Applicability of Flame Temperature Models for Predicting the Upper Flammability Limit in SMR Containment Vessels

Sihyeong Yu [a], Dosu Park [a], Wonung Jeong [a], Joongoo Jeon [b*]
[a]. *Department of Quantum System Engineering, Jeonbuk National University, Jeonju, Republic of Korea*
[b]*Division of Advanced Nuclear Engineering, Pohang University of Science and Technology, Pohang, Republic of Korea*
[*]*Corresponding author: jgjeon41@postech.ac.kr*

Keywords : Combustible Gas, Flame, Flammability limit, Rich hydrogen, UFL, SMR,

1. Introduction

Nuclear power plants (NPPs) are a cornerstone of the global energy supply due to their high energy density and ability to provide stable, large-scale electricity generation. However, in the event of a severe accident, combustible gas can be generated through core cladding oxidation. The accumulation of hydrogen within the containment building can create an explosive atmosphere, posing a substantial threat to containment integrity [1]. Therefore, a quantitative hydrogen risk assessment is essential for ensuring nuclear safety.

Unlike large-scale nuclear power plants (NPPs), where severe accidents generally result in lean hydrogen–air mixtures, small modular reactors (SMRs) are more likely to develop rich hydrogen–air atmospheres due to their adoption of a vacuum containment vessel design [2]. These differences in containment characteristics may lead to distinct air composition and gas distribution patterns, thereby posing challenges to the direct application of existing assessment methodologies.

The hydrogen flammability assessment was performed using the calculated adiabatic flame temperature (CAFT), calculated non-Adiabatic flame temperature (CNAFT) and Shapiro methodologies, which are widely employed to estimate flammability limits under varying temperature, pressure, and steam concentration conditions [3, 4]. The CAFT and CNAFT approaches account for the effects of diluents such as steam or inert gases, whereas Shapiro method provides an empirical correlation based on experimental flammability limit data [5].

The objective of this study is to identify a methodology capable of accurately predicting flammability limits under rich-hydrogen conditions and to assess its applicability to severe accident scenarios in SMRs. To this end, the models were applied to experimental results near the upper flammability limit and to simulation results of severe accident conditions.

2. Methodology

2.1 Existing Methodology

2.1.1 CAFT Methodology

Extensive analytical research has been carried out to simplify the combustion process in a systematic manner, with the goal of developing reliable methods for predicting flammability limits. One common approach is to examine the idealized homogeneous flame, in which heat transfer between burned and unburned gases is neglected. A representative framework for such analysis is the concept of the CAFT, first introduced by Egerton and Zabetakis [3, 6]. They proposed that the adiabatic flame temperature near the flammability limit can be regarded as nearly constant. This temperature can be obtained through an energy balance, as expressed in **Equation (1)**. Under adiabatic conditions, the heat released from exothermic reactions is transferred entirely to the reaction products, resulting in a temperature rise. Here, $\Delta H_{f,i}^{0}$ denotes the enthalpy of formation, T_{ref} is the reference temperature (298 K), and $\overline{c}_{p,i}$ represents the mean specific heat. According to Arrhenius theory, the peak flame temperature occurring at the flame front determines the combustion heat rate. If the heat generated by combustion cannot overcome the heat loss, the flame does not propagate continuously, and consequently, flame extinction occurs. The threshold peak temperature is the temperature at which the minimum amount of combustion heat is generated for propagation.

The CAFT methodology is particularly valuable because it provides a theoretically grounded framework for estimating flammability limits without relying solely on experimental measurements, which can be challenging or impractical in extreme conditions.

$$\sum_{\boldsymbol{reactants}} \boldsymbol{n_i}\left[\boldsymbol{\Delta H_{f,i}^{0}} + \boldsymbol{\overline{c}_{p,i}}\left(\boldsymbol{T_i} - \boldsymbol{T_{ref}}\right)\right] - \sum_{\boldsymbol{products}} \boldsymbol{n_i}\left[\boldsymbol{\Delta H_{f,i}^{0}} + \boldsymbol{\overline{c}_{p,i}}\left(\boldsymbol{T_{CAFT}} - \boldsymbol{T_{ref}}\right)\right] = \mathbf{0} \quad \textbf{(1)}$$

