Hydrogen Flammability Assessment in SMR Containment Using the CAFT Model

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1. Introduction

Nuclear power plants(NPPs) are widely recognized as a valuable energy source capable of stable power generation and carbon neutrality. However, during a severe accident at a nuclear power plant, a large amount of hydrogen can be produced due to oxidation reactions between the fuel cladding and the coolant. The combustion and explosion of this combustible gas can cause overpressure, severely compromising the integrity of the containment building [1].

Small Modular Reactors (SMRs), which are gaining attention as next-generation carbon-free energy sources due to their excellent economics through modular fabrication and passive safety features, are not immune to this hydrogen generation problem. Reactor designs like NuScale or i-SMR adopt vacuum containment vessels, resulting in extremely low initial internal air (oxygen) content [2]. Consequently, it has been assumed that even if hydrogen is generated, the absolute lack of oxygen required for combustion would prevent fires or explosions.

However, a rigorous analysis of the obstprogression of a severe accident suggests a scenario that may differ considerably from simplified assumptions. When large volumes of high-temperature steam released into the confined space of a vacuum containment vessel condense on cold surfaces, the volume ratio of the steam can decrease rapidly. This process may lead to a “hydrogen-rich environment” where the concentration of remaining hydrogen increases significantly [2]. In such a hydrogen-rich environment, even trace amounts of oxygen introduced through cooling-water radiolysis or external valves could potentially approach conditions near the Upper Flammability Limit (UFL). Furthermore, SMRs have structurally limited internal space, making it challenging to optimally position combustible gas control equipment like Passive Autocatalytic Recombiners (PARs). Therefore, a careful flammability assessment reflecting the SMR’s inherent confined space and hydrogen-rich conditions—distinct from the “lean-hydrogen” conditions of existing large reactors—may be important to ensure nuclear safety.

Accordingly, this study introduces the Calculated Adiabatic Flame Temperature (CAFT) methodology, which shows applicability for predicting flammability under hydrogen-rich conditions, to evaluate flammability during severe accidents in SMRs. Based on this, we perform a hydrogen risk assessment over time using representative severe-accident scenario data (ERI/NRC 18-202 report) for the NuScale SMR and quantitatively analyze the hydrogen hazard within the SMR containment building.

2. Methodology

2.1 CAFT-based Flammability Assessment Model

The CAFT model is a methodology that determines flammability by thermodynamically calculating the maximum temperature achievable when a given mixture of gases combusts under adiabatic conditions [3]. It should be noted that this thermodynamic approach inherently assumes a well-mixed, uniform atmosphere, evaluating the macroscopic flammability limit without considering local gas stratification. Through prior research [4], our research team demonstrated that the CAFT model, primarily used for predicting the Lower Flammability Limit (LFL), also exhibits high applicability for predicting the Upper Flammability Limit under hydrogen-rich conditions, such as those found in SMR environments.

In this study, referencing literature by Terpstra et al., the threshold adiabatic flame temperature (Threshold CAFT) determining combustion feasibility under hydrogen-rich conditions was set to 1160 K [5]. That is, a calculated flame temperature of the mixed gas of 1160 K or higher is evaluated as falling within the flammable range. The CAFT model is based on the assumption that the adiabatic flame temperature remains nearly constant at the flammability limit. To evaluate the accuracy of this methodology, the model’s performance was analyzed using two distinct error metrics. Because the CAFT value and the corresponding UFL represent the same flammability-limit condition in temperature and concentration space, respectively, the accuracy was evaluated using both the flame-temperature deviation and the UFL obtained by converting the CAFT result into the concentration domain based on the non-hydrogen species fractions. The first metric quantifies the deviation of the calculated adiabatic flame temperature from the 1160 K threshold, and the second assesses the difference between the measured hydrogen concentration from experimental data and the predicted UFL. This dual-metric approach ensures that both the thermodynamic foundation of the CAFT model and the resulting physical flammability boundaries are rigorously validated against experimental observations. To validate this model, a comparative analysis was performed using U.S. NRC's FITS experimental data [6]. As shown in Figures 1 and 2, the CAFT model was found to predict the critical hydrogen concentration and flame temperature in the hydrogen-rich region with high precision under conditions where the steam concentration is 30% or less.

