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Evaluation and Selection of a Multi-Dimensional Code for H_2 Combustion and Explosion Analysis in the Containment of a Nuclear Power Plant

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1. Introduction

Research into the possibility of a hydrogen explosion, and of a safety device to reduce the hydrogen concentration in the containment of a Nuclear Power Plant (NPP) in Korea, has been intensively conducted since the hydrogen explosion accident of the NPP in Fukushima in 2011. Thus, Passive Auto-Catalytic Recombiners (PARs) were installed in all NPP containments to reduce hydrogen concentration during a severe accident [1]. However, hydrogen combustion is possible during a severe accident if the hydrogen concentration is higher than about 10% at a local position in the containment [2]. Thus, to assure containment integrity, it is necessary to evaluate an overpressure buildup resulting from a propagation of hydrogen flame along the obstacle and wall in the containment during a severe accident. Korea Atomic Energy Research Institute (KAERI) decided to import the computational code for the hydrogen combustion and explosion analysis from a foreign country, to establish a numerical analysis system for considering hydrogen generation in the core, to hydrogen combustion in the containment, as soon as possible.

2. Requirements of a Computational Code for the H_2 Combustion and Explosion Analysis

KAERI has developed a Computational Fluid Dynamics (CFD) analysis methodology to predict the overpressure buildup resulting from hydrogen flame propagation, on the basis of experimental results and application results of the APR1400 IRWST using the commercial code ANSYS CFX [3-7]. An advantage of using the CFX is that it has validated turbulent and combustion models and is an excellent tool to model a complicated geometry configuration. However, the CFX needed a lot of computational time to obtain a converged solution in the transient calculation because the CFX adapted the fully implicit method for the time marching [7]. From the CFX analysis results, we can find the requirements for the hydrogen combustion and explosion code to accurately predict the hydrogen flame propagation in a proper time.

2.1 CFD Analysis for the ENACCEF Experiment

IRSN in France performed the hydrogen flame acceleration test using the ENACCEF facility by varying the initial hydrogen and diluents concentrations and the blockage ratio of an obstacle [8,9]. The hydrogen was ignited at the bottom region and its flame then propagated upward along the test facility. IRSN measured the flame front Time of Arrival (TOA) at 16 locations and the pressure at 9 locations to observe the flame acceleration phenomenon.

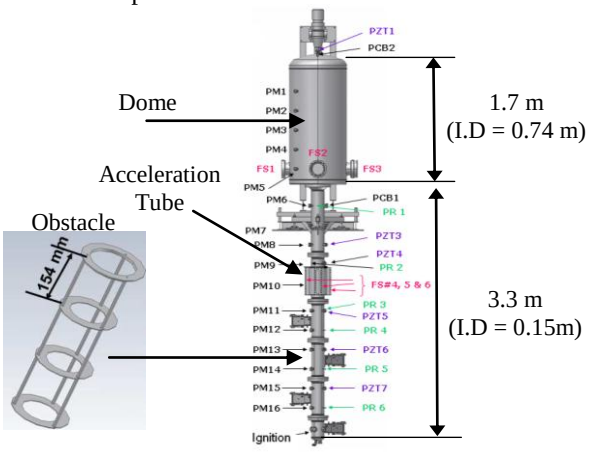
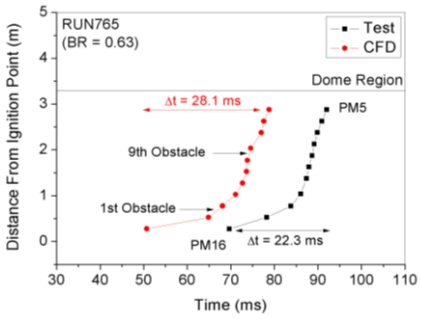
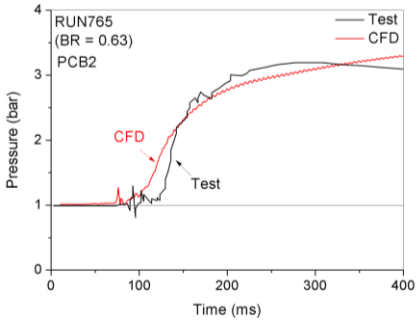


Fig. 1. ENACCEF facility.



