A study on the dependency between turbulent models and mesh configurations of CFD codes.

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1. Introduction

During severe accidents in a nuclear power plants, the generation of hydrogen may occur and this will complicate the atmospheric condition of the containment by causing stratification of air, steam, and hydrogen. This could significantly impact containment integrity analyses, as hydrogen could be accumulated in local region. From this need arises the importance of research about stratification of gases in the containment.

This paper focuses on the analysis of the behavior of hydrogen mixing and hydrogen stratification, using the GOTHIC code and the CFD code. Specifically, we examined the mesh sensitivity and how the turbulence model affects hydrogen stratification or hydrogen mixing, depending on the mesh configuration.

2. Model description

In this section the hydrogen mixing and stratification phenomenon will be examined in comparison with the experimental results of the PANDA facility, using the GOTHIC code and the CFD code. The PANDA facility in Switzerland. It is a multi-compartmental thermal-hydraulic facility concerning the safety of the LWRs. The facility is used for multiple purposes, such as the containment response experiment, component part test, and the primary system experiment.

The four containments were installed in PANDA facility. Each of containments has a height of 4m and diameter of 8m in the form of a dome. An orifice which fluid injection located 3m away from the bottom. Finally, ventilation was installed 0.16m above bottom, in order to keep pressure constant. It is represented in Fig 1.

Experimental outline of the PANDA facility is as follows. First, in order to set up the initially conditions, the mixture of helium and air was filled in PANDA facility. Secondly, the helium, air, and water vapor mixture was injected into the containment through the orifice. Through this, we observed the stratification and mixing phenomena in PANADA facility.

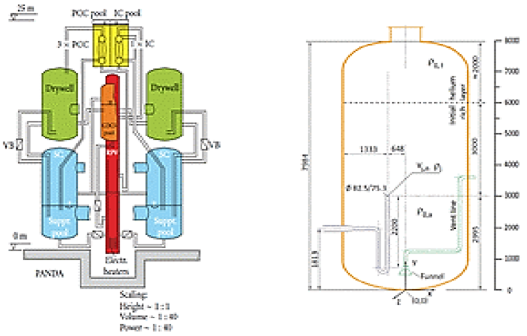


Fig 1. PANDA facility designs [1]

2.1 GOTHIC code model

GOTHIC (Generation of Thermal-hydraulic Information for Containments) is a thermal-hydraulic software to analyze the safety and operation of containment. The finite volume method is used in GOTHIC code. The fluid is modeled in three phase which are vapor, liquid drop and liquid. Computational mesh can be chosen between lumped and 3-D model. The lumped model calculates single value at temperature, pressure, velocity and molar fraction, etc. The 3-D model calculates velocity, pressure, temperature of each rectangular on conservation equations (mass, momentum, energy).

The initial, geometric, and the boundary conditions of the GOTHIC code and modeled in the study used the conditions provided in the Synthesis of the OECD/NEA-PSI CFD Benchmark Exercise [2]. In the PANDA experiment, helium was used instead of hydrogen. And the mixture of helium and air filled nonlinearly from 6m to top initially. The rest of the space was filled with air. The initial pressure of the inside of the containment was 101kPa, and it maintained the temperature 22℃. The experimental condition were summarized Table I[2].

Table I: PANDA experimental conditions [2].

Prssure	101kpa
Air mass flow rate	21.52g/s
Helium mass flow rate	0.42g/s
Gas molar fraction in the inlet flow gas mixture	Air : 0.862
	Helium : 0.134
	Water vapour : 0.004
Injection temperature (℃)	From 20 to 29.3

In this study, the number of the meshes modeled in the GOTHIC simulation 3000 and 5000. To investigate the effectly the mesh aspect ratio, the 5000 meshes model was further modified into the two cases in which the ratios of the width, length, and the height are each 1:1:1.01 and 1:1:1.84 , respectively. The schematic of the GOTHIC model for PANDA experiment is show Fig 2.

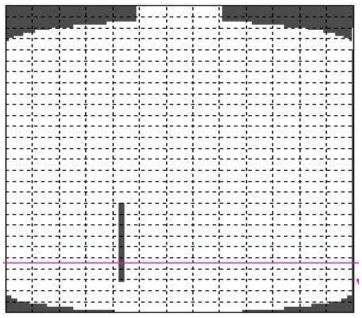


Fig 2. The schematic of PANDA modeled with GOTHIC code.

