Mesh Generation for a Simulation of Hydrogen Behaviors in a Reactor Containment

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1. Introduction

Because it is impractical to experimentally simulate hydrogen behaviors in a containment of a nuclear power plant (NPP) during a severe accident, numerical simulations with separate effect tests using scaled test facilities for validation of the numerical models are commonly used.

Traditionally, the numerical method is split into a lumped-parameter (LP) method and a multi-dimensional computational fluid dynamics (CFD) method. The LP method is based on a relatively coarse nodalization compared to the multi-dimensional CFD method which requires densely nodalized mesh in order to resolve turbulence effect on thermal hydraulic behaviors. In a LP code such as Melcor [1] or Relap [2], turbulence effects are lumped into correlations for heat, mass, and momentum transfers. So parameters of correlations in a LP code must be carefully defined on an appropriate nodalization.

It is well known that numerical simulations are dependent on nodalized control volumes (CV) or meshes used for the simulations. So it is believed that the multi-dimensional CFD method or a turbulence-resolved approach must be applied carefully for an accident analysis. If turbulent characteristics in a flow field are not well resolved by the turbulence-resolved approach [3], the flow field may be poorly distorted, and sometimes it is worse than the correlation-based turbulence-unresolved solution.

In a containment safety analysis, multi-dimensional characteristics in thermal hydraulics are very important because flow paths are not confined (in other words, not well defined) in a large free volume of the containment. But it is difficult to resolve the 3-dimensional behaviors in a containment using the LP method using a small number of CVs because of a difference in length scales between a characteristic length of the flow and representative length of a compartment in the containment.

From 90's, the turbulence-resolved approach has been applied for the containment safety analysis. Royl et al. [4] used GASFLOW to analyze the hydrogen–steam distributions in the Konvoi-type NPP. Houkema et al. [5] compared the results from a LP code and the commercial CFD code CFX, and suggested that a three-dimensional analysis is necessary to predict a non-uniformly distributed hydrogen concentration. Recently, Jiang et al. [6] applied CFD method for an analysis of PCCS (passive containment cooling system) implemented in AP1000.

Though GASFLOW and COM3D [7] are well developed for a real NPP containment analysis, there exist shortcomings in nodalization. They are based on a Cartesian or cylindrical mesh generation, so it is impractical to refine a mesh locally in a region with a physical or geometrical complication. Recently it is known that jet flow of a released gas from reactor cooling system (RCS) is strongly affected in initial distribution and mixing of hydrogen. If the turbulent convection of the released gas augmented by jet momentum and buoyancy force is not well resolved, then the hydrogen distribution during an accident may not be conservative.

Commercial or newly developed CFD codes are using unstructured or hybrid mesh technologies in order to reduce man-hours needed to generate a mesh of a complicated flow field. Use of an unstructured mesh is very attractive because its generation is mostly automated by the help of computational geometry.

In the case of the mesh generation for a simulation of hydrogen behaviors in an NPP Containment, it is not a routine work because of some reasons. Because of the nature of severe accidents such as a wide spectrum of accident progressions, long term transients, and complicated phenomena, the size of a mesh must be carefully controlled base on an available computing power. Without that it is impractical to evaluate hydrogen safety in a NPP containment. And quality of a generated mesh must be also managed to reduce numerical diffusion and enhance stability of used numerical schemes during a fast transient.

Currently it is underway to develop a new generation code founded on modern CFD technology for containment safety analysis. The new code, containmentFOAM [8], is based an open-source CFD library OpenFOAM [9]. In parallel to the containmentFOAM development, it is continuously pursued to improve mesh generation technology specifically for an NPP containment.

In this paper, recently conducted research for the development of a containment mesh generation is introduced.

2. Containment Mesh Generation

An NPP containment is one of most complicated geometry for a CFD simulation. In order to resolve full features of the internal geometry, tens of millions of cells are not enough. When the number of mesh cells increases the required computing time does not linearly increase because a time step is drastically reduced by the limit of the Courant number which is denoted as follows.

$$\Delta t = CFL \min\left[\frac{(V_{cell})^{1/3}}{|\mathbf{U}|}\right] \qquad (1)$$

Based on computational experience using a 64 core moderate-parallel computer (lower performance than massive-parallel computer), a simulation of a hydrogen behaviors in an APR1400 containment using a mesh composed with 1 million cells requires about 2 weeks. So it is thought that a mesh with 1 million cells is appropriate on a moderate-parallel computer for hydrogen safety evaluation in a NPP containment.