(a) Flame front time of arrival



(b) Pressure behavior at PCB2

Fig. 2. Comparison of TOA and pressure between the test and CFX results (RUN765 : H_2 11.6 % to 8%, BR = 0.63).

We used a 3-dimensional grid model with a half symmetric condition to represent the ENACCEF facility. A total of about 3,100,000 hexahedral cells with a cell length of 2 mm - 10 mm were generated in the grid model. A wall condition with a constant temperature of 298 K was applied on the outer surface of the grid model. A turbulent flow was modeled by the DES-SST turbulent model [7]. The turbulent flame closure (TFC) model with a model constant of A = 0.6 - 2.0 according to the hydrogen concentration was used to simulate the hydrogen flame propagation [3,6,8,9]. The time step size for these CFD calculations was 0.005 ms - 0.1 ms to assure a CFL number below 1.0. The laminar flame speeds according to the hydrogen and diluents concentrations [10] were given as the input data of the TFC model.

We calculated 10 test results including RUN765 (Fig. 2) conducted in the ENACCEF facility. The CFD results predicted the measured flame front TOAs and pressure behaviors with an error range of about 20% and 5%, respectively. However, we had to adjust the model constant A according to the hydrogen concentration and find an optimum mesh distribution in the acceleration tube. In addition, the CFD analysis required a long calculation time because the flame propagation was stagnated at the lower corner region in the dome. This may be explained by the fact that an adverse pressure distribution at the corner region disturbed the flame propagation. This phenomenon may disappear if finer mesh distribution at the corner region in the grid model is used [4].

2.2 CFD Analysis for the THAI Experiment

Becker Technologies in Germany performed the hydrogen combustion test using the THAI facility by varying the initial hydrogen and steam concentrations, the initial temperature and pressure, the ignition position, and the presence of a spray operation [11]. An obstacle to accelerate the hydrogen flame was not used in the THAI facility.

A 3-dimensional grid model with a half symmetric condition was used to represent the THAI facility. A total of about 1,500,000 hexahedral cells with a cell length of 5 mm - 20 mm were generated in the grid model. A wall condition with a constant temperature of about 298 K was applied on the outer surface of the grid model. A turbulent flow was modeled by the SST turbulent model [7]. The turbulent flame closure (TFC) model with a model constant of A = 0.8 - 1.6 according to the hydrogen concentration was used to simulate the hydrogen flame propagation [5,8]. The time step size for these CFD calculations was 0.25 ms - 0.5 ms. The laminar flame speeds according to the hydrogen concentrations [] were given as the input data of the TFC model [10].

We simulated 6 test results including HD7 (Fig. 4) conducted in the THAI facility. The CFD results overpredicted the measured temperatures and pressure behaviors with an error range of about 25% and 8%, respectively. The CFD results did not simulate the temperature increase slope in the test results. This may be explained by the fact that the temperature was measured by a thermocouple with a time lag, and heat generation due to the hydrogen-air chemical reaction occurred in an instant in the CFD. In addition, we found that the TFC model cannot accurately simulate the spray effect on the hydrogen flame propagation.

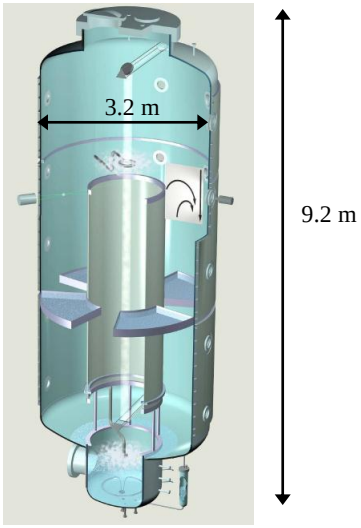
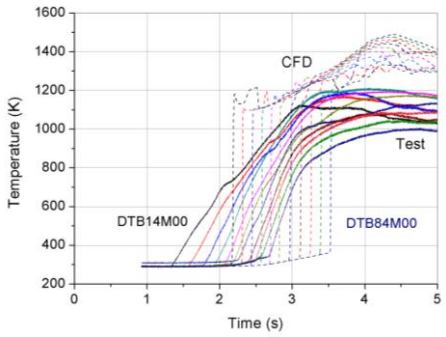
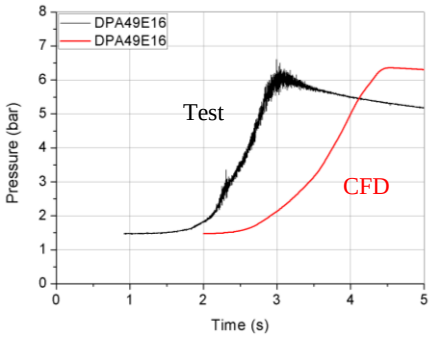


