CALCULATION OF THE PROBABILITY OF DDT DURING SEVERE ACCIDENTS

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ABSTRACT

In this paper, we are proposing a method to quantitatively calculate the likelihood of hydrogen explosions in the form of DDT (Deflagration to Detonation Transition) during a severe accident. Determination of the probability of the DDT during severe accident scenarios thus far has been subjected to qualitative expert opinions. There have been no proposed quantitative methods to calculate such probabilities to the best of the authors' knowledge. The proposed method enables the quantification of probabilities of DDT for any given severe accident sequence that can be simulated by a severe accident analysis code. Different accident sequences will have different characteristics of cladding oxidation, hydrogen production rate and hydrogen release rate, and therefore will have different probabilities of DDT. The proposed method can be used to objectively and quantitatively differentiate the DDT probability of different scenarios due to impacts of equipment availability or operator actions. The proposed definition of DDT probability is intended for two applications. First is the application in PSA level 2 assessments. The second potential application is to help assess the explosive conditions in the reactor building of Fukushima Daiichi units 1 and 3.

KEYWORDS
Hydrogen Explosions DDT Severe Accident Fukushima

1. INTRODUCTION

In this paper, we are proposing a method to quantitatively calculate the likelihood of hydrogen explosions in the form of DDT (Deflagration to Detonation Transition) during a severe accident. Determination of the probability of the DDT during severe accident scenarios thus far has been subjected to qualitative expert opinions. The method of Sherman and Berman [1], which gives the probability of DDT, requires qualitative engineering judgment that could be very subjective. There have been no proposed quantitative methods to calculate such probabilities to the best of the authors' knowledge. The proposed method enables us to quantify a probability of DDT for any given severe accident sequence that can be simulated by a severe accident analysis code. Different accident sequences will have different characteristics of cladding oxidation, hydrogen production rate and hydrogen release rate, and therefore will have different probabilities of DDT. The proposed definition of DDT probability is based on the physics of combustion and an assumption that random ignition is always present at any time as experienced in TMI-2 and Fukushima Daiichi accidents. MAAP analyses are used to simulate accident sequences and to calculate the 7λ criteria. The purpose of MAAP analyses is to determine the containment atmospheric conditions whether flammable or detonable conditions exist during the course of an accident. The concentrations of flammable gases depend largely on the balance between the generation and the consumption of combustible gases during individual accident scenarios. The 7λ criterion is the latest method proposed by an expert group commissioned by OECD/NEA that set the standard for DDT evaluation at present time

[2]. DDT conditions can be calculated at every time step of the accident simulation in every containment node. Here the DDT condition refers to the gaseous mixture that has compositions that meet the criteria of flame acceleration (FA) and the detonation cell size that allows DDT to develop within the characteristic length of the compartment. When the DDT condition is detected in the accident simulation, it means that all necessary conditions for DDT are present.

2. PROPOSED DEFINITION OF DDT PROBABILITY

The proposed definition of DDT probability is based on the physics of combustion that can be modeled in a severe accident code and an assumption that random ignition is always present with equal chance at any time. The probability that DDT occurs is simply assigned as 1 if only detonable conditions exist, i.e. there is a DDT time window that is long enough such that there is no question whether a random ignition is present or not. As shown in Figure 1, if a downwardly flammable non-DDT condition precedes the DDT window, the DDT probability is simply defined as a ratio of the DDT time window to the combined time of DDT window and the downwardly flammable non-DDT window. The downwardly flammable non-DDT conditions that precede the DDT window have a potential to consume the available combustible gases at that time and prevent DDT from occurring afterward. Hence, the preceding flammable non-DDT conditions reduce the probability of DDT during the DDT window.