The fundamental equation of the CAFT model used in this evaluation is given by Equation (1) below.

$$\sum_{reactants} n_i\left[\Delta H^0_{f,i} + \bar{c}_{p,i}\left(T_i - T_{ref}\right)\right] - \sum_{products} n_i\left[\Delta H^0_{f,i} + \bar{c}_{p,i}\left(T_{CAFT} - T_{ref}\right)\right] = 0 \tag{1}$$

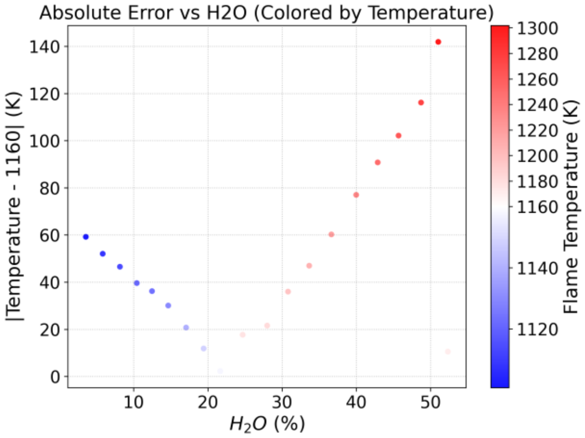

Fig. 1. Deviation of the calculated flame temperature from the 1160 K threshold as a function of steam fraction, with the secondary y-axis indicating the absolute flame temperature.

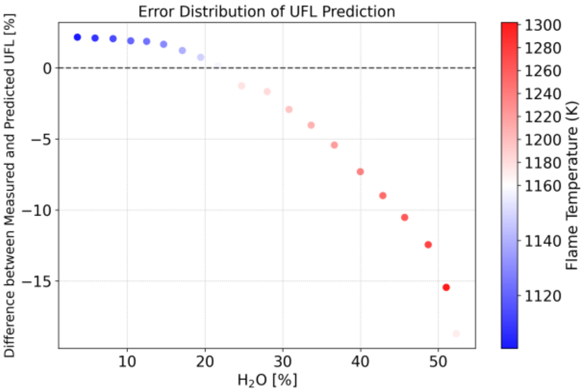

Fig. 2. Difference between measured H_2 concentration and predicted UFL as a function of steam fraction, with the secondary y-axis representing the calculated flame temperature.

2.2 SMR Severe Accident Scenarios in the ERI report

According to the ERI NuScale SMR MELCOR calculation report, the scenarios used in that report are LCC-05T-03 and LCU-03T-01 [2].

The LCC-05T-03 scenario assumes a situation where CVCS piping within the NuScale module ruptures inside the containment vessel [7]. Immediately after rupture, reactor coolant is directly released into the containment vessel's internal space. This leads to an increase in pressure and temperature inside the containment vessel, along with core exposure and cladding oxidation reactions due to coolant loss. Approximately 40 to 50 hours later, active zircaloy oxidation generates large amounts of hydrogen. Due to the relatively small volume of the containment vessel, the oxygen concentration decreases sharply, causing the containment atmosphere itself to reach an inert state initially.

The ERI report's modified LCC-05T-03 scenario, to analyze flammable condition formation, activated the Emergency Core Cooling System(ECCS) valve at 49.38 hours to halt further cladding oxidation [3]. This intentionally halted oxygen dilution by hydrogen and created an environment where oxygen generated via radiolysis of water could reach a flammable concentration (0.05 molar fraction).

The characteristic behavior of this scenario calculated by ERI is as follows. First, the interior of the containment vessel is a closed, single volume, meaning there is no gas exchange with the outside. All hydrogen, oxygen, nitrogen, and water vapor behavior occurs exclusively within the containment vessel in a closed system. Second, oxygen is continuously generated over the long term due to radiolysis. Consequently, the oxygen concentration gradually increases over time, even after the oxidation reactions have ceased.

Furthermore, the LCU-03T-01 scenario considers a situation where the CVCS piping ruptures outside the containment vessel, in the area beneath the bio-shield [8]. The ruptured primary system fluid is ejected directly into the bio-shield cavity, not the containment vessel. This space exchanges air with adjacent modules and the upper pool space via natural convection through structurally open vent paths. Due to this structural difference, this scenario exhibits quasi-open system behavior, where hydrogen and steam accumulate while continuously exchanging with external air, unlike inside the containment vessel.

Hydrogen accumulation behavior is accompanied by strong stratification phenomena. While the well-mixed concentration remains at around 6–10%, it has been reported that hydrogen can accumulate to a maximum of approximately 12.6% in specific localized areas.