2.1.2 CNAFT Methodology

The CNAFT methodology is an extension of the CAFT approach that incorporates indirect radiative heat losses. Unlike CAFT, which was primarily developed to calculate the flammability limits of hydrocarbon fuels such as methane, CNAFT was specifically designed to be more suitable for hydrogen–air mixtures [4]. This

distinction arises from the fact that hydrocarbon flames generally have Lewis numbers greater than one (Le > 1), whereas under severe accident conditions in large-scale nuclear power plants, the environment tends to form lean-hydrogen atmospheres with Lewis numbers less than one (Le < 1). As a consequence, flame extinction in methane–air mixtures typically occurs at the flame tip, while in hydrogen–air flames extinction preferentially initiates at the trailing edge. The CNAFT model was therefore proposed to account for this unique extinction behavior of hydrogen–air systems [7].

In order to incorporate the extinction mechanism unique to hydrogen flames, the CNAFT methodology introduces an additional heat-loss term into the energy balance. The governing equation can be expressed as shown in Eq. (2), where Q_{rad} denotes the indirect radiative heat loss from the reaction zone.

$$\sum_{reactants} n_i\left[\Delta H_{f,i}^0 + \overline{c}_{p,i}\left(T_i - T_{ref}\right)\right] - \sum_{products} n_i\left[\Delta H_{f,i}^0 + \overline{c}_{p,i}\left(T_{CNAFT} - T_{ref}\right)\right] = Q_{rad,1} \quad (2)$$

This term reflects the fact that the negative temperature gradient at the trailing edge enhances heat transfer away from the flame, thus promoting extinction. From a heat-flux perspective, the loss rate can be written as shown in Eq. (3), where k_f is the thermal conductivity, R the volumetric radiation rate, ρ_u the unburned gas density, c_p the average specific heat, and S_u the laminar flame speed. To further simplify, the CNAFT coefficient $\pi = \frac{\alpha}{C}$ is introduced, which allows the indirect radiation loss to be expressed in a linear form as shown in Eq. (4) [4].

$$q_{rad,1} = k_f \frac{R}{\rho_u c_p S_u} \quad (3)$$

$$Q_{rad,1}(\pi) \approx 0.207(\pi - \pi_{ref}) \quad (4)$$

Through this formula, the CNAFT model preserves the simplicity of the CAFT approach while explicitly capturing the role of indirect radiation and trailing-edge extinction in hydrogen–air flames. However, since the CNAFT methodology was originally developed for lean-hydrogen conditions with Lewis numbers less than unity, its applicability under rich-hydrogen conditions with Lewis numbers greater than one remains uncertain.

2.1.3 Shapiro-Moffette Methodology

The Shapiro-Moffette methodology was proposed to evaluate flammability within nuclear power plant containment and provides a systematic framework for assessing the flammability limits of hydrogen-air mixtures. Based on numerous experiments, this methodology examined how flame propagation is affected by vessel wall heat losses (surface-to-volume ratio), pressure variations, and the initial temperature of the mixture, and was subsequently formulated into the Shapiro-Moffette Diagram [5]. In general, the flammability range of hydrogen has been reported to be approximately 4% to 74% by volume. At pressures slightly above atmospheric pressure, the flammability range for downward flame propagation becomes narrower, whereas at higher pressures (10–220 atm) the upper limit expands. Similarly, an increase in the initial temperature broadens both limits, shifting the values from 1.9–76% at 200 °C to 6.3–81.5% at 400 °C.

This structured approach can be applied to scenarios such as a loss-of-coolant accident (LOCA), where hydrogen is generated through zirconium-steam reactions. Therefore, the Shapiro-Moffette methodology provides a valuable basis for evaluating hydrogen detonation risks and ensuring sufficient safety margins in reactor containment analysis.

