is an open-source code of which users can implement required models without limitations. However, it requires model improvement and implementation to reproduce key phenomena for gas mixture behavior in the containment.

In this study, a mass diffusion model of CUPID code was improved for the analysis of condensation heat transfer phenomena in the presence of non-condensable gas mixture containing light gases such as hydrogen. Afterwards, computational simulation using the modified diffusion model was conducted against CONAN facility which used helium-air mixture for non-condensable gas.

2. Modification of CUPID Diffusion Model

In this section, modification of the diffusion model in CUPID is described. The diffusion model is important in the wall condensation analysis as it directly influences the mass transfer of species in company with convection terms [5]. In original CUPID code, non-condensable gas species were analyzed as a mixture which has mass weighted average properties of species. However, since the light gases such as helium have greater diffusivity than air, mass fraction gradient of each species near the condensation wall may be different from each other. Furthermore, energy transfer due to mass diffusion of each species should be calculated separately because enthalpy and diffusive mass flux of each species are different. For this reason, the diffusive source term of the mass transport equation of gas mixture was modified from Eq.(1-a) to (1-b) considering the sum of the diffusion mass fluxes of each species. Each species' diffusivity was calculated using the Chapman-Enskog equation [6]. In general, the energy transfer due to diffusion mass transport is calculated by Eq. (2) [7]. Since the diffusive mass flux of the species must sum to zero, the steam mass fraction is determined as minus the sum of solved mass flux of other species as shown in Eq. (3). Therefore, the energy source term is calculated by Eq. (4).

$$\frac{\partial}{\partial t}(\alpha_g \rho_g X_n) + \nabla \cdot (\alpha_g \rho_g \vec{v}_g X_n) = \nabla \cdot \left(\sum_{i=1}^{n} \alpha_g \rho_g D_i \nabla X_n q_i\right) \quad (1\text{-a})$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g X_n) + \nabla \cdot (\alpha_g \rho_g \vec{v}_g X_n) = \nabla \cdot (\alpha_g \rho_g D \nabla X_n) \quad (1\text{-b})$$

$$S_i = \nabla \cdot \left(\sum_{i=1}^{n} h_i \vec{J}_i\right) = \nabla \cdot \left(\sum_{i=1}^{n} -h_i \left(\rho D_{i,m} \nabla Y_i\right)\right) \quad (2)$$

$$\vec{J}_s = -\sum_{i=1}^{n} \alpha_g \rho_g D_i \nabla X_n q_i \quad (3)$$

$$S_{total} = \nabla \cdot \left(\sum_{i=1}^{n} (h_s - h_i)\left(\alpha_g \rho_g D_i \nabla (X_n q_i)\right)\right) \quad (4)$$

To verify these modifications, analysis of the conceptual problem was conducted in the same geometry of Dehbi's conceptual problem on condensation [8]. As shown in Fig. 1, the height of the computational domain is 24 m and the width is 10 m, and a steam-air-helium mixture is injected at the upper inlet. In the domain, the composition of the gas mixture at the center and the periphery region are different, and it causes diffusion between the two regions. The analysis was performed using both CUPID and a commercial CFD code, STAR-CCM+, for the code to code verification. The standard $k-\varepsilon$ model is used for the calculations of the conceptual problem in both codes. Same meshes which consist of 5,400 cells were used in both codes. The inlet conditions of the problem are summarized in Table. I.

Table. I. Conceptual problem inlet boundary condition of mass fraction

	Central inlet (steam, helium, air)	Periphery inlet (steam, helium, air)
CASE1	(0.35, 0.05, 0.6)	(0.2, 0.1, 0.7)
CASE2	(0.1, 0.45, 0.45)	(0.3, 0.49, 0.21)
CASE3	(0.0, 0.6, 0.4)	(0.0, 0.3, 0.7)

The analysis results of the original CUPID and the modified one are illustrated in Fig. 2 and Fig. 3 and it was found that the unphysical temperature distribution at the diffusion boundary is improved after the modification. The comparison of the outlet mass fraction between STAR-CCM+ and the modified CUPID in case

2 is shown in Fig. 4. As figured, the species distributions analyzed by the modified CUPID code show good agreement with CFD results.