In Table Ⅱ, the aspect ratio is the ratio of the width and height (width/height). For the three cases listed in Table Ⅱ, we investigated the effect of turbulence modes. Two Turbulence models K-epsilon standard and renormalized were tested to check the sensitivity of mesh configuration on turbulence models. The k-Renormalized has been developed model which used alternate source term for the Reynolds stress source term [3].

Table Ⅱ: Aspect Ratio of GOTHIC code model.

mesh	5000(A)	5000(B)	3000
Aspect ratio	1.01	1.84	2.05
Mesh height (m)	0.302	0.1968	0.217

2.2 STAR-CCM+ code model

CFD (Computational Fluid Dynamics) code is one of methodologies that can simulate and predict the performance of fluid systems. In this study, we used STAR-CCM+ which is one of the CFD code popularly used in engineer design. In STAR-CCM+ there are 3 types of turbulence models: Standard K-Epsilon Low-Re, Realizable K-Epsilon Two-layers, and SST K-Omega models. To run the simulation, it's important to generate the mesh. There are many mesh types and generally the trimmer type is efficient for filing large volumes and also uses less capacity than polyhedral mesh type. Besides Prism Layer Mesher, Surface Remesher can be selected. In the volume mesh of 5385 and 266554 cells were generated to simulate the PANDA experiment. So there are 4 simulation cases, i.e. two mesh sizes with three turbulence models for each mesh model. The simulation cases are summarized in Table Ⅲ.

Table Ⅲ: Simulation cases with STAR-CCM+

	Standard K-Epsilon Low-Re	Realizable K-Epsilon Two-layers	SST K-Omega
Mesh size	5385	5385	5385
	266554	266554	266554

The schematic of the STAR-CCM+ model is show in Fig 4.

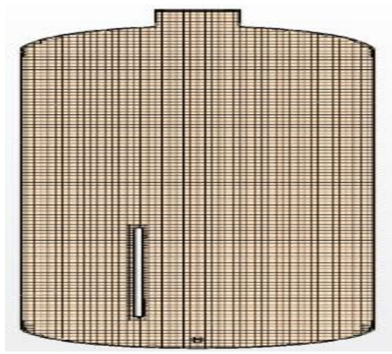


Fig 4. The schematic of PANDA modeled with STAR CCM+ code.

3. Results and discussion

3.1 Results

In PANDA experiments, helium molar fraction was measured in specific points. In Fig 5. the initial helium and air distribution is depicted, which also shows the measurement point.

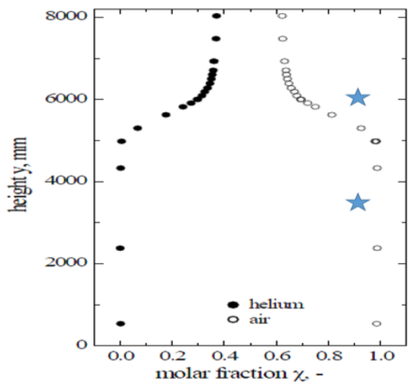


Fig 5. Helium molar fraction monitoring point in PANDA facility and initial helium distribution.

In Fig 6, we marked the locations of comparisons between experiments and code simulations, i.e. the middle section (3.67m from the bottom) and top section (6m from the bottom).

The GOTHIC simulations, six cases i.e. three mesh configuration with two different turbulence models each are analyzed. The results are shown in Fig 6, Fig 6 (a) for the middle section and Fig 6 (b) for the top section. In Fig 6, STD represents standard k-epsilon model, RG represents renormalized k-epsilon turbulence model.