2.2 Limitations of Flammability Assessment Models in Severe Accident Analysis Codes

Although each methodology provides valuable insights into flammability assessment, they all entail inherent limitations [1]. The CAFT methodology, for instance, is effective in evaluating the flammability of gases with Lewis numbers greater than unity by means of the adiabatic flame temperature. However, its inability to account for heat-loss mechanisms makes it less suitable for application in lean-hydrogen environments. In contrast, the CNAFT methodology extends this framework by incorporating radiative heat loss effects into the non-adiabatic flame temperature, making it particularly suitable for hydrogen-air mixtures with Le < 1. Nevertheless, its predictive capability diminishes when applied to gases with Lewis numbers greater than unity. Finally, the Shapiro methodology, while grounded in experimental observations and offering empirical reliability, is constrained by the scope of the experimental conditions from which it was derived, and thus its applicability can be limited under certain circumstances. Accordingly, it is essential to evaluate the applicability of existing methodologies to rich-hydrogen conditions that could occur during severe accidents in SMRs. As a result, severe accident analysis codes such as MELCOR and MAAP still rely heavily on experimental data, which makes it practically difficult to establish a robust flammability assessment within these codes.

2.3 Methodology Applicable to Rich-Hydrogen Conditions

To examine the accuracy of flammability limit predictions under rich-hydrogen conditions, flame temperature calculations were performed under the assumption that the critical flame temperature remains nearly constant in the vicinity of the flammability limits. For validation, experimental data from the FITS experiments conducted by the U.S. NRC were employed,

and, as shown in **Figure 1**, samples near the upper flammability limit were systematically applied to both the CAFT and CNAFT models. Furthermore, a threshold flame temperature of 1160 K was adopted as the reference value at the upper flammability limit (UFL) [8].

In addition to the FITS experimental data, simulation results from the ERI/NRC 18-202 report, specifically the LCC-05T-03 case with 69% oxidation calculated using MELCOR, were also utilized for validation [2].

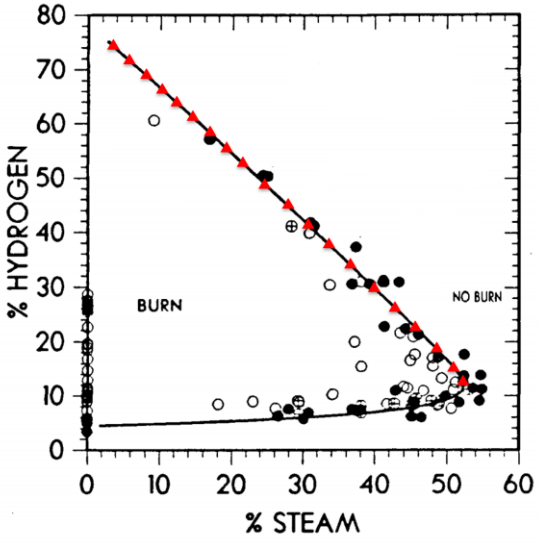

Figure 1. Sampled Point from PITS experiment

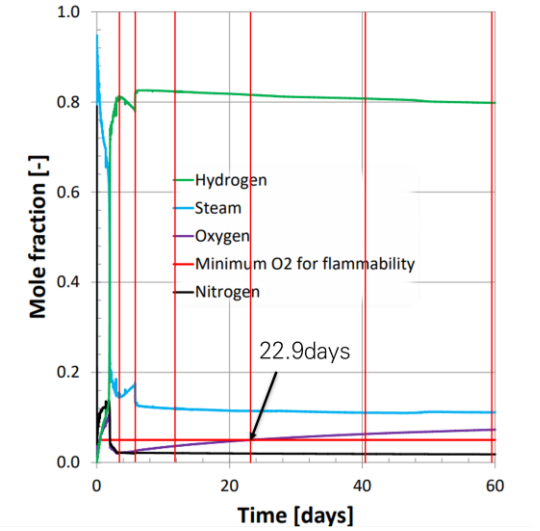

Figure 2. Containment atmosphere composition, scenario LCC-05T-03 with 69% oxidation

3. Result and Discussion

As a result, the CNAFT methodology, which was originally developed for predicting lower flammability limits (LFL), completely failed to provide meaningful flame temperature predictions under rich-hydrogen conditions.

