Coupling of MELCOR and OpenFOAM for an Analysis of Containment Hydrogen Behaviors

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1. Introduction

A nuclear reactor containment building play a very important role as a last barrier to prevent the release of radioactive materials into the external environment in the event of an accident. In particular, pressurized water reactor-type nuclear power plants are designed to minimize the possibility of a large release of radioactive materials into the environment in most severe accident conditions, and to ensure the integrity of containment buildings through accident management guidelines.

In the event of an accident, very complex thermal and hydraulic phenomena occur in the containment building such as release of water vapor and condensation of water vapor released by decompression of the reactor, generation and release of hydrogen by oxidation of the core, mixing and combustion of the released hydrogen, behavior of droplets by water spray with condensation of water vapor, water vapor condensation with heat transfer and development of the liquid film on the surface of the structures inside the containment, release of radioactive materials from the degraded core and its behavior in the containment building, release of the core melt due to reactor failure, reaction of the melt and coolant, and reaction of the melt with concrete of the reactor cavity. These various physical phenomena directly or indirectly affect the integrity of the containment building.

In recent years, IAEA proposes to classify damages in containment buildings in the event of accidents into early and late damages, and try to practically eliminate the possibility of early damages because an early damage of a containment may result in a large early release of radioactive materials into the environment [1]. The practical elimination of the possibility of the large early release is requested to be based on the analysis of accidents by applying realistic and best estimate analysis technology to the representative phenomena affecting the early failure of the integrity of the containment building. And if found, it is to secure safety through back-fitting [2, 3].

Developing detailed and mechanistic analysis technology for various physical phenomena, especially behavior of materials and structures, and thermal and hydraulic phenomena occurring in a containment building in the event of an accident, and applying it to the evaluation of the integrity of the containment building is important for securing the safety of a nuclear power plant. Therefore, the development of a coupled analysis technology for various physical phenomena in the containment building in the event of an accident is required for a best estimation of accident progressions.

2. Methods and Results

Various physical phenomena occurring within the containment building under severe accident conditions affect each other and change over time. As a method for simulating physical phenomena that interact with each other in this way, there are a variety of methods ranging from a method of integrating multiple physics phenomena analysis models in a single analysis code in a module form to a method of linking independent solvers for each physical phenomenon. In this study, we intend to secure an analysis technology using a network connection method of an independent solver in consideration of scalability for various physical phenomena.

In this study, we intend to build a coupling technology of several analysis solvers based on preCICE [11], an open-source library for code coupling. In the previous study [4], it was applied to the fluid-structure conjugate heat transfer (CHT) using the PreCICE library to verify the applicability of the library for coupling separate solvers. And it was confirmed that the CHT problem can be applied to the network connection method of an independent structure heat transfer solver and fluid heat flow solver and it gives the same accuracy as the stand-alone solver including fluid and solid regions.

For a best-estimate analysis of hydrogen behaviors in a NPP containment during a severe accident, a coupled analysis method was applied by coupling MELCOR [5], an integrated analysis code for the phenomena inside the nuclear reactor, and the detailed analysis code, ContainmentFoam [6] which is a hydrogen safety analysis code in a containment developed on the OpenFOAM platform [7] for the analysis of thermal hydraulics in a containment building. To this end, we developed MELCOR's preCICE adapter and performed MELCOR-ContainmentFoam coupled analysis [8].

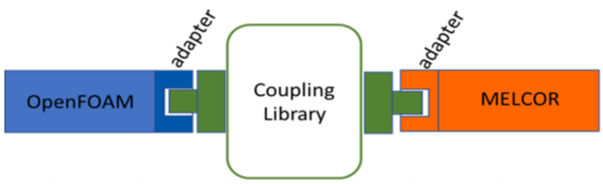

Fig. 1. MELCOR-OpenFOAM coupling by preCICE

Fig. 1 shows the schematic of coupling MELCOR and ContainmentFoam solvers by preCICE adapters. The following describes the development of preCICE adapters for MELCOR and ContainmentFOAM and its application to simulation of a hydrogen release from a vessel to a compartment.

2.1 MELCOR preCICE Adapter

MELCOR is an integrated analysis code developed by Sandia National Laboratory in the United States and managed by the National Regulatory Commission (NRC). Currently, up to version 1.8.6 is obtained as a source code in Korea, and only executable files are provided for later versions. For the development of MELCOR's preCICE adapter, the source code needs to be modified, so version 1.8.6 was used. In particular, in order to extract data necessary for MELCOR-OpenFOAM coupled analysis from the MELCOR code, it is necessary to analyze the variables of the code and at the same time analyze the temporal integration algorithm of the MELCOR code to obtain the latest state values at the current time stage.

