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GOTHIC 3D Applicability to Fast Hydrogen Combustions

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Abstract

Under severe accidents in nuclear power plant (NPP), the hydrogen can be generated by chemical reactions and may threaten the containment integrity via hydrogen combustion. For containment analyses, three-dimensional mechanistic code, GOTHIC had to be applied near source compartments in order to predict whether highly reactive gas mixture can be formed or not under hydrogen mitigation system (HMS) working. For its applicability, this paper presents numerical calculation results of GOTHIC 3D on some hydrogen combustion experiments, which are the FLAME (Sandia National Lab.) experiments, the LSVCTF (AECL Whiteshell Lab.) experiments and the SNU-2D (Seoul National Univ.) experiments. A technical basis for the modeling of the large- and small-scale facilities was developed through sensitivity studies on cell size and combustion modeling parameters. It was found that for large-scale facilities, there were no significant differences in the results with different turbulent burn options, while for small-scale facility, the option using the eddy dissipation concept showed the faster flame propagations. The flame velocity became larger with smaller burn parameters such as the flame thickness δ_f and the burn temperature limit T_{lim}. The best estimate modeling parameters found from this study would be applied to real plant simulation of GOTHIC 3D later.

1. Introduction

During severe accidents in NPP, substantial amounts of hydrogen can be generated from a chemical reaction between the zirconium cladding and the hot water vapor as well as from the core-concrete interactions after a lower head failure of the vessel. Such generated hydrogen may be transported into the compartments in the containment building and has the potential to threaten the containment integrity by over-pressurizing via hydrogen combustion such as deflagration or detonation. Moreover, even local hydrogen burning, which is not a threat to the global containment integrity, may also threaten the survivability of safety-related equipments.

With these backgrounds, three-dimensional mechanistic code, GOTHIC has been applied near source compartments in order to predict whether highly reactive gas mixture can be formed or not under HMS working. However, direct application of GOTHIC 3D to NPP containment without discrimination of the characteristics of each concerned compartment would cause considerable uncertainties in the results of analyses.

In this study, therefore, several sets of sensitivity studies were addressed to identify the effects of GOTHIC modeling on hydrogen combustion phenomena, especially on flame propagation under various conditions of size and geometry. We intended to eventually derive the best estimate modeling parameters in accordance with the compartment conditions. To meet this objective, we investigated a number of experimental works and finally selected three among them. The selected ones are the FLAME (Flame Acceleration Measurements and Experiments) experiments by Sandia National Laboratory, LSVCTF (Large Scale Vented Combustion Test Facility) experiments by AECL Whiteshell Laboratory and the SNU-2D experiments by Seoul National University. In reality, though so many cases were examined in each set of experiments, we choose some representative cases and compared the results of numerical analyses to those of experiments.

2. Experiments considered

Table 1 shows the conditions of experiments selected for this study and the followings describe the brief introductions on each experiment and representative results.

The FLAME is a large horizontal rectangular channel made of heavily-reinforced concrete with dimension of 30.48 m ×2.44 m × 1.83 m (100 ft × 8 ft × 6 ft) as shown in Fig. 1 and it was designed and built for the U.S. Nuclear Regulatory Commission. It is a half-scale model of the upper plenum volume in ice condenser pressurized water reactor (PWR) containments. In FLAME experiments, twenty-nine sets of test were executed and through the experiments, hydrogen mole fraction was varied from 12 % to 30 %. At 12 % hydrogen, there was negligible flame acceleration regardless of the degree of transverse venting or the presence of obstacles. Form the FLAME experiments, the followings were concluded: 1. The reactivity of the mixture as determined by the hydrogen concentration is the most important variable. For very lean mixtures no significant flame acceleration and no transition-to-detonation was observed. 2. The presence of obstacles in the path of the flame greatly increases flame speeds and overpressures, and reduces the lean limit for transition-to-

Table 1. Matrix for experiments.