Fig. 3. THAI facility (Inner cylinder and condensate trays were removed for H2 combustion test).



(a) Temperatures in vessel centerline (from 1.4m to 8.4m)



(b) Pressure behaviors at 4.9 m

Fig. 4. Comparison of temperature and pressure between the test and CFX results (HD7 : H_2 9.93%, initial pressure 1.48 bar, initial temperature 290K).

2.3 CFD Analysis for IRWST Experiment

KAERI performed the hydrogen combustion test with the scaled-down IRWST facility simulating the APR1400 IRWST compartment located in the lower part of the containment, to understand the characteristics of the hydrogen flame propagation in the annulus geometry by varying the hydrogen concentration, the presence of an obstacle, and the presence of a vent hole [12].

The CFD analysis was conducted for the test results obtained with hydrogen concentrations of 15.4%, 18.6%, and 19.5% and without the obstacle and vent hole [3,4]. ANSYS CFX-13 with the TFC model and the model constant of A = 5.0, a grid model with a hexahedral cell length of 5.0 mm, which uniformly divides the annulus width of the test facility as 29 cells, and a time step size of 0.01 ms, can be a useful tool to predict the pressure buildup resulting from the hydrogen flame acceleration in the test results. By comparing the simulated results with the test results, we found that the proposed CFD analysis methodology enabled us to predict the peak pressure with an error range of about ±29% for the hydrogen concentration of 19.5%. However, the error ranges of the peak pressure for a hydrogen concentration of 15.4% and 18.6% were about 66% and 51%, respectively. To reduce the error ranges of the hydrogen concentration of 15.4% and 18.6%, some uncertainties of the test conditions need to be clarified.

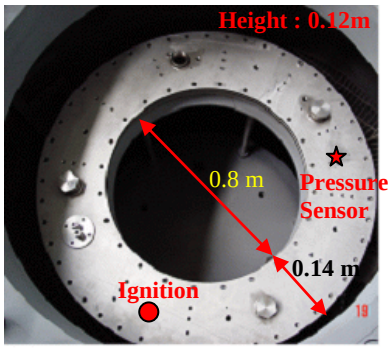
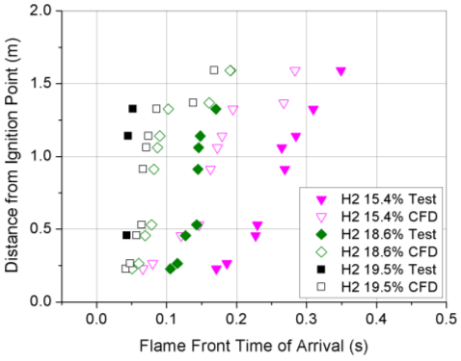
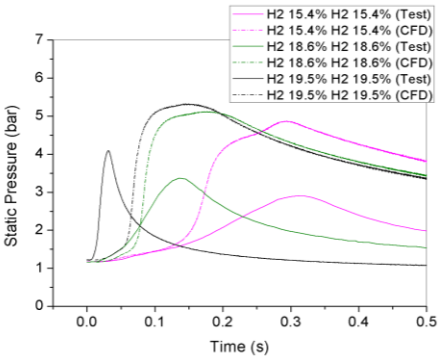


Fig. 5. Scaled-down IRWT facility (top view).



(a) Flame front TOAs



(b) Pressure behaviors

Fig. 6. Comparison of the flame front TOAs and pressures between the test data CFD results for the hydrogen concentration of 15.4%, 18.6%, and 19.5%.

