Preliminary Hydrogen Risk Analysis with Quantitative Criteria for Combustion Step Using Post-Processing Tool for Lumped-Parameter Code

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1. Introduction

The Fukushima Daiichi accident informed that research on severe accident is still necessary. During such severe accident, hydrogen can be generated because of oxidation reaction between high temperature zircalloy cladding and steam within the reactor vessel [1]. The hydrogen produced within the vessel can be released into containment building through safety valves or because of reactor vessel failure. The released hydrogen can experience combustion event and develop into deflagration to detonation (DDT) event through flame acceleration (FA) [1]. Then the hydrogen may bring critical damage on different items related to the reactor system or containment building itself. Because of this potential risk of hydrogen explosion, hydrogen risk analysis became an ever-important task for severe accident analysis [1].

Overall analysis of severe accident can be conducted with lumped-parameter code such as MELCOR. MELCOR is capable of simulating different accident scenarios of light water reactors [2]. MELCOR can indicate when different physical events, such as core uncovering, fuel degradation, and oxidation event, occur and how much chemicals may be produced due to such events. Various packages within MELCOR allow users to analyze specific phenomena including hydrogen accumulation after simulating an accident scenario [2].

However, conventional lumped parameter codes have their own limitations to conduct specialized hydrogen risk analysis. For instance, MELCOR does not include model to predict the likelihood of FA and DDT [2]. Besides, influence of various diluents on flammability limit is not modeled in detail. It means that hydrogen risk analysis with only current MELCOR code is difficult to evaluate adequately the integrity of containment. Therefore, the objective of this study is to propose the concept of post-processing tool including advanced hydrogen risk analysis model needed to improve analytical performance. First, physical models for prediction of flammability limit, FA, and DDT, to enhance hydrogen risk analysis are introduced. After the introduction, brief simulation results are descripted.

2. Physical Model

2.1 Flammability limit

MELCOR has its own flammability limit model. The flammability limit model in MELCOR is described as propagation criteria [2]. Once combustion is initiated, MELCOR judges possibility of propagation by hydrogen concentration of adjacent control volume [2]. The propagation criteria vary depending on direction of the flame. Upward, downward, and horizontal propagation has required hydrogen concentration of 4%, 6%, and 9% respectively [2]. If a control volume adjacent to the initial control volume satisfies the criterion according to its orientation relative to the initiating control volume, MELCOR judges that propagation occurs in the control volume.

Limit of MELCOR related to the propagation criterion is that MELCOR is not able to adjust the criterion depending on concentration of diluent [2]. If diluents, gas not participating on combustion reactions, exist within a control volume, the criteria for hydrogen must be adjusted. In severe accident conditions, tremendous amount of steam, one of many diluents, is released with hydrogen. Therefore, it is important to adjust the criteria to be sensitive on diluent mole fraction for much detailed analysis.

To enhance performance of hydrogen risk analysis regarding hydrogen propagation, prediction of flammability limit using Calculated Non-Adiabatic Flame Temperature (CNAFT) model can be applied. CNAFT model is a modified version of Calculated Adiabatic Flame Temperature (CAFT) model by Jeon et al [3]. CAFT model is designed to calculate theoretical flame temperature when all heat energy from complete combustion of fuel affects the temperature of flame without any heat loss. Then the calculated flame temperature can be used to predict flammability limit because flame temperature is identical along the lean flammability limit [3]. The equation below is simplified form of CAFT model [3].

$$\sum n_i \left[\Delta H_{f,i}^0\right] reactants - \sum n_i \left[\Delta H_{f,i}^0 + \bar{c}_{p,i}(T_{CAFT} - T_{initial})\right]_{propucts} = 0 \quad (1)$$

However, even combustion occurs near flammability limit, certain amount of heat loss always exists, which implies that the CAFT model is not accurate enough. Therefore, CAFT model was modified as CNAFT model with inclusion of heat loss term on calculation of the theoretical flame temperature [3]. Therefore equation (1) changes into [3]:

$$\rho_u S_u \left[c_p T_u + H^a\right] - \rho_u S_u c_p T_{peak} - q_{loss} = 0 \quad (2)$$

With the involvement of the heat loss term, CNAFT model became much accurate on predicting flammability limit. Besides, further modification with regard to polar gas, such as steam, allowed the CNAFT model to have some accuracy on prediction of the flammability limit with mixtures including steam [3]. Figure 1 shows that flammability limit can be well predicted with relative error of 12% [3]. On the other hand, MELCOR has relative error of 67% [3]. Therefore, application of the CNAFT model can provide higher accuracy of flammability prediction on default MELCOR model.