Experiments (Test #)	H_2 Conc. (%)	Remark
FLAME (F-10)	12.3	no top vent, no obstacle, ignition at center of left wall
LSVCTF	11.0	vent area = 1.12 m^2, ignition at center of chamber
SNU-2D	12.0	Obstacle, bottom half vent, top-center ignition

detonation. 3. Large degrees of transverse venting reduce flame speeds and overpressures. 4. Small degrees of transverse venting reduce flame speeds and overpressures for less reactive mixtures, but increase them for more reactive mixtures. In this paper, the test F-10 was selected as the case of GOTHIC simulation.

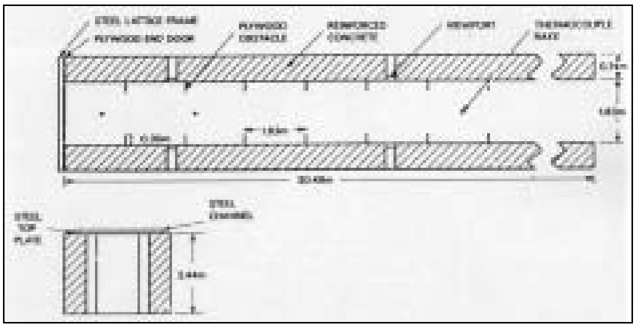


Fig. 1. Schematic of FLAME facility (*M.P. Sherman et al.*).

The LSVCTF is a large-scale combustion test facility with dimension of 10 m × 4 m × 3 m. The schematic of the facility is shown in Fig. 2. The wall consists of 1.25 cm-thick steel plate and 1 m-thick concrete layer outside the steel plate. Two roller-mounted movable end walls are provided to open up the vessel for internal modifications or to move-in bulky experimental equipment when needed. Igniter is located at the center of the facility and a vent is on the one of end walls to guarantee the combustion flows. Area of the vent can be changed with removing or replacing the appropriate number of panels. Temperatures and pressures are locally measured to provide the data of flame propagations. And gas analysis system is adopted to measure the hydrogen concentrations in the chamber. In experiments the hydrogen concentration was varied from 8.5 % to 12 % in accordance with each test and flame speed, pressure and hydrogen concentrations were measured.

In the SNU-2D experiments, the combustion chamber has an upright planar shape with dimension of 1 m × 1 m × 0.024 m. Fig. 3 shows the schematic of SNU-2D combustion chamber, which is made of transparent acrylic plate supported by aluminum frame. Sealing of the chamber is achieved with an inflammable rubber plate inserted between the acrylic plate and aluminum frame. Hydrogen gas is injected into the combustion chamber through a needle valve equipped at the back of the plate and the initiation of combustion is achieved with an igniter equipped in the chamber. Six sets of tests were executed in SNU-2D experiments in accordance with existence of obstacle, positions of igniter (points A, B and C in Fig. 3) and bottom opening condition that is full-open or half-open. Hydrogen concentrations used in experiments were 10 %, 12 % and 12.3 %. Mixing of hydrogen and air after hydrogen injection was achieved by slowly rolling the chamber. When the igniter was positioned at center of the top of chamber (point A), the flame rapidly propagated toward opening section. For the ignition at the corner of bottom (point C), relatively long induction time of propagation was observed and after the induction time, flame propagated from the upper section of chamber.

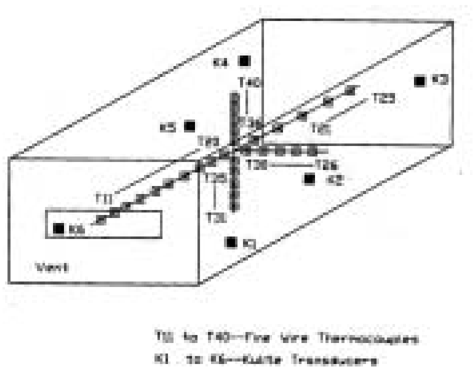


Fig. 2. Schematic of LSVCTF facility and the locations of measuring equipments (*J.L. Sitar et al.*).