2.4 H_2 Flame Propagation in the APR1400 IRWST

We applied the CFD analysis methodology developed on the basis of the scaled-down IRWST test results to the APR1400 IRWST, assuming a closed vent hole to confirm its applicability [6]. A grid model representing the air space of the APR1400 IRWST was generated by a hexahedral mesh with a cell length of about 70 mm. The number of generated cells in the grid model was 3,475,196. A pipe configuration between the spargers was treated as a straight connection between two adjacent spargers as a rectangular shape (Fig. 7) because we did not have detailed information about it. The hydrogen concentration in this calculation was assumed to be a uniform distribution of 15.4% and 19.5% in the grid model, in order to compare the two CFD results with each other.

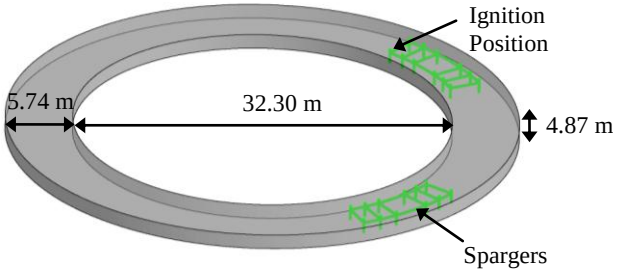
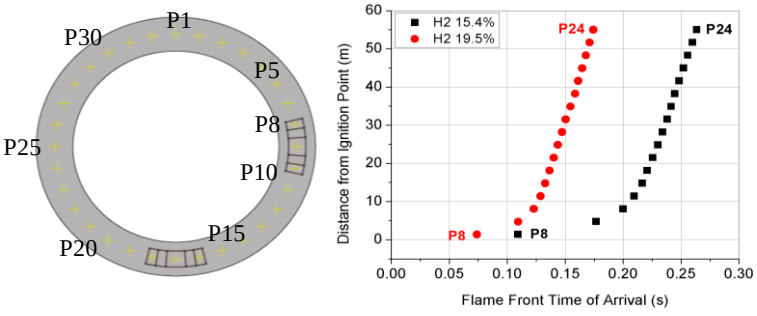
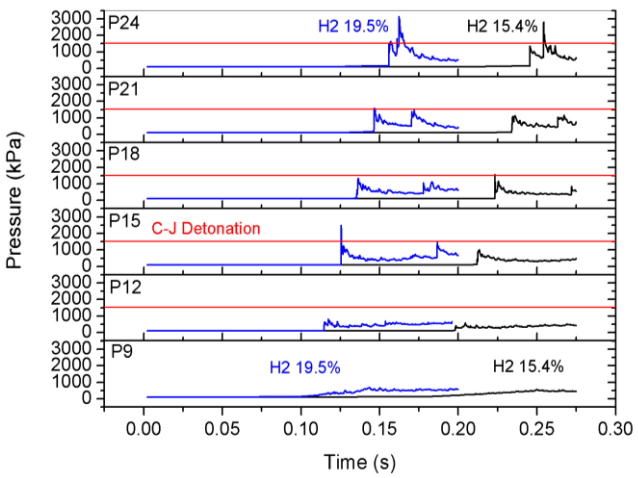


Fig. 7. Grid model of the APR1400 IRWST.



(a) Flame front TOAs



(b) Pressure behaviors

Fig. 8. CFD results according to H_2 concentrations of 15.4% and 19.5%.

The application results (Fig. 8) show that the flame front TOAs for the hydrogen concentration of 19.5% are about 36% faster than those of 15.4%. The flame front TOA is defined as the time instant when the gas temperature increases to about 1000 K. This result may be explained by the fact that the combustion energy of the hydrogen concentration of 19.5% is higher than that of 15.4%. The larger combustion energy induces faster flame propagation. The faster flame speed results in higher pressure at an earlier distance from the ignition location. In the results of the hydrogen concentration of 19.5%, the pressure at P15 increases to about 2400 kPa whereas the pressure at P15 is about 1000 kPa in the results of the hydrogen concentration of 15.4%. Therefore, we can know that the application results using the developed CFD analysis methodology are physically reasonable.