However, this study excluded the LCU scenario from its analysis scope. The reasons are: First, the LCU scenario does not establish the conditions of hydrogen-rich and UFL zones, which are the primary focus of this study, due to the continuous influx of external air. Second, due to its large volume and open structural characteristics, the bio-shield offers ample scope for engineering countermeasures, such as forming a mixed atmosphere and applying hydrogen removal equipment. Therefore, the scenario inside the containment vessel (LCC-05T-03), a relatively high-risk closed system, was prioritized for consideration.

2.3 Transient Gas Fractions and Pressure in NuScale SMR Severe Accident

In this scenario, to control core oxidation reactions, ECCS valves (1 RVV and 1 RRV) are set to be forcibly opened at 49.38 hours. This re-floods the core, halting hydrogen generation. Subsequently, oxygen generated via radiolysis gradually accumulates, reaching the flammability limit of 0.05 mol% (5%) at the 72-hour mark. ERI considered this point the worst-case condition for combustion analysis.

Additionally, since no graph data was provided for the gas temperature, the gas temperature value of 369.65K available in the report was used.

Figure 3, 4 show the change in molar fractions major gas components and pressure within the containment vessel over 72 hours during the progression of the LCC-05T-03 modified scenario.

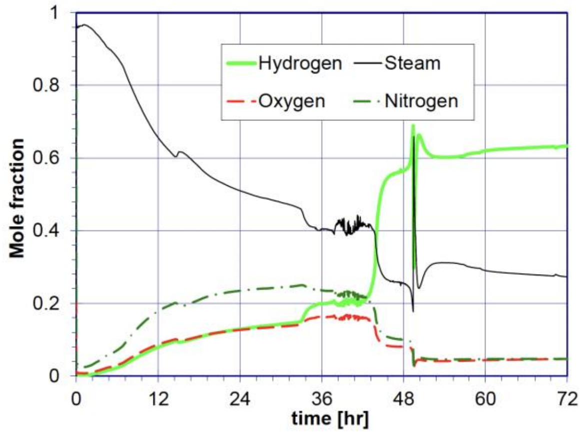

Fig. 3. Evolution of mole fractions for major gas species in the containment during the first 72 hours of the LCC-05T-03 variant scenario (reproduced from Fig. 3.5 in [2]).

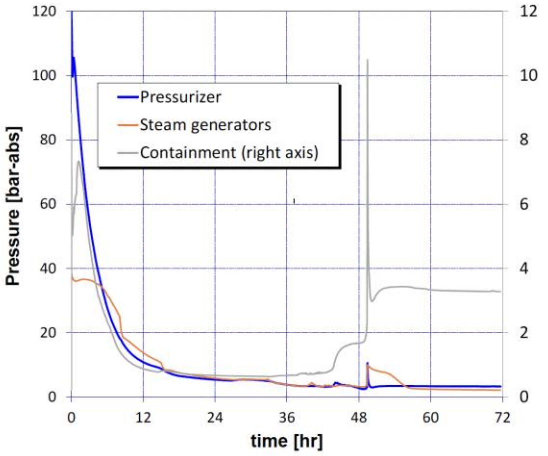

Fig. 4. Evolution of pressure in the containment during the first 72 hours of the LCC-05T-03 variant scenario (reproduced from Fig. 3.1 in [2]).

3. Result

In this study, the CAFT model was applied to evaluate flammability based on hourly gas fraction, pressure, and temperature data inside the containment vessel. Scenario analysis confirmed that the hydrogen fraction increased sharply approximately 44 hours after the accident onset, forming hydrogen-rich conditions. The corresponding pressure and gas mole fractions for each time interval after 44 hours are summarized in Table 1. Accordingly, the adiabatic flame temperature was calculated using this concentration data. The resulting flame temperatures, the predicted UFL, and the comprehensive flammability assessment results are presented in Table 2.

Hour	H_2O(%)	H_2(%)	O_2(%)	N_2(%)	P (Pa)
44	31.42	44.98	10.43	13.63	113044
46	26.13	55.20	8.25	10.52	161535
48	25.38	56.54	8.11	10.01	168244
50	24.41	66.30	4.44	5.04	300857
54	31.19	60.17	4.11	4.58	343244
60	29.01	62.02	4.34	4.76	333842
66	27.98	62.77	4.58	4.76	330569
72	27.37	63.28	4.67	4.86	328967

Table. 1. Evolution of mole fractions for major gas species in the containment during the first 72 hours of the LCC-05T-03 variant scenario.