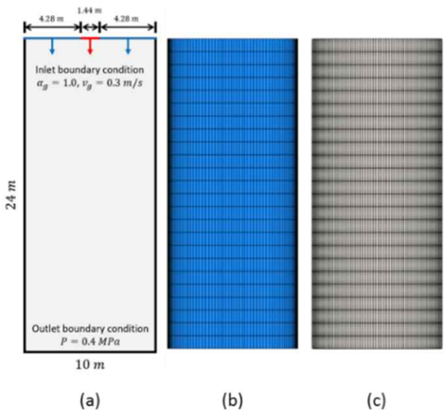

Fig. 1. Schematics of computational domain and meshes (b: STAR-CCM+ mesh, c: CUPID mesh)

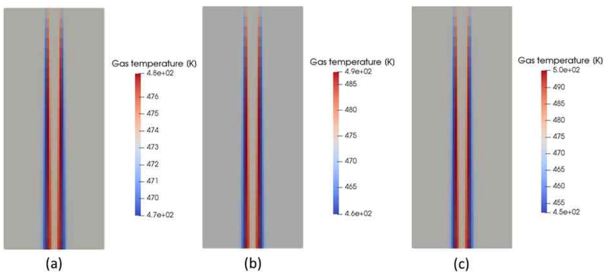

Fig. 2. Temperature contour of original CUPID (a: Case 1, b: Case 2, c: Case 3)

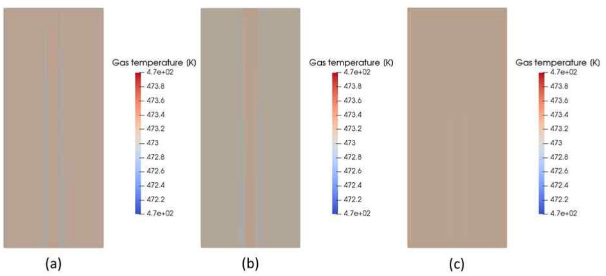

Fig. 3. Temperature contour of modified CUPID (a: Case 1, b: Case 2, c: Case 3)

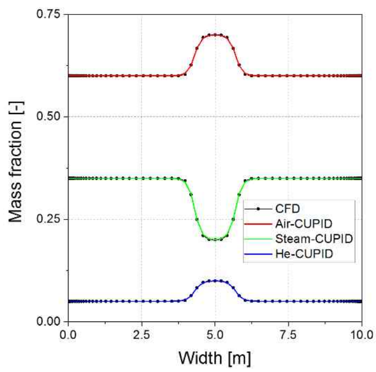

Fig. 4. Comparison of species mass fraction between CFD and modified CUPID at the outlet

3. Computational Analysis of Wall Condensation

In this section, validation of wall condensation model of CUPID against the CONAN experimental facility by using the modified CUPID code is described. The CFD analysis was also conducted to compare the prediction capabilities of the CUPID, as performed in the previous research [9].

3.1. Computational analysis conditions

The CONAN facility is a separate effect test loop for condensation. The CONAN facility consists of two loops. As described in Fig. 5, the primary loop contains the test section, consisting of a 2 m long, 0.34 m channel having a square cross-section, in which a mixture of steam, air, and helium is circulated. The secondary loop of 5 mm in width provides the required cooling of the condensation plate [10, 11]. The incoming gas mixture is saturated and the pressure on the primary side is maintained as 0.1 MPa. Experiments were carried out to investigate both forced and natural convective condensation phenomena by changing the inlet velocity condition. Particularly, in the case of natural convective condensation, reverse flow phenomena occur by buoyancy when the mole fraction of helium is larger than 0.6. The experimental conditions are shown in Table. II [12].

