Flame Acceleration Assessment of Hydrogen Gas in a Severe Accident

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1. Introduction

Hydrogen gas in the severe accident can be generated by various phenomena and can greatly affect the integrity of the containment building due to its gas characteristics (light density, high heat of combustion) [1-3]. In the severe accident, hydrogen combustion may occur due to a certain hydrogen concentration, oxygen concentration, and ignition source in the containment building, and the flame generated by combustion may be accelerated or decelerated depending on the surrounding geometric characteristics, temperature and pressure, etc. If decreasing of flame speed continues, quenching will finally occur, and if increasing of flame speed proceeds, a detonation can occur at the end [1-3]. Therefore, it is necessary to assess the flame acceleration due to hydrogen combustion in the containment building (IRWST, Upper dome and Cavity etc.) according to accident sequence in order to prevent the detonation in the severe accident.

2. Methods and Results

2.1 Methodology of flame acceleration assessment

Many researchers have written a state-of-the-art report on flame acceleration and deflagration to detonation transition in OECD/NEA, and it has been confirmed that the factor that has the greatest influence on flame acceleration is the expansion ratio (density ratio between product and reactant) [1]. The expansion ratio is expressed as Equation (1) according to the definition [4].

$$\sigma = \frac{\rho_u}{\rho_b} \tag{1}$$

where, σ is the expansion ratio, ρ is density, u and b are unburned gas (reactant) and burned gas (product). When calculating the density, it is independent of the pressure, and it is assumed that there is no change in mass and enthalpy before and after the reaction, so Equation (1) can be expressed as Equation (2) through the ideal gas equation.

$$\begin{aligned}\sigma &= \frac{m/V_u}{m/V_b} = \frac{V_b}{V_u} \\ &= \frac{n_b R T_b / P}{n_u R T_u / P} \\ &= \frac{n_b T_b}{n_u T_u}\end{aligned} \tag{2}$$

where, m is mass, V is volume, n is mole number, R is universal gas constant, T is temperature and P is pressure.

Meanwhile, looking at the OECD/NEA state-of-the-art report, GASFLOW, a detailed analysis program for thermal hydraulic phenomena in the containment building, calculates the flame acceleration assessment through σ_{index} as shown in Equation (3).

$$\sigma_{\text{index}} = \frac{\sigma}{\sigma_{\text{critical}}} \tag{3}$$

Through Equation (3), if σ_{index} is less than 1, the possibility of flame acceleration is excluded, and if it is greater than 1, it is evaluated that there is a possibility of flame acceleration. The critical expansion ratio $\left(=\sigma_{\text{critical}}\right)$ in Equation (3) was determined according to the gas temperature and hydrogen-oxygen concentration as shown in Table 1. In addition, in the hydrogen hazard assessment program (DDTINDEX) developed by AECL [5], the critical expansion ratio under the hydrogen-lean condition is expressed as Equation (4) based on Table 1.

$$\begin{aligned}\sigma_{critical} &= 3.75 - 0.0115 \times \left(T_u - 298\right) \\ &+0.00002 \times \left(T_u - 298\right)^2\end{aligned} \tag{4}$$

2.2 Calculated Adiabatic Flame Temperature model

In order to calculate the expansion ratio in the previous chapter, the number of moles and temperature of unburned gas and combustion gas are needed. In the hydrogen combustion, since 1 mole of hydrogen gas and 0.5 mole of oxygen gas produce 1 mole of steam, the number of moles of unburned gas and combustion gas can be calculated relatively simply. The combustion gas temperature is calculated through CAFT (Calculated Adiabatic Flame Temperature) model considering conservatism [7-8]. The assumptions

applied to the CAFT model are as follows:

Table 1 σ_{critical} according to temperature and concentration [5]

Temperature (K)	σ_{critical}	
	$C_{H_2} < 2 \cdot C_{O_2}$	$C_{H_2} > 2 \cdot C_{O_2}$
300	3.75	3.75
400	2.80	3.75
500	2.25	3.75
650	2.10	3.75

(1) During the combustion, all hydrogen gas or oxygen gas is completely combusted.
(Concentration of hydrogen or oxygen gas after completion of combustion is 0 vol.% according to the hydrogen-oxygen concentration ratio in unburned gas)
(2) All energy generated from combustion is transferred to the surrounding flame, and there is no heat loss.
(3) The combustion process is isobaric and isoenthalpy.