The MELCOR data extraction method for an MELCOR-OpenFOAM coupled analysis, that is, selection of variables at the MELCOR's control volumes (CV) or flow paths (FL) for data transfer was designed as follows.

-To minimize the modification of the MELCOR source code for user input.

-To use the existing MELCOR input structure and minimize changes.

-To be convenient for MELCOR users to select the flow path (FL) of the point connected to OpenFOAM and the associated variable.

The MELCOR source code was analyzed based on the above requirements, and it was concluded that the most efficient method is to modify MELCOR's control-function for data extraction. To this end, “SEND” command was added to the function of the existing control-function. Table 1 is the abbreviated list of the commands of the MELCOR’s control functions and addition of “SEND” command for data extraction and transfer to OpenFOAM.

Table 1. Addition of SEND command in the MELCOR’s control functions

CF action	Code Number
ADDITION	110
MULTIPLY	120
DIVIDE	130
…	…
…	…
PIPE-STR	760
SEND	770

By adding the “SEND” command in the MELCOR code, it is possible to use the same structure of the MELCOR input file and the users can easily select locations and values of variables to be transferred to OpenFOAM. Below is an example of the MELCOR data transfer included in MELGEN input file.

Table 2. An example of SEND control function

CF777100	XH2	SEND	1	1.0	0.0	
CF777101	0.0					
CF777111	1.0	0.0	FL-MFLOW.6.360			

The part of the MELGEN input file in Table 2 means that hydrogen mass flow rate from the FL360 flow path is prepared for data transfer. The data prepared by the “SEND” control function is ready to be transferred by preCICE library. The MELCOR preCICE adapter is designed to collect the data from the “SEND” control function and load them on the network communication functions of preCICE.

Table 3. Network communication functions of MELCOR preCICE adapter

```
CALL precicef_set_vertices(meshID, N, GRID, vertexIDs)

CALL precicef_initialize(dtlimit)

CALL precicef_action_required(writeInitialData, bool)
IF (bool.EQ.1) THEN
   WRITE(*,*) "[",IOUTCOUNT,"] writeInitialData ", bool
   IOUTCOUNT=IOUTCOUNT+1

   CALL precicef_write_bsdata(ScalarsID, N, vertexIDs, Scalars)
   CALL precicef_write_bvdata(VectorsID, N, vertexIDs, Vectors)
   CALL precicef_fulfilled_action(writeInitialData)
ENDIF

CALL precicef_initialize_data()

C   // read data if available
CALL precicef_read_data_available( bool )
IF (bool.EQ.1) THEN
  WRITE(*,*) "[",IOUTCOUNT,"] readInitialData ", bool
  IOUTCOUNT=IOUTCOUNT+1

  CALL precicef_read_bsdata(pressureID, N, vertexIDs, pressure)
ENDIF
```

2.2 OpenFOAM preCICE Adapter

The purpose of the current preCICE-based coupled analysis is to simultaneously perform MELCOR analysis of a severe accident in the reactor cooling system (RCS) including the reactor and OpenFOAM (especially ContainmentFoam) analysis of 3-D hydrogen behaviors in the containment building. It was thought that it would be appropriate to apply the associated data of MELCOR to the grid cells of a specific location within the containment volume, not to the boundary surface for detailed CFD analysis.

In the current development, the data to be communicated is largely divided into grids, scalars, and vector variables, and is defined as an array as many as the number of required data. In the current code, for convenience, it is designed to access a specific data variable at a required location by defining it as a one-dimensional array and defining each grid cell in the order of each specific interval. It can be seen that the “pressure” variable is specifically classified for the following communication data variables. This was divided for more convenience by dividing read and write options in data communication between two heterogeneous programs. In MELCOR, pressure data is provided from an external solver (OpenFOAM) and, conversely, scalars and vectors variables such as hydrogen mass flow and its momentum are transmitted to the external solver.

The main point of the OpenFOAM adapter design is to set the source fields for each associated data variable and apply the “fvOptions” method included in OpenFOAM as sources of the governing equations such as species mass equations, energy equation and momentum equation in order to keep the structure of the OpenFOAM solvers unchanged. OpenFOAM includes a library of “functionObjects” which is run-time selectable. The main considerations for development are applying the functionObjects library to apply preCICE to existing OpenFOAM solvers without direct code modification.

2.3 MELCOR-OpenFOAM Coupled Analysis

As a verification of the MELCOR-ContainmentFoam coupled analysis, a test case of hydrogen release from a vessel to a compartment was designed. The SPARC [7] pressure vessel filled with a mixture of hydrogen and air is connected to a compartment through a pipe and a mixture gas of hydrogen and air is released when the pipe nozzle is opened at the lower center of the compartment. The hydrogen release phenomenon was simulated by the MELCOR-ContainmentFoam coupled method. The pressure variation in the SPARC vessel from the hydrogen release was simulated by MELCOR and the hydrogen distribution in the compartment was simulated by the ContainmentFoam solver coupled with MELCOR. Table 4 is the initial conditions of the SPARC vessel.