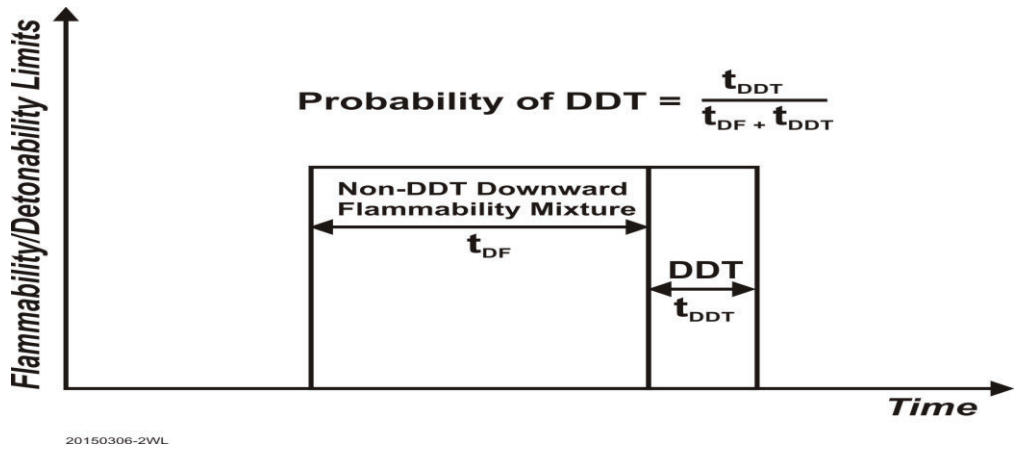

Figure 1. Proposed Definition of DDT Probability.

When DDT occurs, it shall be assumed that the containment will fail catastrophically. Hence, the DDT probability is also the probability of failing containment by DDT. That is, the DDT probability in any building node denoted by "i" according to our proposed definition is given by

$$P_{DDT,i} = \frac{t_{DDT,i}}{t_{DDT,i} + t_{DF,i}}$$

where $t_{DDT,i}$ = DDT time window for node i during which continuous detonable conditions exist
$t_{DF,i}$ = Deflagration time window for node i during which continuous downwardly flammable conditions in node i exist before the onset of the DDT window

The DDT probability is calculated based on the time ratio of detonable mixture conditions. There is no knowledge about ignition sources that can ignite these mixtures. However, it is simply assumed that there is equal likelihood of random ignition over the flammable or detonable periods for the purpose of expressing the probability. Since DDT conditions can occur globally or locally the definition given above

may be applied to either global or local conditions of the containment. However, it is more likely that DDT occurs locally due to local release and accumulation of hydrogen.

3. SEVERE ACCIDENT CODE SIMULATION OF HYDROGEN GENERATION, DISTRIBUTION, AND CONSUMPTION

The proposed approach for the DDT probability requires information of local and global gaseous compositions, pressures and temperatures of the reactor containment during a severe accident. This information can be provided by a simulation of a severe accident scenario of interest with a severe accident code such as MAAP [3], MELCOR [4], SAMPSON [5] or ASTEC. The information will be used for determination of downwardly flammable time window and DDT time window.

In this paper, MAAP5 is used to simulate selected accident sequences. The purpose of severe accident analysis is to determine the containment atmospheric conditions and whether flammable or detonable conditions exist during the course of an accident. The concentrations of flammable gases depend largely on the balance between the generation, the consumption, and transport of combustible gases during individual accident scenarios. The MAAP code simulates the core melt process and generates the hydrogen source terms to the containment. The distribution of hydrogen in the containment will depend on the details and how the containment is partitioned into sub-compartments in the input. The simulation should be as realistic as possible with regard to mechanisms that consume combustible gases. The following models and assumptions are made to reflect the physics of the phenomena in the accident simulation.

1. For plants designed with ignition systems, if the system is available during severe accident, hydrogen would be burned as soon as the lean flammability limits are met. Thus the concentrations of hydrogen will be maintained on average at the lean upward flammability limits. However, depending on the hydrogen release rate and location, a locally high concentration may exist. For the purpose of DDT probability calculation, the ignition system will be assumed to be unavailable during the accident time period of interest.

2. Random ignitions did occur inside the containment during the TMI-2 accident [6] and inside the reactor buildings of unit 1, 3 and 4 during the Fukushima Daiichi accidents [7]. Random ignitions will not be simulated in the analysis. Combustible gases should not be consumed by random ignitions in the simulation so that time-dependent probability of DDT can be calculated for the entire accident time. For each DDT probability calculated as a function of time, random ignition is implicitly assumed but without actual burning in the simulation. This is the same as saying that random ignition is present at any point in time and at equal probability over the entire accident time.