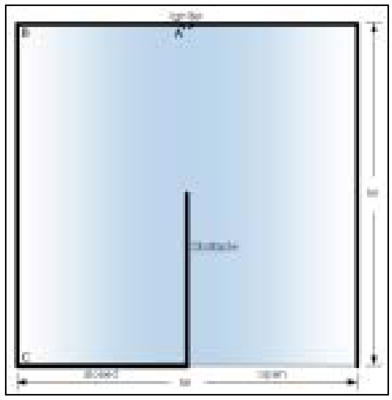


Fig. 3. Schematic of SNU-2D combustion chamber (front view).

3. GOTHIC analyses

3.1. General descriptions of GOTHIC code

GOTHIC (Generation of Thermal Hydraulic Information in Containments) is a general-purpose thermal hydraulics computer program for design, licensing, safety and operating analysis of NPP. Applications of GOTHIC to analyses include hydrogen combustion phenomena in containment as well as overall thermal hydraulic phenomena such as high energy line break, containment heat-up calculations and so on.

3.2. Combustion models

The GOTHIC code includes hydrogen burn models for lumped parameter volumes and distributed (subdivided) volumes. The lumped parameter burn models are almost identical to the burn model described in HECTR and CONTAIN codes, which consist of two separate burn models, a discrete burn and continuous burn. The discrete burn model takes charge of hydrogen combustion within the volume, and the continuous burn model is in charge of hydrogen combustion flows into the volume through junctions. In the discrete burn model, the flame speed is calculated using built in functions of the mole fractions for steam, oxygen and hydrogen. The time required to burn hydrogen within a volume is calculated by dividing the burn length by the flame speed.

Table 2. GOTHIC calculation matrix.

Experiment	Simulation No.	Modeling Features			
		Cell Size (m^3)	Turb. Option	T_{lim} (℃)	δ_f (m)
FLAME	F01[a)]	0.0283[b)]	EDIS	175	0.05
	F02	0.0283	EDIS	175	0.01
	F03	0.0283	EDIS	100	0.05
	F04	0.0283	FSPD	175	0.05
	F05	0.0283	FSPD	100	0.05
	F06	0.0238	EDIS	150	0.005
	F07	0.0238	EDIS	175	0.005
	F08	0.0238	EDIS	190	0.005
	F09	0.2265[c)]	EDIS	175	0.05
	F10	0.2265	FSPD	175	0.05
LSVCTF	L01[a)]	0.1013	EDIS	175	0.05
	L02	0.0156	EDIS	175	0.05
	L03	0.1013	FSPD	175	0.05
	L04	0.1013	EDIS	150	0.05
	L05	0.1013	EDIS	100	0.05
	L06	0.1013	EDIS	175	0.03
	L07	0.1013	EDIS	175	0.01
	L08	0.1013	EDIS	175	0.005
	L09	0.1013	EDIS	180	0.005
	L10	0.1013	EDIS	150	0.005
	L11	0.1013	EDIS	130	0.005
SNU-2D	S01[a)]	1.64×10^{-5}[d)]	EDIS	175	0.05
	S02	1.64×10^{-5}	EDIS	175	0.03
	S03	1.64×10^{-5}	EDIS	175	0.01
	S04	1.64×10^{-5}	EDIS	175	0.001
	S05	1.64×10^{-5}	EDIS	100	0.05
	S06	1.64×10^{-5}	EDIS	100	0.001
	S07	1.64×10^{-5}	FSPD	175	0.05
	S08	1.64×10^{-5}	FSPD	100	0.05

[a)] Base case using default parameters for each experiment
[b)] 0.0283 m^3 = 1.0 ft^3 [c)] 0.2265 m^3 = 8.0 ft^3 [d)] 1.64×10^{-5} m^3 = 1.0 in^3

