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EXPERIMENTAL VALIDATION OF COMBUSTION PREDICTIONS USING THE GOTHIC CODE

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ABSTRACT

During severe accidents in nuclear power plants, formation of hydrogen can pose a serious threat to the integrity of the containment via hydrogen combustion. Recently, the analytical calculation for local hydrogen distribution and combustion has been attempted using the GOTHIC-3D code. However, the results are still not fully accepted due to limited validation of the GOTHIC code.

In this study, the capability of GOTHIC code for hydrogen combustion phenomena was validated with the results of a premixed hydrogen combustion experiment executed by Seoul National University. The experimental chamber has about 24 litre free volume and 2-dimensional rectangular shape. The experiments were performed with 10 % hydrogen/air gas mixture and conducted with combination of two igniter positions (top center, top corner) and two boundary conditions (bottom full open, bottom right half open). Using the lumped parameter and mechanistic combustion model in the GOTHIC code, the SNU experiments were simulated. In case of the lumped parameter simulation, the combustion time was predicted appropriately. But any other local information related combustion phenomena could not be obtained. In the case of mechanistic combustion simulation, the physical combustion phenomena were not matched experimental ones. The GOTHIC code predicted very long combustion time and the flame front propagation phenomena were different from the experimental results. Also, it was found that the combustion model of GOTHIC code had some limitations.

NOMENCLATURE

F *flow*
m *hydrogen consumption rate [kg/s]*
S_l *laminar flame speed [m/s]*
T *temperature [K]*
T_{eff} *effective temperature [K]*
V *actual cell volume [m^3]*
V_{eff} *effective volume [m^3]*
w_l *laminar reaction rate [kg/m^3s]*
w_t *turbulent reaction rate [kg/m^3s]*
X_H hydrogen mole fraction

Λ *interpolation factor*
λ *interpolation factor*

INTRODUCTION

Since the accident at Three Mile Island (TMI), there has been a great deal of interest regarding the problem of hydrogen combustion. During severe accidents in nuclear power plants (NPP), the corium can react with the water or steam to generate hydrogen. Formation of such combustible gas mixture can pose a serious threat to the integrity of the containment via hydrogen combustion such as deflagration or detonation.

Hence, various experimental works were performed around the world to investigate severe accident phenomena related to hydrogen combustion. These experimental works studied characteristics of hydrogen combustion such as flammability limit of hydrogen-steam mixture (SNL FITS), deflagration (SNL VGES), flame acceleration and DDT (SNL FLAME), premixed combustion and continuous injection tests (NTS) and so on.

However, most of the hydrogen combustion analyses have been performed with lumped parameter models such as MAAP, CONTAIN, HECTR and GOTHIC. Though these lumped analysis codes were verified with experimental data and contain correlations from hydrogen combustion experiments, they cannot calculate detonation and cannot simulate characteristics of hydrogen combustion appropriately in the point of local combustion phenomena such as flame front propagation, flame acceleration etc.

Recently, as concern for local hydrogen control has become high, the analytical calculation for local hydrogen distribution and combustion in the containment has been attempted using three-dimensional codes such as GASFLOW or GOTHIC-3D. However, the results are still not fully accepted due to the lack of local experimental data and limited validation works for severe accident conditions.

Therefore, in this study, experimental validation work for GOTHIC-3D code was fulfilled with a hydrogen combustion experiment executed by Seoul National University. This paper presents the results of SNU premixed hydrogen combustion experiments and the results of lumped parameter and subdivided GOTHIC code analyses. Also, some weak points of GOTHIC code for hydrogen combustion analysis were show by a review of combustion models and a comparison between experimental and calculational results.