Table. II. The boundary conditions of the CONAN test

Test case	V_{inlet} $[m/s]$	T_{inlet} [°C]	W_{Air} [-]	W_{He} [-]
P20-T50-V30-H08	3.11	92	0.402	0.005
P20-T50-V30-H65	3.06	89.1	0.223	0.056
P05-T40-V06-H62	(~0.6)	76.9	0.416	0.093
P05-T40-V06-H90	(~0.6)	71.1	0.19	0.219

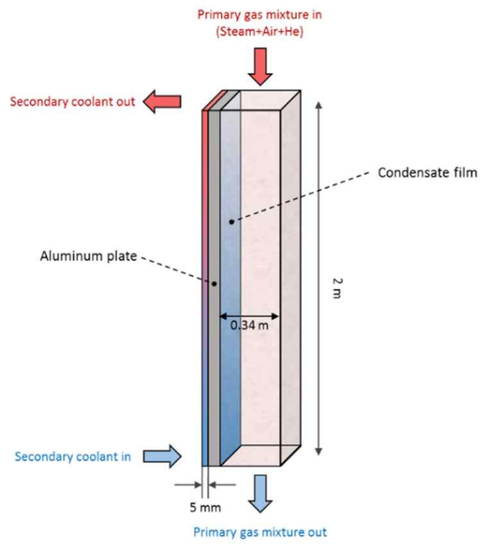

Fig. 5. Sketch of the CONAN facility test section

For the CFD analysis, the computational mesh of 400,000 cells is used shown in Fig. 6 (a), and the wall $y^+$was kept below 1.5. The CUPID analysis mesh which is consist of 63,000 cells is figured in Fig. 6(b). The average wall y^+ is 2 or less.

Generally, the high computational cost is required and many iterative calculations should be conducted until convergence when the conjugate heat transfer analysis including the two-phase flow analysis is used. Therefore, the steady-state analysis of the secondary side is preceded to predict the condenser wall temperature of the primary side. Then, condensation phenomena were analyzed in the primary side by using the pre-determined condenser wall temperature from the preceding calculation. The turbulence model is the realizable $k-\varepsilon$ model, which matches well with experimental results in the preliminary calculations. Two-phase flow analysis approach was used with fluid film model in STAR-CCM+.

In CUPID, in the same way as the CFD analysis, only the primary side where steam is condensed were analyzed. The condensation wall temperature condition was the same as the CFD analysis condition. For the turbulence model, standard $k-\varepsilon$ model was used and the RBLA condensation model was used and condensate film was not considered.

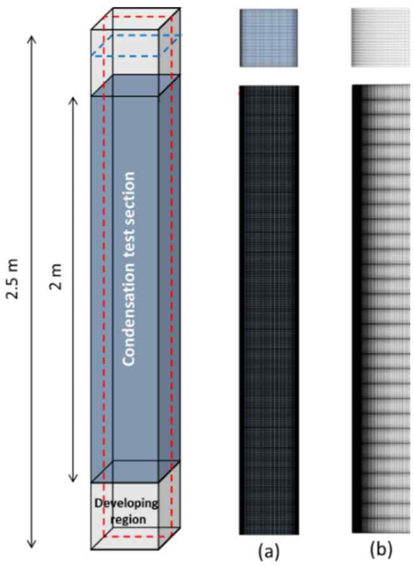

Fig. 6. Computational domain and cross-sectional and side view of meshes of CONAN test section
(a: STAR-CCM+, b: CUPID)

3.2 Simulation results

The analysis results of forced and natural convective condensation conditions are reported in Fig. 7 and Fig. 8, respectively. Both codes were suitable for the analysis of forced convective condensation phenomena. The local condensation heat flux was well predicted to be less than 8% by both codes. However, in the natural convective condensation cases, P05-T40-V06-H62 and P05-T40-V06-H90, both codes could not predict local heat flux peak which can be observed from experimental results. In particular, CUPID underestimated the measured local heat flux and CFD results about 25% under the condition of P05-T40-V06-H62. This is because, in CUPID analysis results, the turbulence generation rate and the species mass transfer rate were underestimated, so that the diffusion layer is thick and the mass fraction gradient of the vapor is relatively small which is directly related to condensation rate. Nevertheless, the STAR-CCM+ code confirmed the possibility of prediction of the local condensation peak near the inlet. As shown in Fig. 9, non-condensable accumulation near the condenser wall leads to reverse flow near the wall since the density of helium is much lower than air. Thus, collision between upward flow at near the wall and bulk flow rapidly generate turbulence kinetic energy. CUPID calculation results also showed a near-wall reverse flow and local heat flux peaks as observed in Fig. 8(b), but the peak height was much lower than the experimental results.