The mechanistic burn model is applicable to subdivided volumes. When this option is specified, burning of hydrogen requires that the mole fraction limits be satisfied. If the mole fraction limits are satisfied, then combustion of hydrogen is continuously calculated. The combustion rate of hydrogen is determined from the maximum of the laminar and turbulent combustion rates. Laminar combustion is preset to zero and is not calculated unless the effective temperature for combustion exceeds the user specified lower temperature limit. The laminar burn model is given by Lewis and von Elbe. The turbulent burn model has two options which are the eddy dissipation concept of Magnussen and Hjertager and turbulent flame speed based concept of Damköhler. In the model for the turbulent reaction rate, two empirically based limitations are imposed. The first is referred to as cold quenching and the second condition is referred to as high turbulence flame quenching.

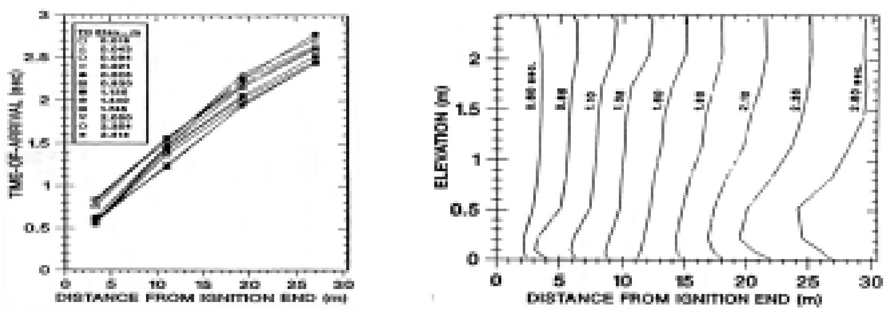
4. Results

4.1. Analysis of FLAME experiments

The experimental data of time-of-arrival and flame propagation produced by four thermocouple rakes, pressure transducers and additional thermocouples, are illustrated in Fig. 4 (*M.P. Sherman et al.*). Lines in time-of-arrival data shown in Fig. 4(a) indicate the flame velocity at each level suffering variation as flame propagates. This can be clearly found in Fig. 4(b), which is the vertical cross-sectional plot of Fig. 4(a). Test results indicate the flame propagation toward the exit of channel was finished in 3 seconds and weak flame acceleration occurred. Because of buoyancy force the flame propagation has concave shape with slower velocities at lower part in channel. Fig. 5 shows the results of GOTHIC calculations for some representative cases described in Table 2.

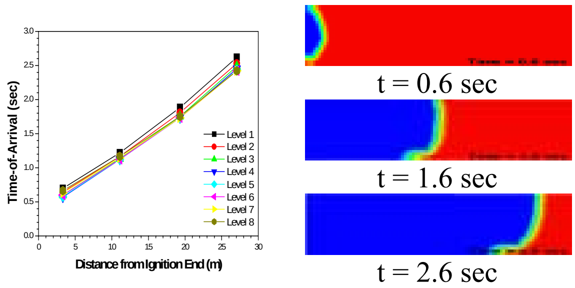
Comparison of Fig. 5(a) and Fig. 5(b) gives the cell size dependency in GOTHIC model. Firstly, the case F01 with default values of burn parameters shows good agreement both in scale of time-of-arrival and in flame propagation shape, compared to the results of experiment, except that the flame acceleration could not be found in case F01 while the experimental data shows it. However, when the length of the cell dimension is increased as about a factor of 2, that is the case F09, the flame propagation becomes much slower than that in the case F01. Because the overall flame velocity is slow, the buoyancy effect becomes relatively more dominant so that the gradient in flame surface becomes larger.