PREMIXED HYDROGEN COMBUSTION EXPERIMENT

Experimental Apparatus and Instruments

Figure 1 shows pictures of the two-dimensional combustion chamber. Figure 2 shows a picture of the experimental apparatus. The combustion chamber has an upright rectangular shape of dimensions $1 \times 0.024 \times 1$ m^3. This chamber is sufficient to examine the two-dimensional flame propagation characteristic because the chamber

depth is very small compared with the chamber width and height. The hydrogen flame propagation in the direction of depth can be ignored. The chamber is made of transparent acrylic plate and aluminum frame. For the sealing of the gas mixture, an inflammable rubber plate is inserted between the acrylic plate and aluminum frame. To fill up a gas in combustion chamber, a valve is installed at the back acryl plate and an electric igniter is equipped. The igniting system is composed of capacity discharge igniter (CDI) and ignition coil. A high-speed CCD camera (motion analyzer : KODAK Ekta Pro EM1012) was used to visualize the hydrogen flame. Though the hydrogen flame wavelength is not in visible range, the high-speed photography could be obtained because the high temperature steam generated at the hydrogen flame front emits red series wavelength. Considering the distance between hydrogen flame and steam is less than 1 mm, it is proper that the steam be regarded as hydrogen flame. For the operation of high-speed CCD camera, simple circuit synchronizer utilized photo-coupler (PC817) was used. A mass flow controller compensated by wet test gas meter was equipped to precisely control the composition of the gas mixture.

Figure 1: Pictures of 2-D Combustion Chamber.

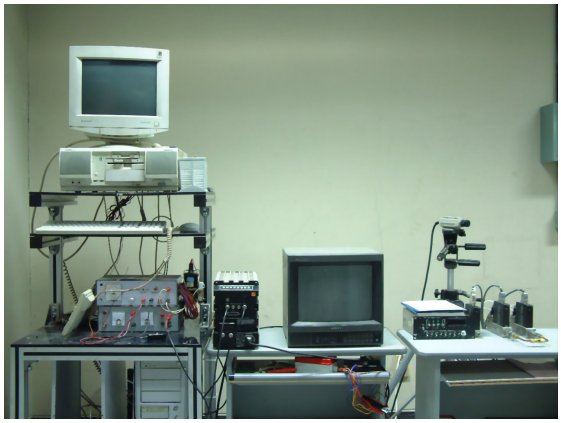


Figure 2: Experimental Apparatuses.

Experimental Conditions and Methods

The premixed combustion tests were conducted. Since the composition of gas mixture concerned during severe accidents in NPP is about 10 % hydrogen and this lean condition suitable for safety problem, the gas mixture composed of 10 % chemically pure hydrogen (>99 %) and 90 % dry air was used. The tests were performed with the chamber bottom open to prevent damage due to combustion and the igniter was located at the top of combustion chamber. Because the density of the gas mixture is smaller than air, this condition can maintain most of the chamber volume as a homogeneous gas mixture composition. The tests were conducted with combination of two ignition positions (top center, top corner) and two boundary conditions (bottom full open, bottom right half open). Because the chamber bottom wall is open, the test condition is constant pressure.

GOTHIC CODE ANALYSIS

The GOTHIC code is a general-purpose thermal hydraulics computer program that models the design, licensing, safety and operating analysis of the nuclear containments, auxiliary building and related equipments. It solves the mass, energy and momentum balances for three separate phases: vapour continuous liquid and dispersed liquid. The vapour phase can be a mixture of steam and non-condensing gases. A separate mass balance is maintained for each component of the vapour mixture. The phase balance equations are coupled by mechanical models and the correlations for the interface mass, energy and momentum transfer. The GOTHIC has a flexible nodding structure that allows both lumped parameters and 3-D modelling capability. This makes it possible to use of a variety of nodding arrangements in order to accommodate a wide range of containment modelling needs. For the solution methods, the GOTHIC uses a finite volume approach with a first order upwind method. A semi-implicit method is used (with either the direct or iterative methods) to solve the reduced balance equations for the volume pressure. Generally, the GOTHIC code aims at practical containment analysis calculations using relatively large spatial meshes for a large simple geometry. In practice, however, very fine meshes in relatively small and/or complex geometry can be needed to predict local hydrogen combustion phenomena properly. Especially, in the aspect of local flame propagation, the fine mesh analysis of the GOTHIC code is not fully investigated yet. Despite the GOTHIC code has modified burn models, the assessment of GOTHIC burn models combined with fine mesh calculations is still remained to be checked in order to use it for hydrogen combustion analysis in a relatively small geometry. The version of GOTHIC code used in this study is 6.0.