However, a lot of computational time, about 2 - 3 months, was consumed to obtain the converged solutions using parallel computation with 20 CPUs because the fully implicit scheme in the CFX used an iterative method. In addition, a very small time step size of about 0.01 ms was used to capture the overpressure buildup phenomenon. Thus, we judged that the CFX was not the proper tool for predicting the overpressure buildup resulting from the hydrogen flame acceleration, considering that the gas volume in the APR1400 containment is about 88,000 m^3.

2.5 Requirements of the H_2 Combustion and Explosion Code

On the basis of the validation and application results, we found the numerical models and functions which should be implemented in the multi-dimensional code for the hydrogen combustion and explosion analysis. These may be used as the requirements for choosing the hydrogen combustion and explosion code from a foreign country:

- A time marching method should be the explicit scheme.
- Model constants of the combustion model should be proposed based on the validation against the test results with various hydrogen concentrations.
- The grid generation tool should be convenient for modeling of a complicated obstacle geometry.
- Various combustion and turbulent models should be provided to simulate hydrogen propagation under a severe accident.
- Application results for a real plant should be presented.
- The ability to import the hydrogen distribution results calculated with the GASFLOW should be provided because KAERI uses the GASFLOW code for predicting hydrogen distribution.

3. Selection of the H_2 Combustion and Explosion Analysis Code

3.1 Investigation on the H_2 Combustion and Explosion Analysis Code

The available computational codes for analyzing hydrogen combustion and explosion in the containment of a NPP include TONUS-CFD [13,14], COM3D [14-16], REACFLOW [17], CRECOM [18], and GOTHIC [19,20]. These codes have been intensively reviewed and evaluated for their numerical methods, physical models, a solver algorithm, an ignition model, validation and application results, and connection ability with the GASFLOW (Table I). In particular, TONUS-CFD, COM3D, and GOTHIC have been actively used in an international benchmark problem of hydrogen combustion, and in research papers [8,9,19,20]. Unfortunately, no real plant application results using the CRECOM and GOTHIC were found in the literature survey.

As a result of the investigation, the COM3D was the determined to be an excellent code for the hydrogen and combustion code analysis in the containment. When compared to other codes the COM3D most accurately predicted the flame quench shown in the ENACCEF test results, and the flame acceleration the occurred due to an acoustic instability measured in the THAI test results [8,15]. The COM3D is currently used for analyzing hydrogen flame acceleration in the European Pressurized Reactor (EPR) containment with the validated analysis methodology [14,16]. In addition, the hydrogen distribution results available by GASFLOW can be automatically transferred to an initial condition of the COM3D when the Cartesian grid model is used [10].

Table I: Investigation Results on Hydrogen Combustion and Explosion Analysis Codes

	TONUS CFD (CEA, France)	**COM3D** (FZK, Germany)	**REACFLOW** (JRC, Italy)	**CREBCOM** (Kurchatov, Russia)	**GOTHIC** (EPRI, USA)
Grid Model	Fixed cartesian grid (Hexa mesh)	Fixed cartesian grid (Hexa mesh)	Fixed & Adaptive grid (Tetra mesh)	Fixed cartesian grid (Hexa mesh)	Lumped parameter code (Volume & Junction)
Parallel Computation	Unclear	O	Unclear	Unclear	O
Hydrodynamic Solver (Algorithm)	N-S eq. (low Ma) Euler eq. (high Ma)	N-S eq. & Euler eq. (fully compressible flow)	N-S eq. & Euler eq. (fully compressible flow)	Unclear (3D gas dynamic model)	General mom. eq.
Energy Equation	Temp. base (low Ma)	Total enthalpy	Total enthalpy	Unclear	Static enthalpy
Thermodynamic Properties (ρ, C_p, h)	-C_p: JANAF polynomial -ρ: Ideal gas law	-C_p: JANAF polynomial -ρ: Ideal gas law	-C_p: JANAF polynomial -ρ: Ideal gas law	-C_p: Constant -ρ: Ideal gas law	-C_p: Correlation -ρ: Ideal gas law
Turbulent Model	-Mixing length model -Standard k-ε model	Standard k-ε model	Standard k-ε model	Unclear	-Mixing length model -Standard k-ε model
Combustion Model 1) Ignition model 2) DDT simulation 3) Model constant 4) PAR model	Arrhenius/ EBU/Detonation 1)Combusted region 2)Unclear 3)Variable for H2 % 4)O	EDM/KYLCOM 1)Forced chemical reaction over predefined volume 2)Possible 3)Unclear 4)X	EDM 1)Forced chemical reaction over predefined volume 2)Possible 3)Variable for H2 % 4)X	BVM/Burning rate model 1)Unclear 2)Unclear 3)Unclear 4)X	Burn model/EDC 1) Forced chemical reaction over predefined volume 2)X 3)Unclear 4)O
Multi-component (H2-Air-Steam)	O	O	Unclear	Unclear	O
Validation Test Facility (S, H2) S: Small scale M: Medium scale L: Large scale	-DRIVER (S, ?) -ENACCEF (S, 10-14%) -RUT (L, 10%) -HYCOM -HDR -BMC	-DRIVER (S, 13%) -ENACCEF (S, 14%) -THAI (M, 10%) -RUT (L, 10%)	-DRIVER (S, 13%) -ENACCEF (S, 10-14%) -RUT (L, 10%)	-Explosion channel (S, ?) -RUT (L, 10%)	-SNU-2D (S, 12%) -THAI (M,) -LSVCTF (L, 11%) -FLAME (L, 12.3%)
Application	-EPR containment	-EPR containment	-EPR containment	-None	-Unclear