Dependency of turbulent burn options in GOTHIC was investigated. While most cases presented in this paper used EDIS model, cases F04 and F05 adopted FSPD model. Fig. 5(c) shows the results of calculation using FSPD model, case F04. The difference of case F04 from case F05 is that case F04 used default burn parameters while case F05 used 100℃ as T_{lim}. Because if the FSPD model is selected, the model in itself cancels out the flame front thickness parameter δ_f, the effect of δ_f was not considered. FSPD model resulted in somewhat faster values in flame propagation as illustrated in Fig. 5(c). In additional calculation, case F05, we could find the much faster than case F04 because of using the lower burn temperature limit. The resultant effect was also similar in that from the comparison between case F01 and case F03, in which the EDIS model was used.

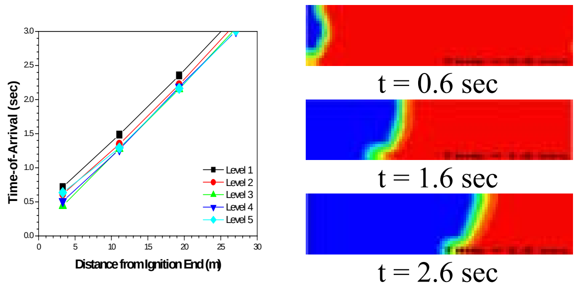


(a) Time-of-arrival (b) Flame propagation

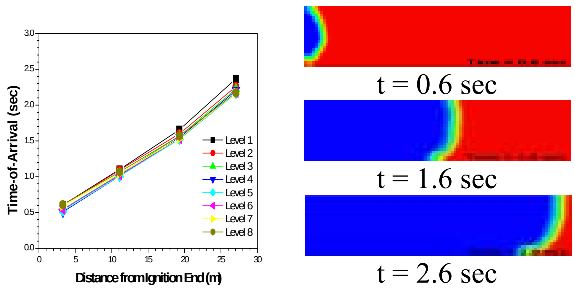
Fig. 4. Results of test F-10, FLAME. (*M.P. Sherman et al.*)



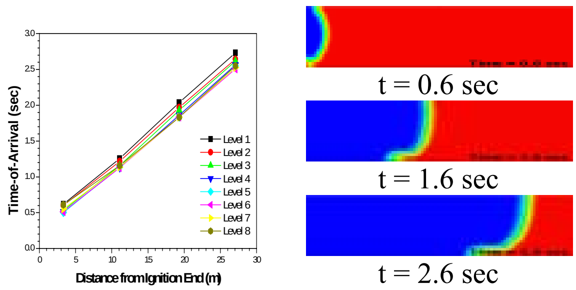
(a) Results of case F01



(b) Results of case F09



(c) Results of case F04



(d) Results of case F07

Fig. 5. Time-of-arrival data and contours of flame propagation in FLAME chamber, GOTHIC.

Fig. 5(d) illustrates the results when δ_f is set to 0.005 m. Since the empirical value of laminar flame thickness is about 10^{-4} m and that of turbulent flame is 10 to 100 times thicker (*F.A. Williams*), we considered 0.005 m as approximate value of δ_f. In this case we hardly feel the difference in flame propagation compared to case F01 using default values. However it can be found that time-of-arrival data was improved in the flame acceleration viewpoint.

From the parametric effect calculations, we could find the dependencies of cell size, turbulent burn models and two of burn parameters on GOTHIC results. In case of test F-10, the best agreement was achieved in case F07. This case uses EDIS model as turbulent burn option and default value of T_{lim} with modification of δ_f as a factor of 0.1. However, the dependency of cell size in subdivided volume was found as somewhat critical factor when modeling a facility. In this study, two cell dimensions were applied and those are 1 ft-based (F01~F08) and 2 ft-based (F09, F10) dimension. Fortunately one of the two agreed well with experimental data so that 1 ft-based modeling could be thought as a basic guideline to apply GOTHIC to other tests in FLAME experiments.

4.2. Analysis of LSVCTF experiments

In the LSVCTF experiments, there was combustion duration before the start of flame propagation. However, the code could not simulate this physical phenomenon. Thus the location of the first thermocouple in each direction from the igniter was set as the reference point for the comparison of time-of-arrival data in both experiments and code simulations. Fig. 6 comparably shows the results of the representative cases. As seen in the figure, a significant difference could not be found in all cases, but there were slight distinctions in accordance with modeling parameters.