Brief Review of GOTHIC Combustion Models

GOTHIC 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 code and it consists of two separate burn models, a discrete burn and continuous burn. In the discrete burn model, the flame speed is calculated using built in functions of the volume steam, oxygen and hydrogen mole fractions. The time required to burn the hydrogen within a volume is

calculated by dividing the input or default burn length by the flame speed.

The mechanistic burn model is applicable to subdivided volumes and this model contains laminar and turbulent combustion of hydrogen. The laminar burn model is given in an expression by Lewis and von Elbe(1961). The turbulent burn model adopted the eddy dissipation concept of Magnussen(1989) and Magnussen and Hjerthager (1976). 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.

In the mechanistic burn model, the hydrogen consumption rate is given by

$$\dot{m} = Max(w_l, w_t)V_{eff} \quad (1)$$

where the effective burn volume is approximated by

$$V_{eff} = V(\frac{T_j}{T_{eff,j}})^3 \quad (2)$$

where V is the actual cell volume.

And, the weighted average effective temperature for cell j is calculated as following.

$$T_{eff,j} = \frac{\phi_j T_j + \sum_{i=\varepsilon_j} Max(F_i, 0)(T_j + \lambda_i \Lambda_j (T_i - T_j)}{\phi_j + \sum_{i=\varepsilon_j} Max(F_i, 0)} \quad (3)$$

GOTHIC Modeling and Analysis Methods

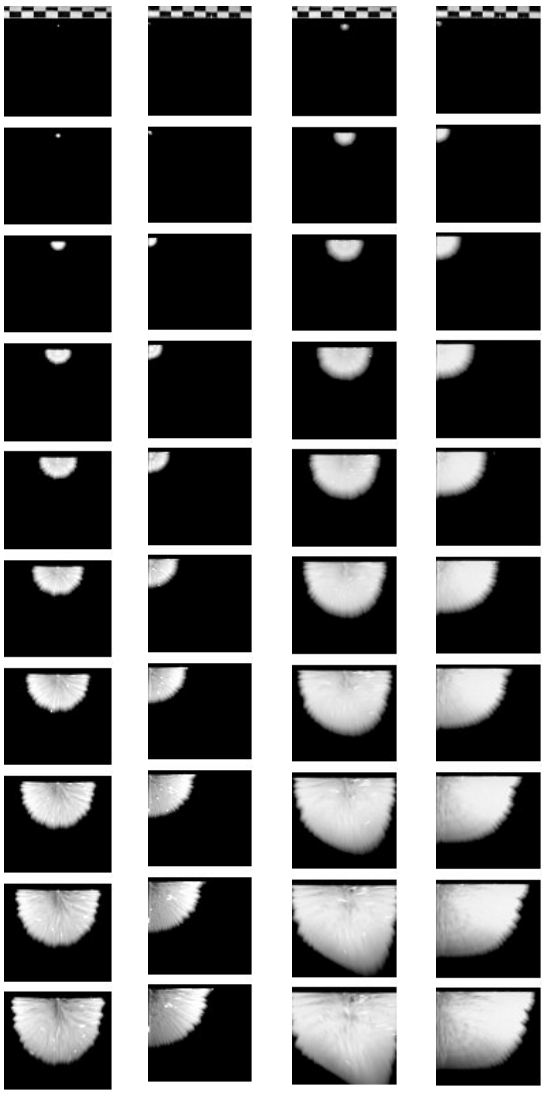
The SNU premixed hydrogen combustion experiments were simulated using lumped parameter and mechanistic burn models respectively. In the analysis, the same conditions were adopted as those in the experiment. The initial temperature of the combustion chamber set to room temperature (298 K) and the initial pressure set to 101.3 kPa. The gas mixture was composed of 10 % hydrogen and 90 % air. Because the GOTHIC code cannot use air as oxidizer, it is assumed that the air consists of 21 % oxygen and 79 % nitrogen. Therefore, the calculations were performed with a premixed gas mixture composed of hydrogen, oxygen and nitrogen. GOTHIC's built-in physical properties of each gas were used.