Table 4. Initial conditions in SPARC

Pressure	**5 bar**
Temperature	100 °C
H2 mole concentration	30 vol%

Fig. 2 shows the results of the coupled analysis of MELCOR-ContainmentFoam. As expected, the pressure in the SPARC vessel, which is the region of the MELCOR analysis, is gradually decreasing as the internal gas (a mixture of hydrogen and air) is released into the compartment. The data of hydrogen and air mass flow rates and their temperatures calculated by MELCOR are transferred to the ContainmentFoam solver by the preCICE communication library. It is seen in the figure that the transfered gas mixture is injected in the compartment and released as a buoyant jet in the compartment by the low density of the hydrogen gas mixture.

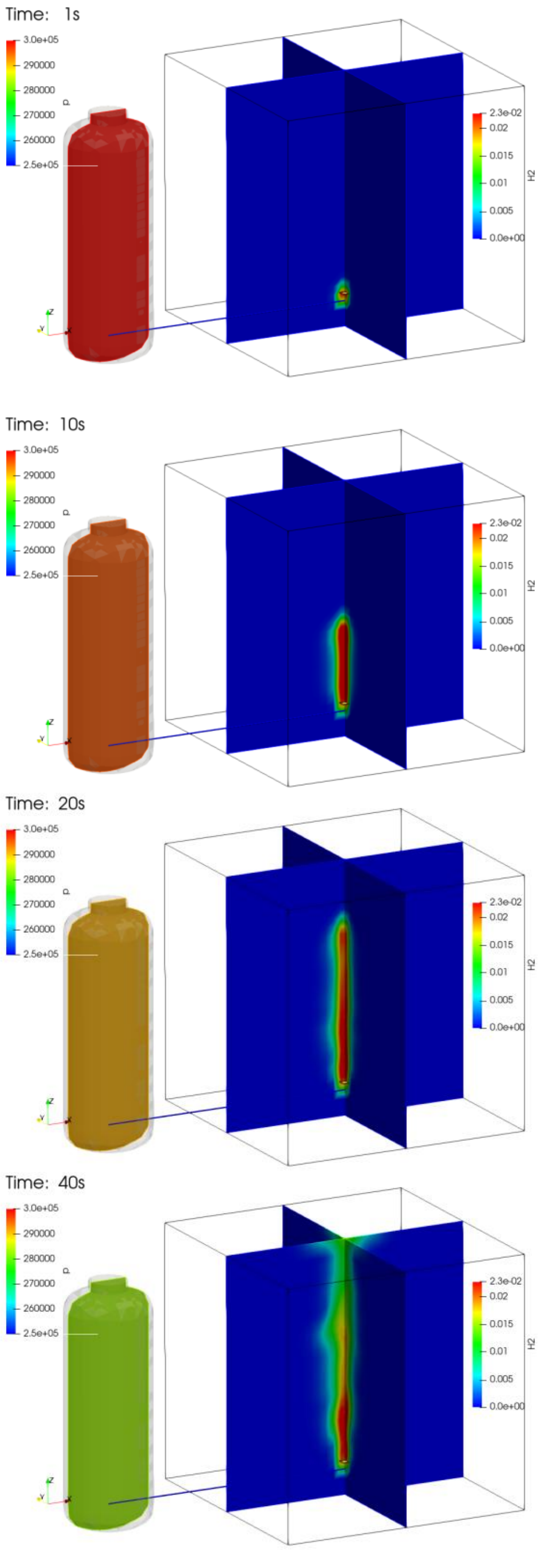

Fig. 2. MELCOR-ContainmentFoam coupled analysis, pressure field in SPARC and hydrogen distribution in the compartment along time.

3. Conclusions

In this study, based on preCICE, an open-source library for coupling stand-alone applications, we developed a coupling technology of independent analysis solvers. For a best-estimate analysis of hydrogen behaviors in a NPP containment during a severe accident, a coupled analysis method was applied for coupling MELCOR, an integrated analysis code for the phenomena inside the nuclear reactor, and the detailed analysis code, ContainmentFoam for the analysis of thermal hydraulics in a containment building. To this end, we developed MELCOR's preCICE adapter and performed MELCOR-ContainmentFoam coupled analysis to verify its applicability.

It is planned to apply the network-based coupled analysis technology developed in this study to simulations of hydrogen behaviors in nuclear power plants during a severe accident and to evaluate the hydrogen safety of a nuclear power plant.

ACKNOWLEDGEMENT

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