As illustrated in **Figure 3**, the CAFT approach, in contrast, yields flame temperatures in the range of 1100–1300 K near the UFL boundary.

In **Figure 4**, it can be observed that the prediction error becomes minimal when the hydrogen fraction is approximately 53%. Overall, the calculated temperatures remain close to the threshold of about 1160 K; however, larger deviations are observed in atmospheres with relatively lower hydrogen concentrations and higher steam fractions.

Furthermore, as demonstrated in **Figure 5** and **Figure 6**, when the hydrogen concentration exceeds 50%, the predicted UFL values retain a safety margin of up to ~2%, indicating non-flammability. In particular, **Figure 6**, which illustrates the difference between the actual hydrogen concentration and the calculated UFL, shows that for hydrogen fractions below 50%, this difference becomes negative, suggesting deficiencies in reliably predicting combustion behavior in this region.

Overall, it is observed that when the hydrogen concentration falls below approximately 50%, there is a tendency for increased difficulty in accurately calculating both the flame temperature and the UFL. It should also be considered that when the hydrogen concentration drops below about 50%, the higher steam fraction could contribute to uncertainties in the experimental data.

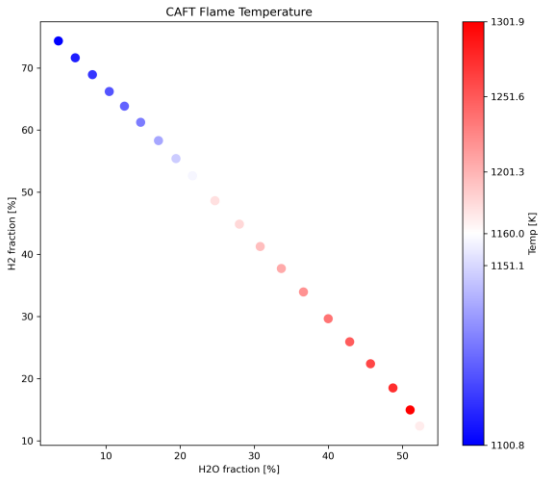

Figure 3. CAFT Flame Temperature

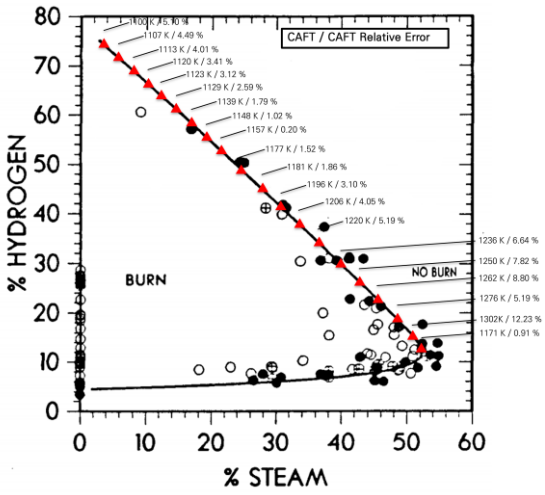

Figure 4. CAFT Temperature and Relative Error

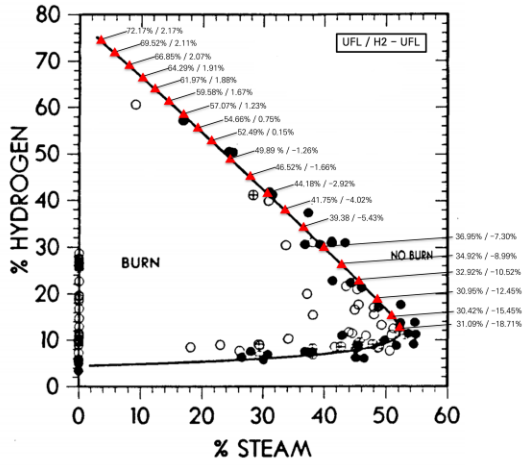

Figure 5. Distribution of UFL Prediction

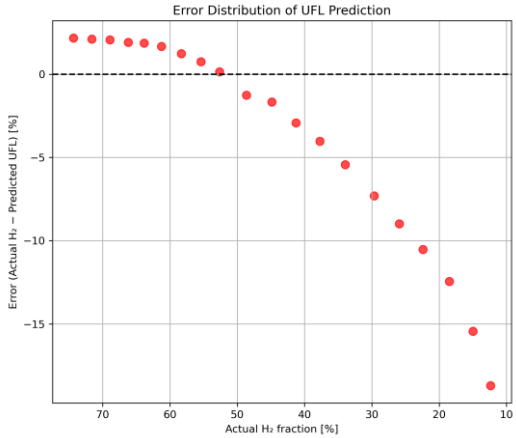

Figure 6. Error Distribution of UFL Prediction

As shown in **Table 1**, by extracting values from the LCC-05T-03 scenario with 69% oxidation and applying the CAFT methodology, it was confirmed that the predictions aligned well under severe accident conditions in SMRs.

Day	CAFT(K)	UFL(%)	H2 – UFL (%)
3.8	740.8	53.22	27.78
5.7	814.81	55.72	22.23
11.9	980.53	76	6.41
22.9	1198.7	82.11	-0.28
40.8	1420.32	85.23	-4.18
59.3	1572.07	86.45	-6.16

Table 1. CAFT and UFL calculations from scenario LCC-05T-03 with 69% oxidation

4. Conclusion