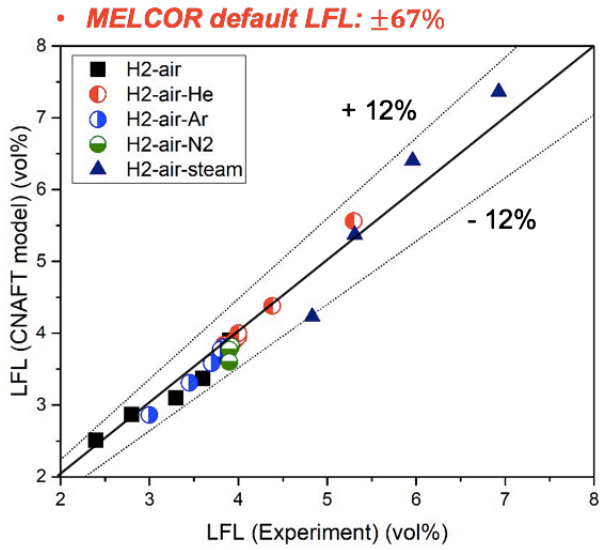

Figure 1. Linear relationship between LFL with CNAFT model and experiment result [3]

2.2 Flame acceleration

FA is phenomenon that may occur after combustion event under certain conditions. If FA occurs, it may lead to DDT, which gives critical damage on surroundings. Even it is important to figure out whether FA occurs or not, there is no model to predict occurrence of FA in MELCOR [2].

Because of its possibility to be developed into DDT, it is important to estimate whether the flame would accelerate fast enough and result in fast turbulent combustion event, such as sonic or choked flames. Among different parameters that affect possibility of FA event, experimental results showed that L/δ, ratio of integral length scale of turbulence to laminar flame thickness, and σ, ratio of densities of reactants and products (expansion ratio), are the main factors that defines flame acceleration rate [4]. However, in a large scale, σ is the value that gives dominant dependency on the type (slow or fast) of final regime of flame [4]. Therefore, criterion of FA can be suggested as [4]:

$$\sigma > \sigma^*(\beta, Le) \quad (3)$$

where σ^* is critical expansion ratio, a function of β, Zeldovich number, and Le, Lewis number. It is expected that the model is plausible to predict the occurrence of FA as part of hydrogen risk analysis.

2.3 Deflagration to detonation

Criteria of DDT for practical applications can be obtained by separating DDT as different phases. DDT consists of two phases, generation of localized explosion and onset of detonations [4]. Second phase, the onset of detonation is influenced by several factors. The criteria introduced below are conservative enough because the criteria are not a complete set [4]. Therefore, even the provided criteria are satisfied, possibility exists that DDT may not occur.

Criteria of initiation of phase 1 consists of fast flame requirement. Fast flame requirement implies that the flame should accelerate fast enough to result in 'choked' or 'sonic' combustion regime for phase 2 [4]. Because of its characteristics, FA criterion can be used for the phase 1 [4]. Onset of detonation can be modeled with detonation cell size, λ, to characterize the sensitivity of the mixture to detonation initiation [4]. With assumptions of uniform volumetric energy content, typical fuel-air mixture, and detonation initially developed as planar wave, detonation onset was estimated to be about 7 λ [4]. To formulate criterion for the onset of detonations, it is necessary to know characteristic geometrical size, L_c [4]. If 7 λ is smaller than L_c, then it can be judged that DDT may occur [4].

3. Simulation and results

3.1 Post-processing tool

As a part of development of post-processing tool, an open source tool is under modification. An open source tool called readptf is a Linux based tool first created by a researcher Vokáč from Czech Republic [5]. Original intention of the tool was extraction of intended data out of plot file of MELCOR under Linux platform computer [5]. By modifying source code of readptf, it would be possible to extract required data out of MELCOR plot file to perform hydrogen risk analysis.

Other part of the post-processing tool is actual simulation of hydrogen risk analysis with the extracted data out of plot file. The extracted data and nodalization of nuclear power plant will be used as initial input for the analysis. The extracted data, which would be different gas released to containment over time, will be used for calculation of possibility of combustion event. If possibility of combustion event is detected on a certain control volume, occurrence of flame propagation, FA, and DDT will be checked. If DDT occurs, then it can be judged that the containment is not intact anymore and no further analysis would be performed. If DDT does not occur, resultant temperature and pressure would be different after the FA event or deflagration event [4].

Therefore, even occurrence of FA only without DDT may be violence of nuclear safety act [6]. Besides, if deflagration occurs without FA event, propagation direction would vary depending on hydrogen concentration. After verification of events that may occur in initiating control volume, further risk analysis will be conducted on adjacent control volumes depending on resultant propagation direction. The simulation would be performed over the initial SA analysis simulation time or time until DDT occurs. With the hydrogen risk analysis, it would be able to obtain detailed hydrogen behavior sequence including combustion, FA, and DDT in each control volume. Currently, only preliminary analysis of flammability limit is conducted. FA and DDT analysis are needed as future tasks.