In Fig. 6, the effect of cell size can be found comparing the case L01, which is the default case, to the case L02. The difference between the two cases is the volume of three dimensionally subdivided cells, as mentioned in Table 2. In default case, the volume was subdivided with 0.1013 m^3 cells, while 0.0156 m^3 cells for case L02. As revealed in the figure, which case is the better one cannot be said because the default case showed better agreement with experiment in the vent direction, while the opposite result in the counter-direction. For the case L02 with about 7 times large number of cells, the much larger computational efforts were required and this is an uneconomical work. Accordingly, the three-dimensional model of case L01 was considered as the basic three-dimensional modeling for LSVCTF simulations.

Comparison between EDIS and FSPD turbulence options with the default values on other modeling parameters was achieved. The results of this analysis correspond to case L01 and case L03 in Fig. 6. The results on both directions in the chamber show little differences in time-of-arrival data and also show some differences compared to experimental data.

With the three-dimensional model of case L01 and EDIS turbulence option, the sensitivity studies for the parametric effects were examined. As shown in Table 2, the attempts finding the best agreement with experimental data were achieved. We could find the general trends that the results of code calculations approach the experimental values with decreasing the values of T_{lim} and/or δ_f. T_{lim} did affect less significantly than δ_f. As the additional considerations, the empirical flame front thickness reported by Williams, was used to model the problem, which are the cases L08 to L11. These cases showed somewhat better agreements with experimental data. However, the results did not show the large differences and we found the best agreeable values for those variables.

From various sensitivity studies, the most suitable values of modeling parameters for the LSVCTF experiments were found. And those are the default value, 175℃ and 0.005 m for T_{lim} and δ_f, respectively, with three-dimensional model of case L01 and EDIS turbulence option. As mentioned above, though we selected the most estimate value of δ_f as 0.005 m (case L08), case L07 competes with it.

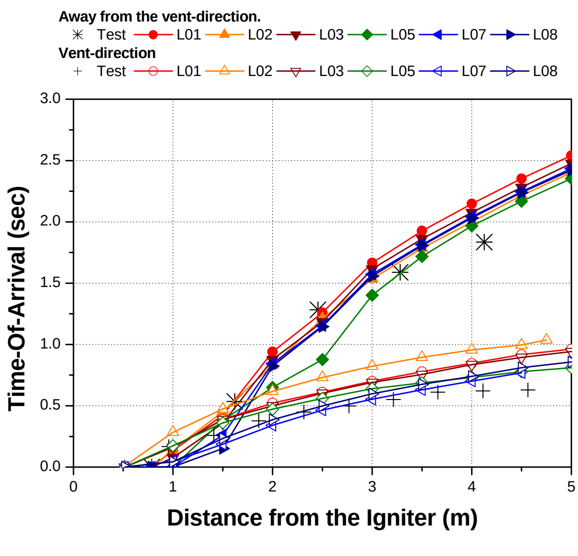


Fig. 6. Time-of-arrival data for flame propagation in LSVCTF chamber, GOTHIC.