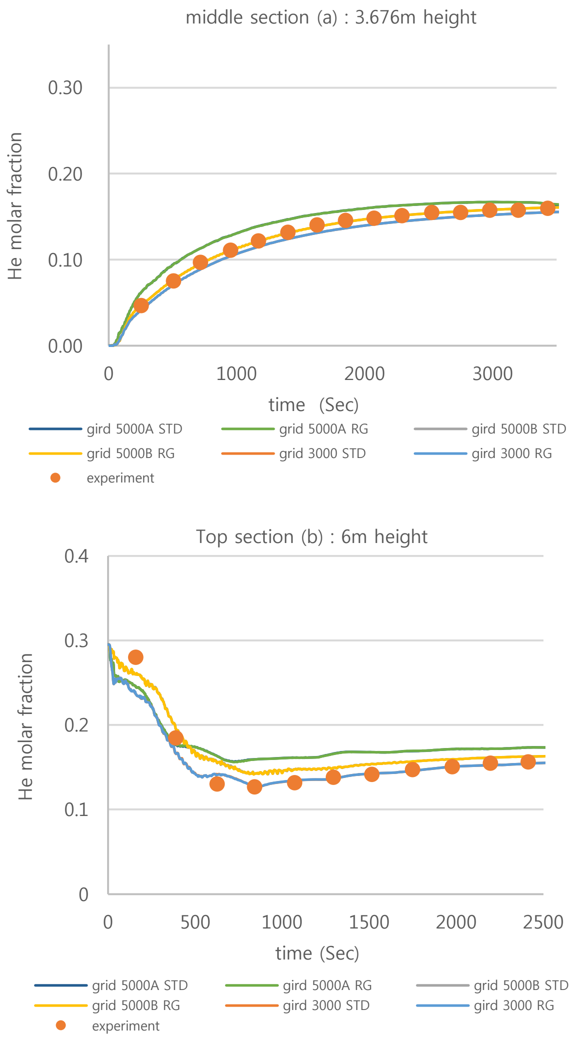
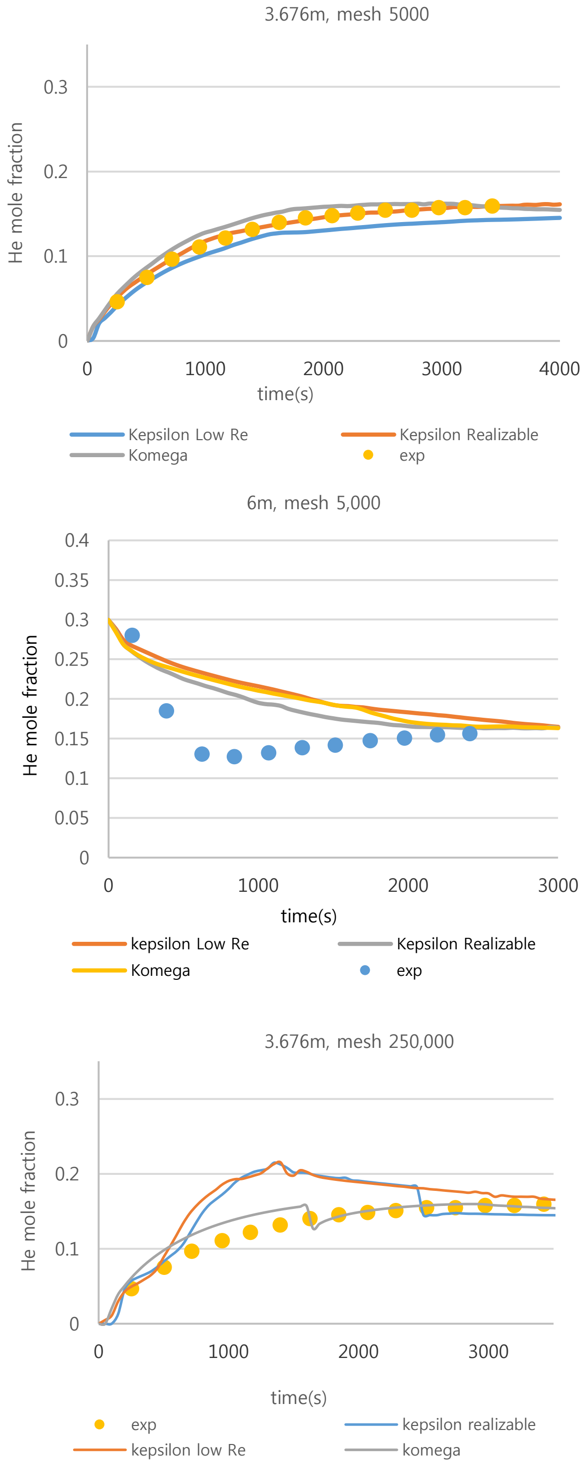


Fig 6. Helium concentration time-histories at the two position using the Gothic code (middle: 3.767m, top: 6m.).

In case of STAR-CCM+, the same simulation results like those of GOTHIC are shown in Fig 7. In Fig 7, the helium mole fractions at 6m and 3.676m are presented for 5,000 and 25,000 mesh cases, each with three turbulence models, i.e. k-epsilon low realizable, k-epsilon realizable, and k-omega model.