3. Combustible gases such as hydrogen (and carbon monoxide if molten core concrete interaction (MCCI) occurs) should be consumed by passive auto catalytic recombiners (PARs) as realistically as possible in the simulation if PARs are available in the plant design. PAR is a hydrogen control device designed to operate by recombining hydrogen and oxygen molecules on the catalyst surfaces at H_2 concentrations below the lean flammability limits. With this the impact of PARs during a severe accident on reducing the DDT probability can be studied by comparing the calculated DDT probability.

4. PAR-induced ignition is a real physical phenomenon that should also be simulated. At hydrogen concentrations even slightly higher than the lean flammability limit, PARs can become overloaded. The catalysts can heat up excessively, and ignite the hydrogen mixture nearby the PAR outlet

opening. The ignition is caused by the high temperature of the catalysts that serve as ignition sources. At moderate H_2 concentrations, the combustion can be a benign deflagration causing a moderate pressure transient with no damage to the recombiners. Experimental data on the conditions that lead to PAR-induced ignition are available to allow realistic simulation. PAR-induced ignition has been observed in several experiments including (1) HR Test series in the OECD Thai program [8], (2) H2PAR program conducted by IRSN [9], and (3) KALI-H2 program conducted by CEA [9]. According to the HR tests, the minimum H_2 required for ignition by PAR was 6.9% H_2 with 0% steam, and 8.3% H_2 with 45% steam. The line connecting these two points on the flammability limit diagram is shown in Figure 2. The line defines the PAR-induced ignition limits on the flammability limit diagram based on the HR test data. According to the H2PAR and KALI-H2 test data (which is summarized in [9]), PAR-induced ignition was observed at the following mixture concentrations: (1) between 5.5%-6.8% H_2 in dry air, (2) 8.5%H_2 with 9.2%H_2O, (3) 8.6%H_2 with 31%H_2O, and (4) 10%H_2 with 45%H_2O. These data points are plotted on the flammability limit diagram in Figure 2. Also shown in this figure is the PAR-induced ignition limits calculated by the SPARK code for the complete range of the flammability diagram. Ignition conditions are very close to downward flammability limits and below the conditions for DDT. This should lead to a deflagration that will consume substantial amount of hydrogen and reduce the DDT probability.