In this study, the CAFT and CNAFT methodologies were applied to improve the accuracy of upper flammability limit (UFL) predictions. The CAFT approach shows limitations in predicting flammability limits under lean-hydrogen conditions (Le < 1), which led to the development of the CNAFT model. However, under rich-hydrogen conditions (Le > 1), CAFT was expected to perform better, and its application demonstrated reasonable agreement with both high-hydrogen FITS experimental data and severe accident environments in SMRs.

Future work should focus on developing an improved non-adiabatic flame temperature model that accounts for high steam fractions and accurately predicts UFL behavior under all hydrogen concentrations.

ACKNOWLEDGEMENT

This work was supported by the Nuclear Safety Research Program through the Regulatory Research Management Agency for SMRs (RMAS) and the Nuclear Safety and Security Commission (NSSC) of the Republic of Korea. (No. RS-2024-00509653) and the National Research Council of Science & Technology (NST) grant by the Korea government (MIST) (No. GTL24031-000)

REFERENCES

[1] J. Jeon, and S.J. Kim, Recent progress in hydrogen flammability prediction for the safe energy systems, International Journal of Hydrogen Energy, Energies, vol. 13, no. 23, art. 6263, Nov. 2020,

[2] U.S. Nuclear Regulatory Commission, Assessment of Hydrogen Combustion During Severe Accidents In a NuScale Plant Module, NRC Staff Report, ML19312A082, 2019.

[3] M. Vidal, W. Wong, W.J. Rogers and M.S Mannan, Evaluation of lower flammability limits of fuel–air–diluent mixtures using calculated adiabatic flame temperatures, Journal of Hazardous Materials, vol. 130, pp. 21–27, 2006.

[4] J. Jeon, Y. S. Kim, and H. Jung, A mechanistic analysis of H_2O and CO_2 diluent effect on hydrogen flammability limit considering flame extinction mechanism, Int. J. Hydrogen Energy, vol. 44, no. 59, pp. 31238–31247, Dec. 2019.

[5] H. M. Shapiro, The flammability limits of hydrogen–air mixtures, Symposium (International) on Combustion, vol. 3, no. 1, pp. 53–64, 1951.

[6] Zabetakis, M.G. Flammability Characteristics of Combustible Gases and Vapors; Bureau of Mines: Washington, DC, USA, 1965.

[7] J. Jeon, Extinction Mechanism of Ultra-Lean Hydrogen Flames for Safety of Clean Energy Systems, Department of Nuclear Engineering, Hanyang University, Republic of Korea, 2022.

[8] M. Terpstra, Flammability limits of hydrogen and methane in air with added diluents, Dept. Chem. and Petroleum Eng., Univ. of Calgary, Calgary, AB, Canada, 2012.