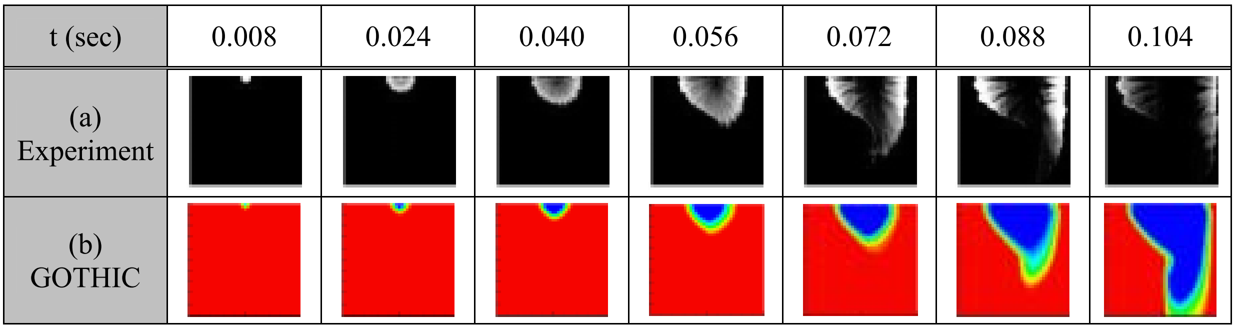


Fig. 7. Comparison of the results between SNU-2D experiment and GOTHIC simulation (case S06). The flame front exited the end of chamber in about 0.1 second.

4.3. Analysis of SNU-2D experiments

SNU-2D experiment is a very small-scaled test for the application to GOTHIC. For this experiment, the cell size dependency was not examined but the volume was two-dimensionally subdivided with similar length of thickness of the chamber, about 1 inch. In this analysis the code with the default model or a model in which one parameter was modified, could not predict well the fast flame propagation transient as measured in experiments. Accordingly, the parametric effect simulations were executed with various T_{lim}s and δ_fs to find the best estimate modeling values.

In most simulations addressed in Table 2, the times-of-arrival of flame at the opening region of the chamber were about in one second after ignition. Therefore we could not help modify both the δ_f and T_{lim}. Fig. 7 illustrates the most acceptable result compared to that of experiment. Fig. 7(a) is the high-speed CCD camera images from the test while Fig. 7(b) for GOTHIC simulation of case S06. As shown in the figure, the GOTHIC prediction shows good agreement with experimental data in which δ_f and T_{lim} are 0.001 m and 100℃, respectively.

5. Summary of results and discussion

From the results described above, it can be said that the smaller cell size, the larger flame propagation velocity and that if the length of the cell comes closer to δ_f, the same result comes out as decreasing the δ_f. For large-scale facilities such as FLAME and LSVCTF, similar results were found for both EDIS and FSPD turbulence models, while for small-scale facility like SNU-2D, the EDIS option showed the faster flame propagations. The resultant best estimate modeling parameters for each experiment are shown in Table 3.

For FLAME experiments, GOTHIC simulations did not show the flame acceleration phenomena and the variation of δ_f does not give a significant effect on the results, while the variation of T_{lim} does with fixed flame thickness. Essentially we recommend 0.005 m for δ_f, which is based on an empirical value and the best estimate modeling case, therefore, can be found in which it uses 0.005 m and 175℃ for δ_f and T_{lim}, respectively.

Table 3. Best estimate GOTHIC modeling parameters for each experiment.

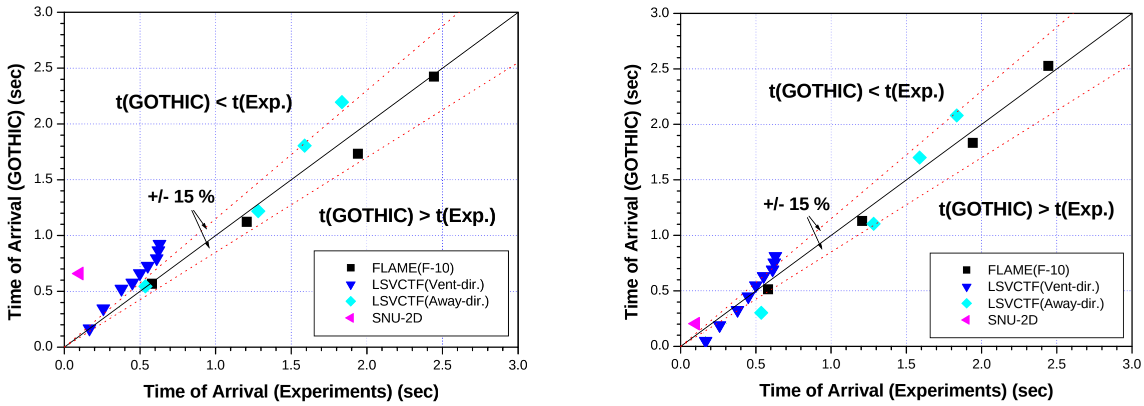
Experiment	Volume (m^3)	H_2 Conc. (%)	Modeling parameters		
			Basic length of a cell (m) [a)]	δ_f (m)	T_{lim} (℃)
FLAME	135.92	12.3	0.3048	0.005	175
LSVCTF	120.0	11.0	0.45	0.005	175
SNU-2D	0.025	12.0	0.025	0.001	100