Another important consideration for a containment mesh generation is its quality. Nominally mesh quality is defined by skewness and non-orthogonality. Aspect ratio of a cell can be a parameter of the mesh quality for a high Reynolds number flows. But it can be neglected in the case of hydrogen behaviors in a containment.

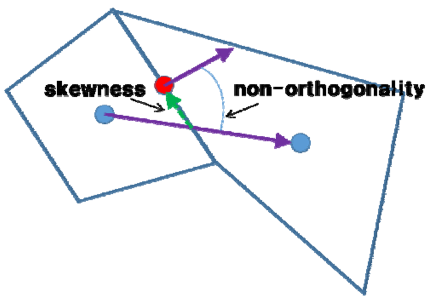


Fig. 1. Skewness and non-orthogonality of a mesh

The skewness and non-orthogonality are depicted schematically in Fig. 1. They are important parameters of the mesh quality because a very skewed or non-orthogonal mesh can increase a computing time by an increased work load to converge iterative matrix solvers of discretized equations. And sometimes they make numerical solutions diverged.

In this study, an APR1400 containment was chosen for an evaluation of mesh generation technology. The micro-scale features of the containment geometry compared to the diameter of the containment outer wall was trimmed out. Fig. 2 shows a modeled geometry of the APR1400 containment. The total volume of Apr1400 containment is approximately 120,000 m^3, and the volume to be used for calculation except internal structure is 92,670 m^3 (Table 1).

Table 1. Geometries of APR1400

	Volume (m$^{3)}$
RCS	1,400
Compressed vessel	470
Internal wall	26,500
Containment	121,000
Computational	92,670

Fig. 2. Modeled geometry of the APR1400 containment

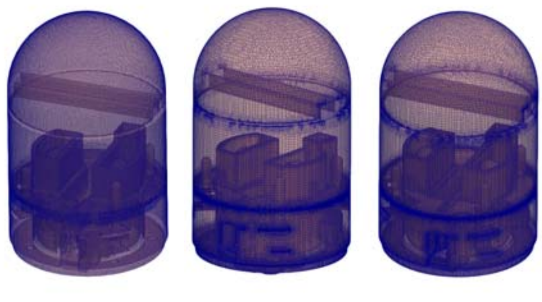
There are two methods to create the mash for OpenFOAM solver. One is using the open-source software 'SALOME', and the other is to use OpenFOAM's internal modules 'cfMesh' or 'snappyHexMesh(SHM)'.

When using the SALOME, grid creation is intuitive and convenient, but in complex structures, such as internal geometry of APR1400, it is advantageous to use the module 'cfMesh' or 'SHM'. 'cfMesh' generates grids easier and faster, but is more likely to produce irregular grids. SHM requires a complex 'Dict' file and generates grids slower, but most cells are hexagonal and the grid is regular.

The mesh was created in three cases using these two internal modules. The results of the generated cells are shown in Table 2

Table 2. The results of generated cells

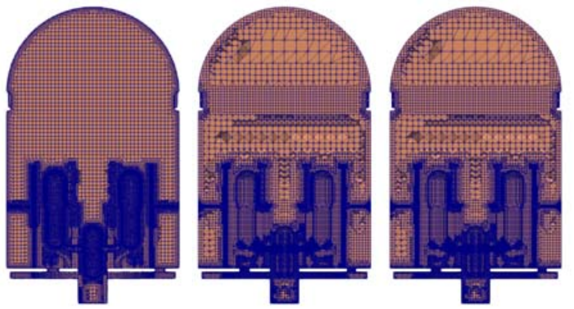
Cell type	cfMesh (cells)	SHM (cells)	SHM_refine (cells)
Hexahedral	962,923	917,537	918,154
Prisms	22,698	66,029	66,113
Pyramids	70,455	0	0
Tetrahedral	56,658	1469	1465
Polyhedral	56,482	164,263	164,529
Total	1,169,216	1,149,298	1,150,271



(a) (b) (c)
Fig. 3. Mesh generation result (a) – cfMesh, (b) – SHM, (c) – SHM_refine

Figure 3 shows the mesh generation results. 1,169,216(cfMesh) and 1,149,298(SHM) cells were generated. The average cell volume is approximately 0.08 m^3 for APR1400 containment.