In cases of lumped volume analysis, the combustion chamber had only one volume of which the dimensions were $1 \times 0.024 \times 1$ m^3. The discrete burn model was applied to the volume and an igniter was assigned in the volume. The GOTHIC built-in igniter model was applied and other parameters related to hydrogen combustion criteria were assigned default values.

In cases of subdivided volume analyses, the mechanistic burn model was applied to the volume and an igniter was assigned to the same location in the experiment. The combustion chamber was simulated with 750 cells ($25 \times 1 \times 30$ cells). For the easy convergence of GOTHIC code, the section close to the ignition cell was divided small (2 cm) and the other section was divided relatively large (4 cm). The calculation results were almost identical for more than 750 cells. Pressure boundary condition was applied at the chamber bottom and an adiabatic wall condition was applied to the other parts of walls.

RESULTS AND DISCUSSION

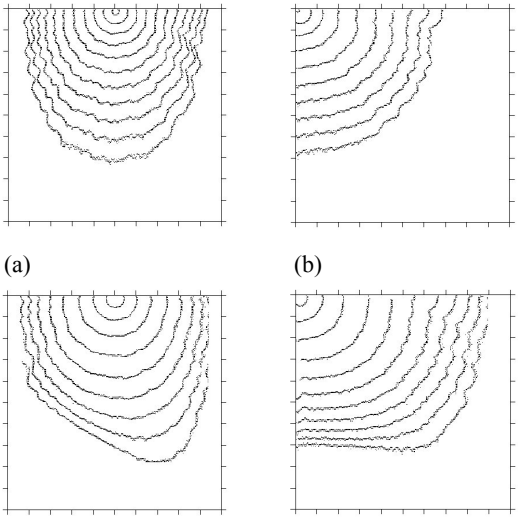
Figure 3: Direct Photograph Images of 10 % H2/Air premixed Flame Propagation (250fps) ;
(a) Top ignition, bottom full opened,
(b) Corner ignition, bottom full opened,
(c) Top ignition, bottom right half opened,
(d) Corner ignition, bottom right half opened



Experimental Results

Figure 3 shows the high-speed CCD photograph images (250 fps) of premixed hydrogen combustion experiments. The time step between each image correspond to 4 ms. The grid on the first image indicates the chamber size and one grid correspond to 10 cm. Figure 3 (a) shows the result of top center ignition and bottom full open case. After the ignition, the hydrogen flame propagated in the radial direction. With the lapse of time, the hydrogen flame front changed to a more and more wrinkled shape. Generally, when highly diffusive gas such as hydrogen is mixed in lean condition, the generation and growth of flame cell structure is highly dependent on a diffusive thermal instability. It is accepted that this jagged shape of flame front reflected the effect of diffusive thermal instability. Figure 3 (b) shows the result of top corner

ignition and bottom full open case. The characteristics of hydrogen flame propagation were similar to the top center ignition case results. And the reason to relatively weak flame intensity near the wall was due to the heat loss through the wall. Figure 3 (c) represents the result of top center ignition and bottom half open case. And figure 3 (d) shows the result of top corner ignition and bottom half open case. In comparison with bottom full open cases, the bottom half open cases results showed stronger flame intensity. This phenomenon can be explained by following reason. After ignition of the gas mixture, it discharged by expansion effect of combustion through the bottom open end. In bottom half open test cases, the opened area is small compared with full open test cases one. Thus, the amount of discharged gas mixture decreased and combustion rate of gas mixture was increased. Because the expansion of combusted gas generated a flow toward the open end, the flame had a tendency to rapidly propagate toward the open end of chamber.