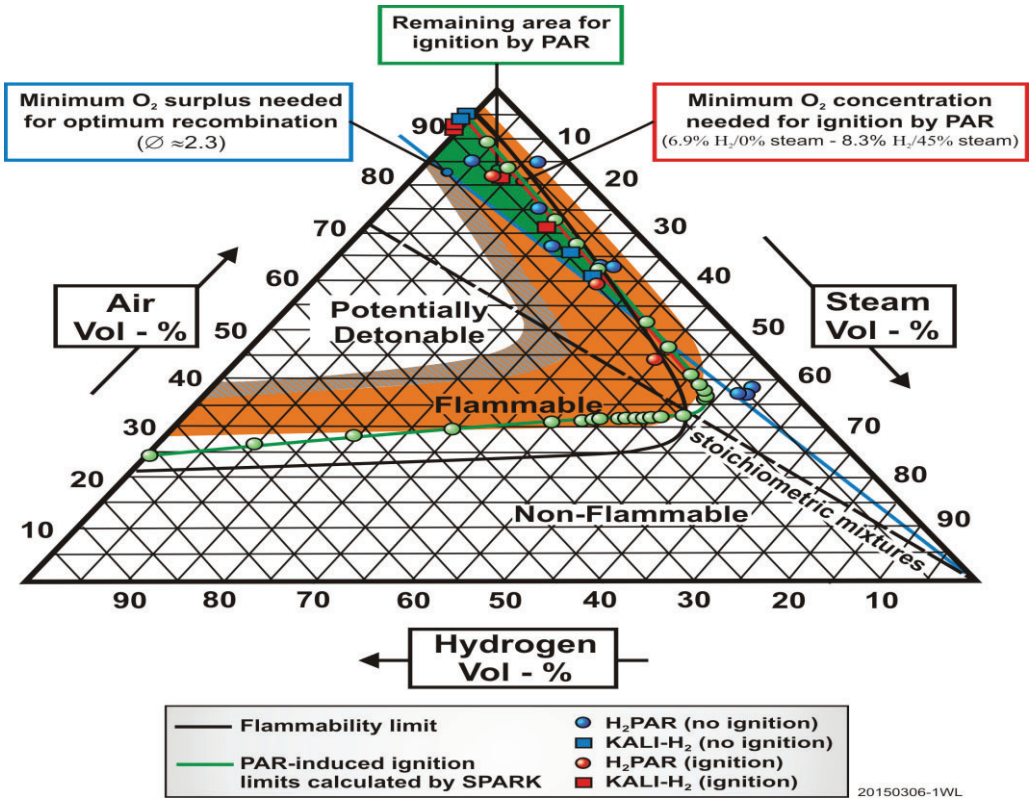

Figure 2: Flammability Limits [8] and PAR-induced Ignition Limits [9].

5. Another requirement for PAR-induced ignition is the oxygen surplus [8]. It was concluded from the HR test data that for PARs to have optimal performance (which corresponds to high catalyst temperatures), the oxygen surplus factor which is defined as $\varphi=2(O_2\% / H_2\%)$ must be at least 2.3.

When the oxygen surplus factor φ = 1, i.e. when the mixture is stoichiometric, the PAR performance falls below 50% of the PAR performance when φ=2.3. The low performance corresponds to low catalyst temperatures due to low recombination rates. This criterion becomes important for accident sequences where the oxygen concentration has been substantially reduced by PARs to the extent that the original composition of air is highly distorted and that PAR-induced ignition may no longer be likely due to oxygen starvation.

6. The potential of PAR-induced ignition in the presence of H_2 and CO was also observed in the more recent experiments performed at JÜLICH for PAR performance test in the presence of CO [10]. It was found that the efficiency of CO recombination in terms of molar rates is significantly smaller (by about a factor of 2 depending on flow rate) than the corresponding H_2 conversion efficiency. It was also found that due to exothermic reactions, the parallel CO/H_2 conversion at a combined 4%CO and 4%H_2 concentration produced high catalyst temperature sufficient for ignition. The catalyst temperatures increased as CO concentration was added to the constant 4%H_2 mixture. The maximum catalyst temperature was 772°C.

7. Self-ignition (or auto-ignition) at high temperatures of hydrogen mixture is another relevant combustion phenomenon for the accident simulation. However, temperature and required hydrogen concentration at which auto-ignition occurs is not very well defined and that large variations exist in reported data. Most auto-ignition temperatures were quoted without specifying hydrogen concentration. At high temperatures but not high enough for auto-ignition, experiments showed that hydrogen oxidation in air occurs in the absence of ignition sources. Slow chemical reaction between hydrogen and air occurred at temperatures of 500°C for lean mixtures [11] and as low as 300°C for H_2-rich mixtures [13]. For example, reduction of hydrogen concentration from 50 to 44 percent hydrogen, and from 15 to 11 percent hydrogen, were observed on a time frame of minutes at 377°C [12]. At sufficiently high temperature, the mixture would "auto-ignite" on a short time frame. According to experiments performed by [13], auto-ignition could occur at 12.5%H_2 at 714°C. At higher H_2 concentration (into the detonable regime), auto-ignition could occur even at much lower temperatures. From the simulation point of view, it is more realistic to model the consumption of hydrogen by slow oxidation at temperatures and concentrations below the criteria for auto-ignition at 12.5% combined H_2+CO and 714°C. The auto-ignition temperature of CO in air with some moisture is about the same as that of hydrogen [14]. It is reasonable to assume that the auto-ignition temperature of the H_2/CO mixtures formed in the reactor cavity during MCCI is similar to that of the hydrogen mixture.

8. Hot corium surface and hot flying corium particles during MCCI are potential ignition sources. Corium surface temperature in the cavity of at least 800°C is required for auto-ignition in the cavity. The surface temperatures of these hot objects can be well above the auto-ignition temperatures. The required surface temperature for ignition can be derived from the NRC-sponsored experiments performed at Sandia National Laboratories for testing the thermal igniter performance [15]. It was found that the glow plug igniter consistently ignited mixtures at surface temperatures between 700°C and 800°C with the upper value corresponding to the higher temperatures necessary to ignite mixtures with steam. It is reasonable to assume that the hot surface temperature required for ignition is at least 800°C in the simulation.