3.2 Preliminary results

A preliminary analysis of an accident scenario indicates that hydrogen behavior analysis may be much accurate with the post-processing tool. A preliminary analysis was conducted for OPR1000 under SBO scenario with MELCOR 1.8.6 code. During the accident sequence, large amount of hydrogen gas was released to reactor cavity. Figure 3, hydrogen concentration on a single control volume over time, is shown below. The graph tells how much hydrogen will be remaining without any combustion event because burn package for hydrogen risk analysis was not turned on during simulation. Figure 4 is graph of CNAFT of gas mixture in same control volume over the same time. Based on ignition criteria of MELCOR, flammable gas mixture exists almost for an hour. However, CNAFT model indicates that based on theoretical flame temperature, flammable gas mixture exists for less than a quarter of an hour. Therefore, the roughly estimated flammable region on the figure 3 becomes much narrower with advanced flammability estimation model, CNAFT model.

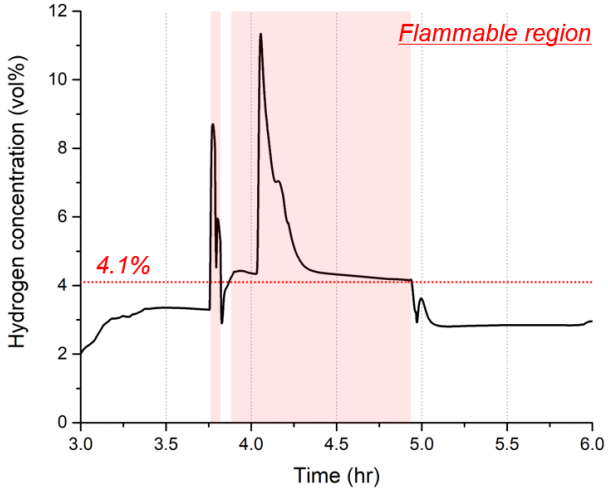

Figure 3. Hydrogen concentration limit over time with flammable region based on MELCOR code

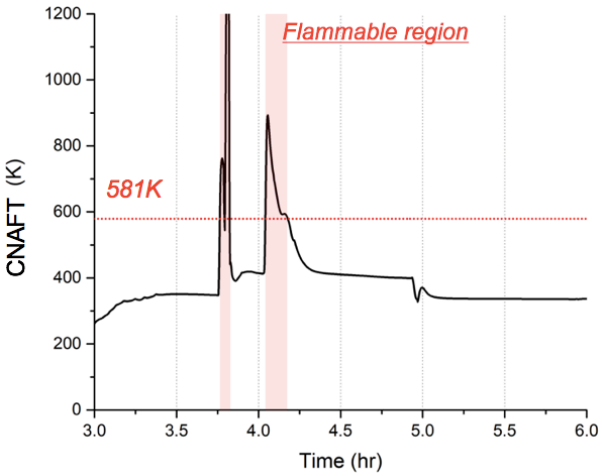

Figure 4. CNAFT over time with flammable region based on CNAFT model.

4. Conclusions

In this study, physical models of flame propagation, FA, and DDT were introduced. With comparison between the CNAFT model and models in MELCOR, benefit of having CNAFT model for higher accuracy could be observed. Besides, by modifying open source post-processing tool of MELCOR plot file, data extraction can be done for production of input file. The produced input file can be used for further hydrogen risk analysis such as one introduced as a preliminary result. Major findings can be summarized as follows.

(1) CNAFT model can predict flammability limit depending on change in concentration of diluents when MELCOR has a fixed value of hydrogen concentration as a criterion.
(2) FA can be predicted with σ, expansion ratio by comparing it to the critical expansion ratio.
(3) 7 λ method can be used to predict possibility of DDT. The method includes possibility of not having DDT event, so it can be judged that the method is conservative.
(4) Post-processing tool is able to extract data out of MELCOR output for hydrogen risk analysis.
(5) Result of preliminary analysis indicates that the modeling is effective enough to remove overly conservative analysis done by MELCOR.
(6) Supplemental preliminary analysis of FA and DDT with the physical models, and further development of the post-processing tool are left as future work. Because FA is not modeled in MELCOR at all, precision of the DDT model would be compared with MELCOR result and experiment results.

If development of the code is complete with adjustment on the models for combustion step, assessment of the its ability to accurately conduct hydrogen risk analysis can be accomplished. After

development of the code is done, future work would be comparison of the code with other hydrogen risk analysis software. With a single output from a lumped-parameter code for SA analysis, the different hydrogen risk analysis method can be used to assess ability of the post-processing tool.

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