Hour	Flame Temperature(K)	Predicted UFL(%)	Flammability
44	1834.52	71.71	O
46	1552.52	70.96	O
48	1536.48	71.41	O
50	1006.03	57.01	X
54	943.93	42.53	X
60	981.62	49.19	X
66	1017.81	53.43	X
72	1032.57	55.21	X

Table. 2. Calculated adiabatic flame temperatures, predicted UFLs, and flammability assessment results based on the CAFT model.

Calculations indicate that the flame temperature between 44 and 48 hours after the accident exceeded approximately 1500K, significantly surpassing the critical temperature of 1160K established in this study. Therefore, this interval was analyzed as falling within the flammable region from a thermodynamic perspective.

In contrast to the ERI analysis suggesting that flammability emerges near the 72-hour mark, the model calculations indicated that flammability actually weakened beginning at approximately 49.38 hours after ECCS valve operation. This divergence is consistent with the physical mechanisms described in the source text, which notes that:

"The time dependence of Equation (1), plus the imposed time dependence for the cumulative cladding oxidation, imply that prior to 72 hours the containment atmosphere is inflammable due to oxygen concentration less than 0.05. Flammability arises at 72 hours due to the cumulative oxygen mass generated by radiolysis; the particular oxygen concentration of 0.05 at that time reflects the imposed cumulative amount of hydrogen generated by cladding oxidation [2].”

By directly applying this description, the weakening of flammability observed at 49.38 hours can be understood as a consequence of the containment atmosphere dynamics following valve opening. The rapid influx of steam caused a pronounced dilution of oxygen between 50 and 72 hours, which in turn reduced the adiabatic flame temperature below 1050 K—well below the level necessary to sustain combustion. Therefore, even though the ERI analysis identifies 72 hours as the point at which oxygen concentration reaches 0.05 due to radiolytic generation, the model results show that the flame temperature at that same time fails to reach the critical energy-based threshold of 1160 K.

Analysis revealed that while the ERI report concluded no flammability existed before 72 hours post-accident due to oxygen concentrations not exceeding 5%, actual oxygen levels around 44 to 48 hours were confirmed to reach approximately 8%. Furthermore, since the steam fraction was low at that time, making it difficult to expect a flame-suppressing effect, it can be concluded that flammable conditions were already present even during the 44 to 48-hour period prior to 72 hours.

4. Conclusion

This study evaluated the potential for flammability under hydrogen-rich conditions from a thermodynamic perspective by applying the Calculated Adiabatic Flame Temperature (CAFT) model to the internal thermal-hydraulic data of the NuScale SMR severe accident scenario (LCC-05T-03). The key observations derived from this study are as follows.

First, the 44–48 hour interval after the accident onset was identified as a period during which the CAFT model predicts the possibility of flammability. In this time window, zircaloy oxidation leads to a marked increase in the hydrogen fraction while oxygen concentration remains at approximately 8%. Because the steam fraction is relatively low, limited steam inerting effects can be expected. As a result, the adiabatic flame temperature was predicted to exceed 1500 K—well above the energy-based threshold of 1160 K—indicating that sufficient combustion energy could be present under the modeled conditions. These findings suggest that this period may require additional confirmatory analysis.

Second, the analysis revealed thermodynamic behavior that differs from the flammability assessment presented in the existing ERI report. While the ERI evaluation considered the pre-72-hour period to be non-flammable due to insufficient oxygen (<5%) and identified the 72-hour point as the time at which flammability would arise due to radiolytic oxygen generation, the application of the CAFT model in this study suggests an alternative interpretation. After the ECCS valve opened at 49.38 hours, a substantial steam influx diluted the oxygen concentration and increased the heat-absorption capacity of the gas mixture.

Consequently, the predicted adiabatic flame temperature at the 72-hour point decreased sharply to below 1050 K, falling short of the threshold required for combustion.

These results indicate that reliance solely on simple single-gas concentration criteria (e.g., 5% oxygen) may lead to an underestimation of combustion risks within the containment during severe accident transients. The findings suggest that the CAFT model—capable of simultaneously reflecting gas-mixture composition changes and the deactivation effects of water vapor—may provide a more comprehensive and conservative framework for assessing hydrogen hazards in SMRs. Further studies, including broader sensitivity analyses and confirmatory modeling, are recommended to validate the predicted flammability behavior and to strengthen the technical basis for hydrogen risk evaluation under severe accident conditions.

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