According to the above assumption and the 1st law of thermodynamics (the law of conservation of energy), the enthalpy between the burned gas and the unburned gas is the same, so it can be expressed as Equation (5).

$$\sum n_i \left[\int_{T_{\text{ref}}}^{T_u} c_{p,i} dT \right]_{\text{unburned}} = \sum n_i \left[\int_{T_{\text{ref}}}^{T_b} c_{p,i} dT \right]_{\text{burned}} + \Delta n_{H_2O} \Delta H^0_{f,H_2O} \quad (5)$$

where, unburned is unburned gas, burned is burned gas, n_i is the number of moles of *i* gas in unburned gas and burned gas, $\Delta H^0_{f,H_2O}$ is standard heat of formation of water vapor, $c_{p,i}$ is specific heat at constant pressure of *i* gas, T_u is temperature of unburned gas, T_b is temperature after completion of combustion and T_{ref} is reference temperature $(= 298\text{K})$.

2.3 Comparison with ANSYS CHEMKIN program

The ANSYS CHEMKIN program is a commercial combustion analysis program considering detailed chemical reactions. Through the ANSYS CHEMKIN program, it is possible to calculate the temperature, enthalpy, volume and pressure of the gas after completion of combustion by considering all detailed chemical reactions [9]. When calculating the gas status after completion of combustion, various reaction stages and various radicals are considered, and some hydrogen gas is present in the mixed gas after combustion due to a complex dissociation reaction, which leads to relatively non-conservative results in terms of combustion compared to the CAFT model. Therefore, in terms of the regulation, it is necessary to calculate through the CAFT model for flame acceleration assessment in severe accident. Also, the conservatism of the CAFT model should be checked through comparison with the ANSYS CHEMKIN program. To check the conservatism of the CAFT model, the expansion ratio should be calculated and compared for the same case as the ANSYS CHEMKIN program. The cases applied to the calculation are as shown in Table 2, where the hydrogen mole fraction is 0.01 to 0.15 (#11), the oxygen mole fraction is 0.005 to 0.10 (#11), the water vapor mole fraction is 0.0 to 0.5 (#9), and the temperature is 285 to 500K. (#5), for a total of 5,445. Figure 1 shows the expansion ratio calculated through the CAFT model and the ANSYS CHEMKIN program for all cases. σ_{CAFT} is the value calculated using the CAFT model and σ_{CHEMKIN} is the value calculated using the ANSYS CHEMKIN program. The solid line shown in the graph means that the expansion ratio calculated using the CAFT model and the ANSYS CHEMKIN program in the same case are equal, and the area below the solid line means that the CAFT model results are larger than the ANSYS CHEMKIN results. As shown graph, it was confirmed that the expansion ratio calculated using the CAFT model are similar to the results of the ANSYS CHEMKIN program considering the detailed chemical reaction within an average error of 8%. Also, for all cases, the expansion ratio calculated using the CAFT model is always larger than that of using the ANYSYS CHENKIN program. Considering the detailed chemical reaction, as the heat of combustion increases (high concentration of hydrogen gas), the rate of the reverse reaction in which hydrogen gas is generated during various dissociation reactions increases [9-10], so the expansion ratio is relatively small.