*N-S eq.: Navier-Stokes Equation, EDM: Eddy Dissipation Model, BVM: Burning Velocity Model

3.2 COM3D Analysis of the ENACCEF Test Results

We performed a preliminary analysis for the ENACCEF test results with the hydrogen concentration of 13% and an obstacle blockage ratio of 0.63 using the COM3D to compare results with the CFX results. In the COM3D analysis, a 3-dimensional grid model with a quarter symmetric condition was generated. A total of about1,177,000 hexahedral cells with a cell length of 7 mm were generated in the grid model. The Eddy Brake Up (EBU) model with a model constant of C_{EBU} = 6.0 was used to simulate the hydrogen-air chemical reaction [10]. A turbulent flow was modeled by the standard k-ε turbulent model. A wall condition with a constant temperature of 298 K was applied on the outer surface of the grid model. The time step size for the COM3D calculations was automatically controlled to assure a CFL number below 1.0.

The COM3D results overpredicted the peak pressure of the test results with an error range of about 20% (Fig. 9). However, the computational time to complete the hydrogen flame propagation in the grid model was 10 times faster than that of the CFX results even though the number of mesh between the grid models is different. Therefore, we know that the COM3D is a very efficient code for hydrogen flame acceleration. A precise calculation for the ENACCEF test results with a variety of conditions will be performed before applying the COM3D analysis to the APR1400 containment.

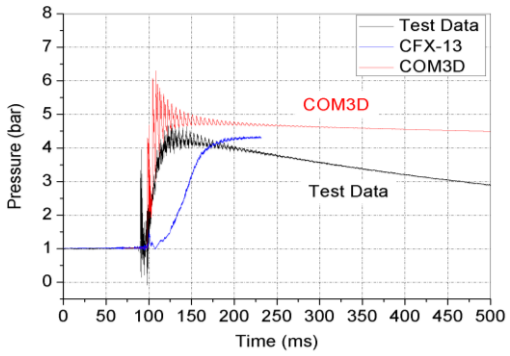


Fig. 9. Comparison of pressure behaviors between the results predicted by COM3D and CFX, and the test results.

4. Conclusions and Further Work

KAERI chose the COM3D as the computational code for hydrogen combustion and explosion analysis by evaluating for its numerical methods, physical models, a solver algorithm, validation and application results, and its ability to connect GASFLOW for calculating hydrogen distribution. In addition, the COM3D is currently used to evaluate the integrity of the EPR containment by predicting the overpressure buildup resulting from the hydrogen flame acceleration with the validated analysis methodology. However, we have to find a way to transfer the GASFLOW results, with a cylindrical grid model, as the initial condition of COM3D with a Cartesian grid model, because the COM3D can automatically import the GASFLOW result only when the Cartesian grid model is used, whereas KAERI has performed the GASFLOW analysis with the cylindrical grid model.

ACKNOWLEDGMENTS

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