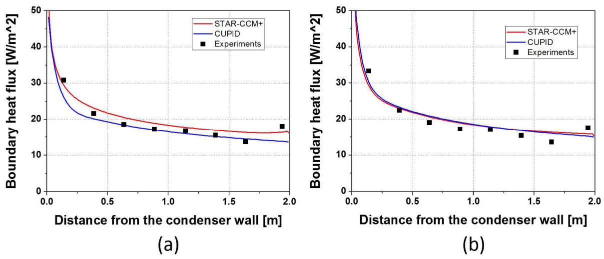

Fig. 7. Comparison between calculated and experimental heat fluxes: forced convective condensation
(a: P20-T50-V30-H08, b: P20-T50-V30-H65)

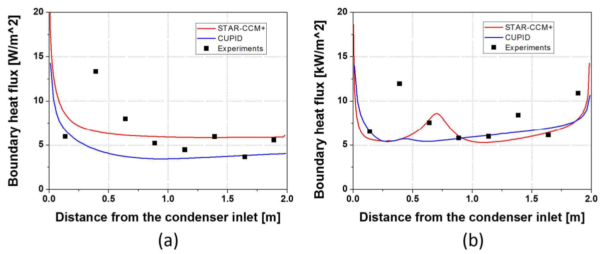

Fig. 8. Comparison between calculated and experimental heat fluxes: natural convective condensation
(a: P05-T40-V06-H62, b: P05-T40-V06-H90)

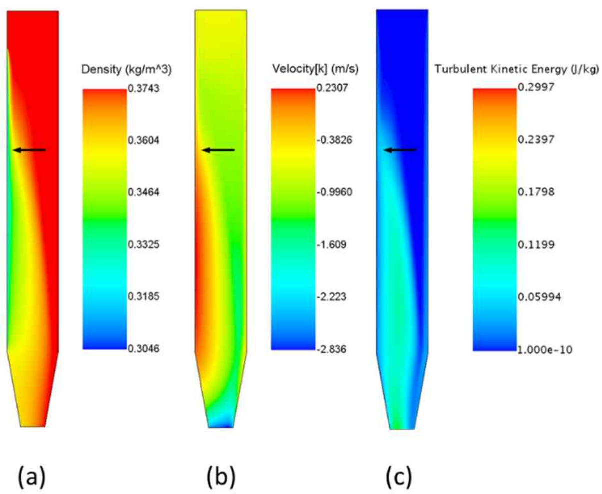

Fig. 9. Properties contour of gases mixture
(a: density, b: axial velocity, c: turbulent kinetic energy)

4. Conclusion

In the present study, the mass and energy transfer evaluation method due to mass diffusion in CUPID were improved by treating each species separately rather than a single mixture. This corrected the non-physical temperature distribution in the diffusion boundary region caused by violation of the energy conservation. The modification can contribute to simulating the gas mixture behavior that has more than two non-condensable gas species.

As a result of the computational analysis of wall condensation phenomena, it was confirmed that the modified CUPID shows reasonable agreements with the CFD code and the experimental results of CONAN. Especially, under forced convective condensation conditions, both codes show good agreement against CONAN experimental results. However, in the case of natural convective condensation, local condensation heat flux calculated by modified CUPID is much lower than experimental results and CFD results. Therefore, under natural convective condensation case, more code to code validation will be performed with CFD code for properly analyzing buoyancy-driven turbulence generation phenomena under the condensation environment and for improvement of condensation analysis capability of CUPID code.

Acknowledgement

This work was supported by the Seoul National University Electric Power Research Institute and the Korea Radiation Safety Foundation (KORSAFE) grant funded by the Korean government (MSIP & NSSC) (Nuclear Safety Research Center Program: 1305011)

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