9. When calculating detonation cell widths of a H2-CO mixture, one mole of carbon monoxide can be treated as if it is one mole of hydrogen [14]. A significant amount of carbon monoxide can be generated during severe accidents from interactions of ex-vessel molten core with limestone-sand concrete in the reactor cavity. During this phase of an accident, the combustible gases will be mixtures of hydrogen, carbon monoxide, steam and air. In the OECD-sponsored study of

combustion characteristics of H2-CO-air mixtures [14], it was found that for a given total concentration of H2-CO in the mixture, the detonation cell width of the H2-CO mixture is about the same as the detonation cell width of the H2-only mixture with the same total fuel concentration. In other words, these results show that a mole of CO can be treated approximately as if it is a mole of H2 in the detonation cell width calculation.

4. DDT EVALUATION METHODS

Two methods for DDT evaluation have been proposed. The older method of Sherman and Berman [1] which assigns the probability of DDT in five categories, i.e., DDT is highly likely (p=0.99), DDT is likely (p=0.9), DDT may occur (p=0.5), DDT is possible but unlikely (p=0.1), and DDT is highly unlikely to impossible (p=0.01). This method classifies the combustible gaseous mixture into five mixture classes based on detonation cell widths. The method also classifies the compartment that contains the combustible mixture into five geometric classes according to the degree to which the geometry of the compartment and obstacles inside it promote flame acceleration. Large but confined geometries with obstacles in the path of the expanding unburned gases are considered most favorable for flame acceleration. If transverse venting is added to the above path, it is considered a feature that hinders flame acceleration. If obstacles are removed from the path, the geometry is considered neutral to DDT. Large volumes with hardly any obstacles and large amount of venting transverse to the flame path are classified as unfavorable to flame acceleration. Last but not least, a totally unconfined geometry at large scale is classified as so unfavorable to flame acceleration. Based on which mixture class and which geometric class are assigned to the conditions of interest, one of the five DDT probability categories is assigned. The problem and the difficulty with this method lie in the determination of geometric class which requires too much qualitative engineering judgment. Actual plant geometries can be very complicated such that subjective judgment by different people can lead to diverse answers.

The more recent method proposed by an expert group commissioned by OECD/NEA. The group issued the so-called "State-of-the-Art Report (SOAR) on Flame Acceleration and Deflagration-to-Detonation Transition in Nuclear Safety" that set the standard for DDT evaluation at the present time [2]. The SOAR approach is based on theoretical consideration and experimental data on flame acceleration (FA) and deflagration to detonation transition (DDT) up to the year 1999 with most experiments performed from 1993 to 1999. The SOAR approach is the work of an international group of 11 highly respected hydrogen safety experts collaborating under the OECD NEA program. The SOAR approach is supported by extensive experimental data performed with large scale geometries in the 1990s. It is important to realize that the detonation cell width approach based on literature up to the 1980s is not the same as the SOAR approach. The SOAR approach uses a σ-criterion for flame acceleration and a 7λ criterion for DDT as pre-requisite conditions. The σ-criterion is a measure of mixture reactivity to promote flame acceleration. σ refers to an expansion ratio defined as unburned-to-burned mixture density ratio. The expansion ratio must be greater than the critical expansion ratio ($\sigma_{critical}$) for flame acceleration (which is a prerequisite to DDT) to occur. While the expansion ratio represents the reactivity of the mixture, the critical expansion ratio is regarded as a boundary between slow flames and fast accelerated flames. The critical expansion ratio is a function of temperature. The critical expansion ratio decreases with increasing temperatures. The detonation cell width (λ) is a basic parameter used for characterizing the sensitivity of a mixture to detonation initiation. The 7λ criterion is a measure of the effect of scale on the detonation onset. Experimental data performed extensively in the 1990s to support the SOAR report generally showed a good agreement with the 7λ criterion over a wide range of scales and mixture compositions. Both criteria are as necessary conditions for onset of DDT. Meeting or exceeding these criteria does not necessarily result in DDT. The criteria are only necessary conditions. The criteria are not sufficient conditions for DDT. Using this methodology for quantifying DDT likelihood is the same as assuming that these criteria are sufficient conditions for the onset of DDT.