(a) (b)

(c) (d)

Figure 4: Flame Propagation Sequences of 10% H2/Air Premixed in 2-D Combustion Chamber ;

(a) Top ignition, bottom full opened,

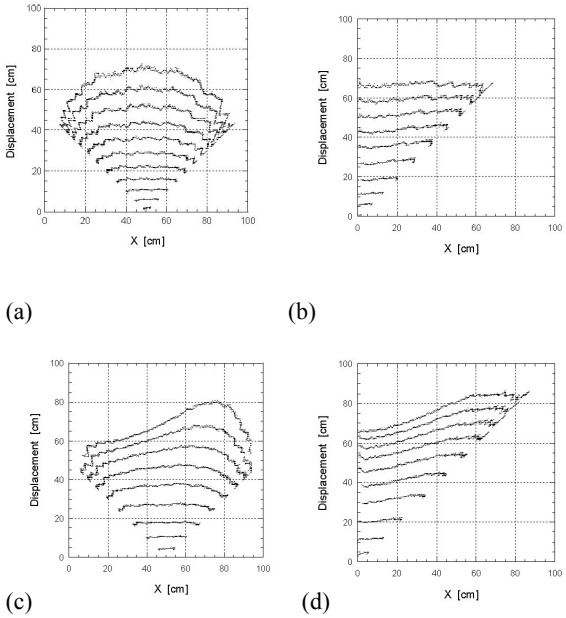
(b) Corner ignition, bottom full opened,

(c) Top ignition, bottom right half opened,

(d) Corner ignition, bottom right half opened

Figure 4 represents the hydrogen flame propagation sequence. This figures indicated the hydrogen flame front at every 4 ms. In this figure, it was possible to confirm the flame cell generation and growth. In the early stage of combustion, the flame front propagated with almost equal velocity and in the radial direction. With the lapse of time, the flame approaching the wall slowed in propagation velocity and the flame near the open end propagated rapidly. The flame toward the wall was affected by the compression effect of wall and the flame near the open end was affected by the expansion effect. Figure 4 (d) shows this phenomenon clearly. In the bottom left wall part, the flame propagation velocity slowed as time progressed, whereas the flame in the bottom right part rapidly propagated toward the open end.

Figure 5 shows the distance between the flame front and the ignition position. The slow flame velocity near the wall part and the fast flame velocity toward the open end are depicted clearly



(a) (b)

(c) (d)

Figure 5: Flame Edge Displacement from Ignition Position ;

(a) Top ignition, bottom full opened,

(b) Corner ignition, bottom full opened,

(c) Top ignition, bottom right half opened,

(d) Corner ignition, bottom right half opened

GOTHIC Analyses Results and Discussions

Figure 6 shows the result of GOTHIC lumped parameter analysis. The combustion of 10 % hydrogen and air mixture completed in about 100 ms. This agreed well with the experimental result. But any other information related to local combustion phenomena could not be obtained.

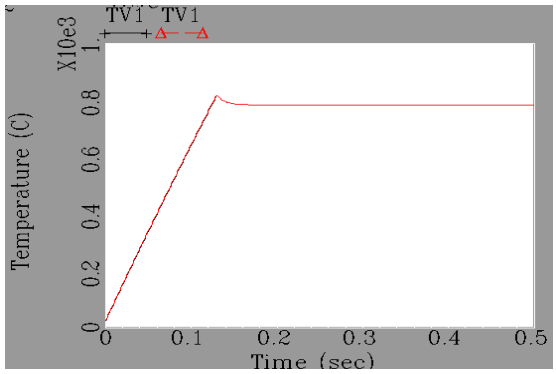


Figure 6: GOTHIC Lumped Parameter Combustion Analysis result

Figure 7 represents the GOTHIC mechanistic analyses results of 10 % hydrogen and air mixture combustion. The

lines in this figure show the different hydrogen mole fraction. It is assumed that the highest mole fraction line from a burned part implies the flame front. Because of the limitation of cell based calculation, the flame front shape was not exactly obtained and because of the wall adiabatic condition, the variation of flame intensity was not found. In the early stage of combustion, the combustion of gas mixture progressed in the radial direction and the flame front propagated rapidly toward the open boundary. Although these results showed the characteristic of flame propagation, it is still not well matched with the experimental results for the flame propagation sequence and combustion time. In the experiments, the combustion completed within 50 ms. Whereas, in the GOTHIC-3D calculation, the combustion was finished after several seconds.