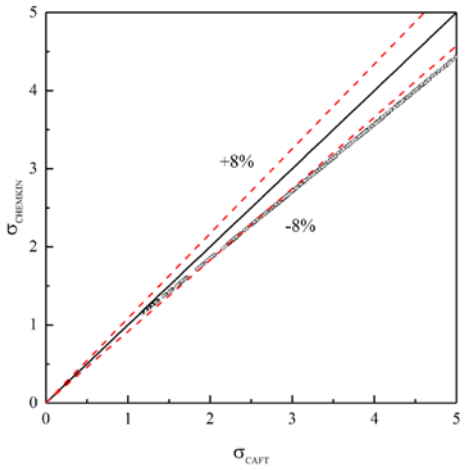

Fig. 1. Calculated σ using the CAFT model and the ANSYS CHEMKIM program

Table 2 Factor and value in case

Factor	Value
Hydrogen mole fraction (-)	0.01, 0.02, 0.04, 0.06, 0.08, 0.10, 0.11, 0.12, 0.13, 0.14, 0.15 (#11)
Oxygen mole fraction (-)	0.005, 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09, 0.10 (#11)
Water vapor mole fraction (-)	0.0, 0.025, 0.05, 0.10, 0.15, 0.20, 0.30, 0.40, 0.50 (#9)
Temperature (K)	285, 300, 350, 400, 500 (#5)

3. Conclusions

In this study, the assessment of flame acceleration due to hydrogen combustion in the containment building in the severe accident was analyzed. Among the flame acceleration assessment methodologies analyzed in the OECD/NEA report, in GASFLOW and DDTINDEX, flame acceleration is determined based on the ratio between the expansion ratio and the critical expansion ratio. The expansion ratio can be calculated from the number of moles and temperature of unburned gas and combustion gas, and the critical expansion ratio is calculated from the hydrogen and oxygen concentrations and the mixed gas temperature. When calculating the expansion ratio, the combustion gas temperature can be obtained by applying the CAFT model in consideration of conservatism. Finally, as a result of comparing the results of flame acceleration assessment using the ANSYS CHEMKIN program, a commercial detailed combustion analysis program, and the CAFT model, the expansion ratio calculated using the CAFT model was always calculated to be larger than the expansion ratio calculated using the ANSYS CHEMKIN program, within the average error range of 8% due to the conservatism of the CAFT model.

REFERENCES

[1] OECD/NEA, Flame Acceleration and Transition to Detonation in Hydrogen/Air/diluent Mixtures, NEA/CSNI/R(92)3, 1992
[2] OECD/NEA, Flame Acceleration and Deflagration-to-Detonation Transition in Nuclear Safety, NEA/CSNI/R(2000)7, 2000
[3] OECD/NEA, ISP-49 on Hydrogen Combustion, NEA/CSNI/R(2011)9, 2012
[4] W. Breitung, S.B. Dorofeev, Criteria for Deflagration-to-Detonation Transition (DDT) in Nuclear Containment Analysis, SMiRT-15 Post-Conference Seminar on Containment of Nuclear Reactors, Seoul, Korea, August 23-24, 1999.
[5] C.K. Chan, L. Wojciechowski, CODE PACKAGE FOR ASSESSING THE POTENTIAL FOR DDT IN A POST-ACCIDENT NUCLEAR CONTAINMENT, IAEA-IHMTFCV, Cologne, 18-22 June 2001
[6] J. Jeon et al., Development of Calculated Non-Adiabatic Flame Temperature Model to Predict Flammability Limits of H2-Air-Diluent Mixtures Based on Heat Transfer Mechanism, Trans. Korean. Nucl. Soci., Jeju, Korea, 2018
[7] C. V. Mashuga & D. A. Crowl, Flammability Zone Prediction Using Calculated
[8] W.C. Reynolds, The Element Potential Method for Chemical Equilibrium Analysis : Implementation in the Interactive Program STANJAN, Dept of Mechanical Engineering Stanford Universtiy, Palo Alto, CA, 1986
[9] Mascarenhas, V.J., Weber, C.N., Westmoreland, P.R. (2020). Estimating flammability limits through predicting non-adiabatic laminar flame properties, Proceedings of the Combustion Institute, In Press.
[10] Karanam, A., Sharma, P.K., Ganju, S., Singh, R.K. Chemical equilibrium analysos of dry hydrogen combustion, Proceedings of the ThEC15, Mumbai, India, 2015.