Figure 4 is a vertical cross-section view of the containment mesh. As shown in the figure 4, the cell density around the reactor cooling system(RCS) boundary is given a sufficient number to calculate hydrogen behavior due a jet flow from RCS.



(a) (b) (c)
Fig. 4. Cross-section view of containment (a) – cfMesh (b) – SHM, (c) – SHM_refine

Table 3 shows the mesh quality results. A skew face means a face with skewness 4 or more, and a non-orthogonal face means a face with a non-orthogonality of 70 degrees or more. The number of non-orthogonal faces and skew faces is extremely small in case 'SHM'. Non-orthogonal faces and skew faces incur computational time delays and reduce the accuracy of the computation results. Thus, more accurate calculation results can be expected in case 'SHM'. The mesh with four skew faces was manually refined to reduce the number of skew faces to zero(SHM_refine - 1,150,271 cells).

Table 3. Mesh quality

	cfMesh (faces)	SHM (faces)	SHM_refine (faces)
Non-orthogonal	693	0	0
Skew	288	4	0

Test simulations were conducted to see how each generated grid affected computation time. The test is hydrogen flame propagation analysis inside APR1400 using XiFoam. Testing conditions and results are shown in Table 4 below. The computer used for the calculation was intel(R) Xeon silver 4110 CPU(8 core) x 2ea and 96GB memory, calculated in parallel using 6 cores in each case, analyzed 0.1s problem time. In the result, the cfMesh case failed calculate due to the high skew faces, which failed to converge. The SHM case has only 4 skew faces than the SHM_refine case, but the total computation time increased by about 1%.

The effect of skew faces on future real calculations can be greater if we use a turbulence model that requires more equations to be solved, and if the analyzing time is more than 2000 seconds, the final computation time is expected to vary by more than a few days

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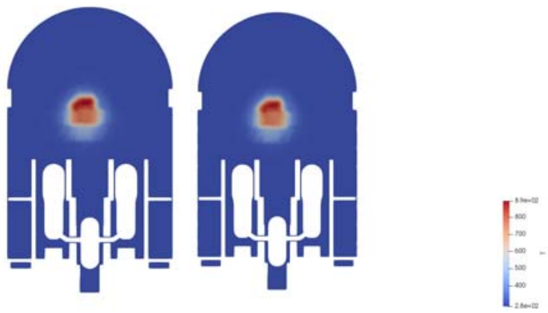
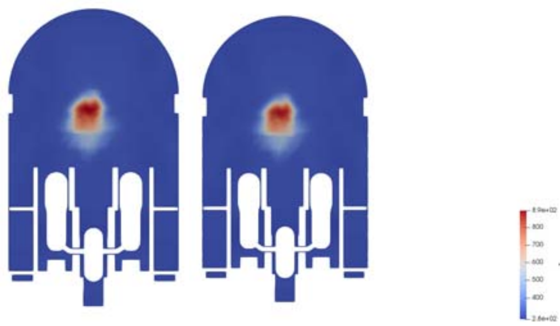
Table 4. Testing condition

	cfMesh	SHM	SHM_refine
Solver	XiFoam		
Reactant	Air(O_2, N_2), Wet hydrogen(H_2, H_2O)		
Stoichiometric air-fuel mass ratio	43.823		
Turbulent model	k-ε		
Analyzed time	0.1		
dt	0.0001		
Computation time	Failure	3113s	3087s



(a) (b)
Fig. 5. Gas temperature at 0.01s (a) – SHM, (b) – SHM_refine



(a) (b)
Fig. 6. Gas temperature at 0.1s (a) – SHM, (b) – SHM_refine

3. Conclusions

A mesh generation of an NPP containment for transient simulation of hydrogen behaviors during severe accidents is still challenging.

In this work, mesh generation technology was tested for the APR1400 containment and some guide lines such as mesh size and quality are applied to evaluate appropriateness of the generated meshes for the hydrogen safety evaluation of APR1400. During the work reasonable meshes for the APR1400 containment were obtained. But it is thought some technology to improve mesh quality are needed to enhance numerical stability of the simulations.

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