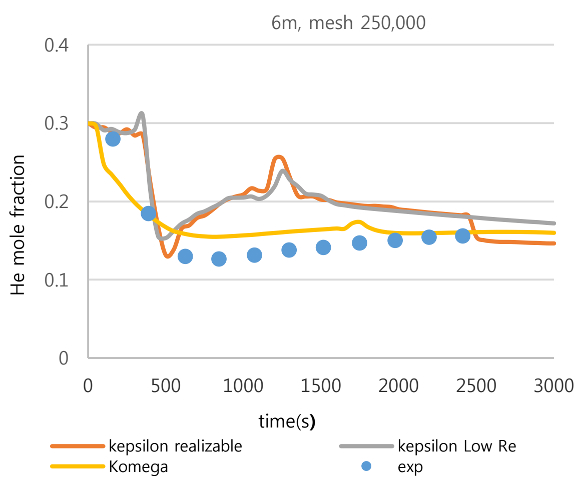


Fig 7. Helium concentration time-histories at the two position using the STAR-CCM+ code (middle: 3.767m, top: 6m.)

3.2 Discussion

In case of GOTHIC code simulations, the difference between calculation and experimental data was analyzed by estimating relative errors by equation (1).

$$\text{Relative Error} = \frac{1}{n}\sum_{i=1}^{n}\frac{|m_{i,exp} - m_{i,CFD}|}{m_{i,exp}} \quad (1)$$

Where $m_{i,exp}$ is the molar fraction of experiment, $m_{i,CFD}$ is the molar fraction calculated by GOTHIC. And n is total number of data. The relative error estimation is summarized.

Table Ⅳ: Relative error estimation of GOTHIC code simulations.

	Ke-STD			Ke-Renomalized		
mesh	5000A	5000B	3000	5000A	5000B	3000
3.376m	0.0131	0.0009	0.0064	0.0130	0.0009	0.0064
6m	0.0198	0.0130	0.0076	0.0191	0.0131	0.0075

It is noticed in Table Ⅳ that two choice of turbulence models affects the simulation results very little regardless of number of meshes. In Fig 6, it is observed that the case with large aspect ratio shows better results than that with small aspect ratio if the number of meshes is the same. As large aspect ratio means smaller height of meshes, it could be concluded that a mesh configuration with smaller size in the vertical direction is more important to predict the experimental results. In terms of the mesh number, the cases that the number of mesh is 3000 and 5000B are well matched with experiment data without significant error. On the other hand, in the case of 5000 meshes with aspect ratio of 1.01(5000A) a significant deviation of computational result from the experiment was observed. By interesting the results of cases of 3000, 5000A, 5000B mesh configurations, it could be concluded that the vertical height of a mesh is more important than the number of meshes in order to make better predictions, because the stratification phenomena can be better simulated with a fine mesh structure in the vertical direction. In the case of STAR-CCM+ code simulations, as shown in Fig 7, the effect of the turbulence model becomes in significant as the number of the mesh decrease. It is thought that the turbulence mixing effects becomes subdued and the turbulence motion becomes averaged out in large mesh volume.

Another observation is that the deviations between turbulence models are large for the monitoring point farther away from the injection orifice. This may be due to the fact that when the monitoring point is located near the injection orifice the forced mixing is so dominant that turbulence models may result in almost same level on mixing. In the meanwhile, the vortex mixing may develop in a region some distance away from the injection point. Since the flow injected in mono-direction initially becomes diverging and mixing with surrounding atmosphere, that would create vortex turbulence. This may explain the k-omega turbulence model show better performance than k-epsilon models in particular for the experiment data at 6m.

4. Conclusions

In this work, sensitivity analyses for the meshes and the turbulence models were conducted for missing and stratification phenomena. Two computation fluid dynamics code, i.e. GOTHIC and STAR-CCM+ were adopted and the computational results were benchmarked against the experimental data from PANDA facility. The main findings observed through the present work can be summarized as follows:

1) In the case of the GOTHIC code, it was observed that the aspect ratio of the mesh was found more important than the mesh size. Also, if the number of the mesh is over 3,000, the effects of the turbulence models were marginal.
2) For STAR-CCM+, the tendency is quite different from the GOTHIC code. That is, the effects of the turbulence models were small for fewer number of the mesh, however, as the number of mesh increases, the effects of the turbulence models becomes significant. Another observation is that away from the injection orifice, the role of the turbulence models tended to be important due to the nature of mixing process and inducted jet stream.

In summary, it is stressed that when a CFD code is used for thermal mixing and stratification the selection of a turbulence model should be considered in conjunction of the mesh configurations including the number of mesh, aspect ratio, in order to reflect phenomena.

Acknowledgments

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