[a)] This value reveals the representative length of a cell three-dimensionally subdivided volume in GOTHIC analysis.

In LSVCTF simulations, there were no significant effects of both parameters. However, through the sensitivity analyses, the most feasible case whose values are exactly same with those of FLAME was found.

However, for a small-scale facility, the above results were not valid any more. The SNU-2D facility is a very small-scaled one compared to others. In reality, the best estimate set of modeling parameters was found in absolutely different ranges, which are 0.001 m and 100℃ for for δ_f and T_{lim}, respectively.

Fig. 8 summarizes again the results of all the simulations. It compares the time-of-arrival data from the experiments to those from the GOTHIC calculations. Considering the size of a compartment in real plants, because the scales of FLAME and LSVCTF facilities are relatively similar compared to that of SNU-2D facility, the points in the graphs were plotted based on the modeling parameters from the analyses of large-scale facilities, those are 175℃ in T_{lim} and 0.05 m and 0.005 m in δ_f. Comparing two figures, it can be found that the better agreements between experiments and GOTHIC simulations were seen in the result using modified parameters, rather than in that using the default modeling parameters.



(a) Default modeling using EDIS option, T_{lim} = 0.05 m and δ_f = 175℃.

(b) Modified modeling using EDIS option, T_{lim} = 0.005 m and δ_f = 175℃.

Fig. 8. Comparison of the results between GOTHIC analyses and experimental data.

6. Conclusion

The GOTHIC 3D applicability to fast hydrogen combustion and flame acceleration was investigated, and technical basis for the modeling of the large- and small-scale combustion facilities was developed through sensitivity studies on combustion parameters and turbulent burn options in the code. For large-scale facilities, there were no significant differences in the results with different turbulent burn options, while for small-scale facility, the option using the eddy dissipation concept showed the faster flame propagations. With smaller burn parameters such as the flame thickness and the burn temperature limit, the flame velocity became larger. Therefore, selection of the proper combustion modeling parameters would play an important role in the prediction of hydrogen concentration in the reactor containment.

References

1. Damköhler, 1949, Z. Electrochem, Vol. 46, pp. 601.
2. George, T.L., Wiles, L.E., Claybrook, S.W., Wheeler, C.L., McElroy, J.D. and Agee, L., April 2001. GOTHIC Containment Analysis Package Technical Manual – Version 6.1b. NAI 8907-06 Rev. 11, NAI, Washington, pp. 10.1-10.13.
3. Lewis, B. and von Elbe, G., 1961. Combustion, Flames and Explosions of Gases. Academic Press, Inc., New York, Chapter VI.
4. Magnussen, B.F. and Hjertager, B.H., 1976. On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion. In: 16th International Symposium on Combustion, The Combustion Institute, pp. 719-729.
5. Sherman, M.P., Tiezen, S.R. and Benedick, W.B., March 1989. The Effect of Obstacles and Transverse Venting on Flame Acceleration and Transition to Detonation for Hydrogen-Air Mixtures at Large Scale. NUREG/CR-5275, SNL, Albuquerque, pp. 1-49.
6. Williams, F.A., 1996. Combustion Theory, The second edition. Addison-Wesley Publishing Company, pp. 130-136, 373-440.