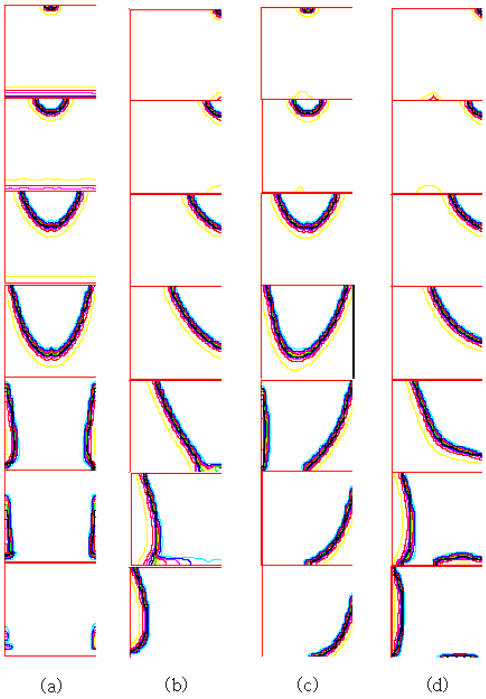


Figure 7: GOTHIC Analyses Results of 10 % H2/Air Combustion – Hydrogen Mole Fraction ;

(a) Top ignition, bottom full opened,

(b) Corner ignition, bottom full opened,

(c) Top ignition, bottom half opened,

(d) Corner ignition, bottom half opened

To explain the combustion time difference between GOTHIC-3D and experimental result, it is useful to examines the following reasons.

First, a review of the GOTIHC-3D burn models is necessary. The laminar mechanistic burn model is given in an expression by Lewis and von Elbe model and the GOTHIC adopted this model with some modification. The Lewis and von Elbe expression was verified with their combustion tests. But, the compositions of gas mixture used in the verifying tests had a range from 20 % hydrogen to 80 % hydrogen mixed with oxygen and steam. Therefore, in case of the different geometry tests and the lean condition of 10 % hydrogen and air mixture, this model should be applied carefully.

And the effective volume in equation (1) means actual burn volume. This effective volume is calculated with relation to the weighted averaged temperature (effective temperature). It refers in the GOTHIC technical manual that the verification of this weighting method was conducted with the FLAME tests. But the FLAME facility has very large free volume and the geometry is rectangular channel about 30 meters. Although the weighting method gives good predictions in FLAME tests, it cannot be said that the weighting method was verified a small scale and low contents of hydrogen gas mixture combustion cases. Because, in the GOTHIC code, there are no parameters which can affect the propagation process, like flame thickness, burned and unburned hydrogen mole fraction and so on. It cannot be said that the combustion analysis using default values in GOTHIC code always agreed with the experimental ones.

Also, the interaction between the hydrogen flame and the flow in the chamber should be confirmed. In the GOTHIC code, the hydrogen flame propagation was related to the mole fraction of mixture gas only. So, the flow due to the combusted gas is not well matched between the flame propagation and the flow in the chamber.

In case of 20 % hydrogen/air mixture and adiabatic chamber wall, the flame greatly accelerated after a few seconds. And the combustion was finished within 50 ms. This results imply that the GOTHIC-3D code doesn't have combustion analysis capability for the early stage of combustion.

CONCLUSION

In this study, the premixed hydrogen combustion experiments were conducted and GOTHIC code analyses were performed with lumped parameter and subdivided volume. Comparing the experimental and analytical results, the capability of GOTHIC code in predicting the hydrogen combustion phenomena was validated.

The GOTHIC lumped parameter burn model predicted reasonably to the time required to burn the hydrogen. But any other information such as flame propagation, flame front shape, gas expansion or compression effect etc. cannot be obtained.

In the GOTHIC-3D simulation results of SNU premixed hydrogen combustion, the GOTHIC-3D code could not predict the flame propagation in the early stage of combustion appropriately. And the characteristics of flame propagation could not be predicted. Moreover, it was found that the mechanistic model had some limitations in calculation of hydrogen combustion in case of low hydrogen contents and small geometry chamber.

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