As with any engineering correlation or methodology based on test data, there is uncertainty (not error) in the SOAR approach. The SOAR approach as it stands now is the industry standard for evaluating hydrogen risk for probabilistic safety assessment. The major uncertainty lies in how to define the characteristic length L that will be used to compare with 7λ. The DDT criterion is that L must be greater than 7λ. The characteristic length of a compartment is a very important parameter required in the 7λ criterion. Characteristic length in the context of the 7λ criterion refers to the distance available while the 7λ length refers to the minimum distance required for DDT propagation. Determining characteristic length of the compartments of a nuclear plant can be quite ambiguous because of the complex geometry of the plant. The rules for determination of characteristic size for a lumped-parameter code approach are given in Appendix F of the SOAR report [2]. In these rules, 4 simple shapes of rectangular boxes including long box, flat box, tall box and cubic box are used to characterize the geometrically complex compartments found in the containment. For compartment that can be flooded with water, actual compartment height, determined by taking into consideration the water height in the compartment, should be used. Due to the complexity of the containment geometry, rather than deciding the shape of an individual compartment and calculating the characteristic length, a simple approach can be taken such that the characteristic lengths of all 4 shapes are first calculated and the maximum is selected as the characteristic length. The calculated characteristic length cannot be longer than the longest dimension of the compartment. The characteristic length is therefore determined according to this simplification of the geometry. As discussed above, the difficulty with the Sherman and Berman method is its dependence on qualitative judgment of the geometry whether the geometry favorable to flame acceleration or not. The SOAR method removes this difficulty by quantitatively determining the characteristic length of the compartment.

The overall DDT criteria to be used in the analysis are the 7λ criterion and the σ criterion: both must be satisfied simultaneously for the necessary conditions for DDT, i.e.

$$\text{Characteristic length } L > 7\lambda \text{ and expansion ratio } \sigma > \sigma_{critical}$$

When the DDT condition is detected in the accident simulation, it means that all necessary conditions for DDT are present. Whether or not the condition is sufficient for DDT is beyond the capability of the criteria. However, as a conservative approach, one may assume that the presence of DDT condition locally or globally in the containment means DDT will occur if ignited.

5. EXAMPLE

As examples, the proposed definition is applied to severe accidents in a typical 1000 MWe PWR with a large dry containment. The first example assumes failure of core cooling during a hot shutdown that leads to core melt, vessel failure, and MCCI. A large amount of hydrogen gas was produced but the containment atmosphere was inert by steam. Late into the accident long after vessel failure, containment spray actuation was assumed to reduce containment pressure by condensation of steam, and the cavity was eventually flooded by spray water. Figure 3 shows gaseous volume fractions of steam, H_2, CO, and O_2 as a function of time for the case when the cavity is flooded by spray water. Figure 4 shows gaseous volume fractions of steam, H_2, CO, and O_2 for another case when the cavity flow path does not allow cavity flooding by spray water. The DDT probabilities calculated and monitored for more than 3 days for each case are also shown in both figures. For the flooded cavity case, the DDT probability changes from zero to non-zero values when H_2 volume fraction increases to 14% while steam volume fraction (which is high initially) decreases to 15%. The DDT probability increases to a value of 0.75 after 3 days

into an accident as an ultimate result of a large amount of combustible gases (mostly hydrogen) generated from MCCI in a basaltic concrete.

However, for the case when the cavity is assumed not to be flooded by spray water and to remain dry under MCCI conditions, the molten debris pool remains very hot inside the cavity. The MCCI-driven molten debris pool can generate hot "flying particles" through the gas bubbling and melt eruption process [16]. These hot particles are assumed to ignite the flammable gas mixture formed in the cavity. This process can potentially continue until sufficient amount of oxygen has been consumed to the point of the containment-wide oxygen-starved condition. As a result, the DDT probability remains zero through the entire accident sequence (Figure 4). This example demonstrates that the concentration of combustible gases (which is produced by the MCCI process) is controlled to low levels by the high temperature nature of the MCCI process itself provided that the cavity flow paths are not too restricted to allow oxygen to be brought to the cavity from the rest of the containment. There is uncertainty in the combustion mode over the MCCI molten debris. The combustion mode assumed in this study is multiple hot-surface-induced deflagrations. However, burning as diffusion flames over the molten debris is also possible. In either mode, hydrogen would be consumed, and the trend would be the same.

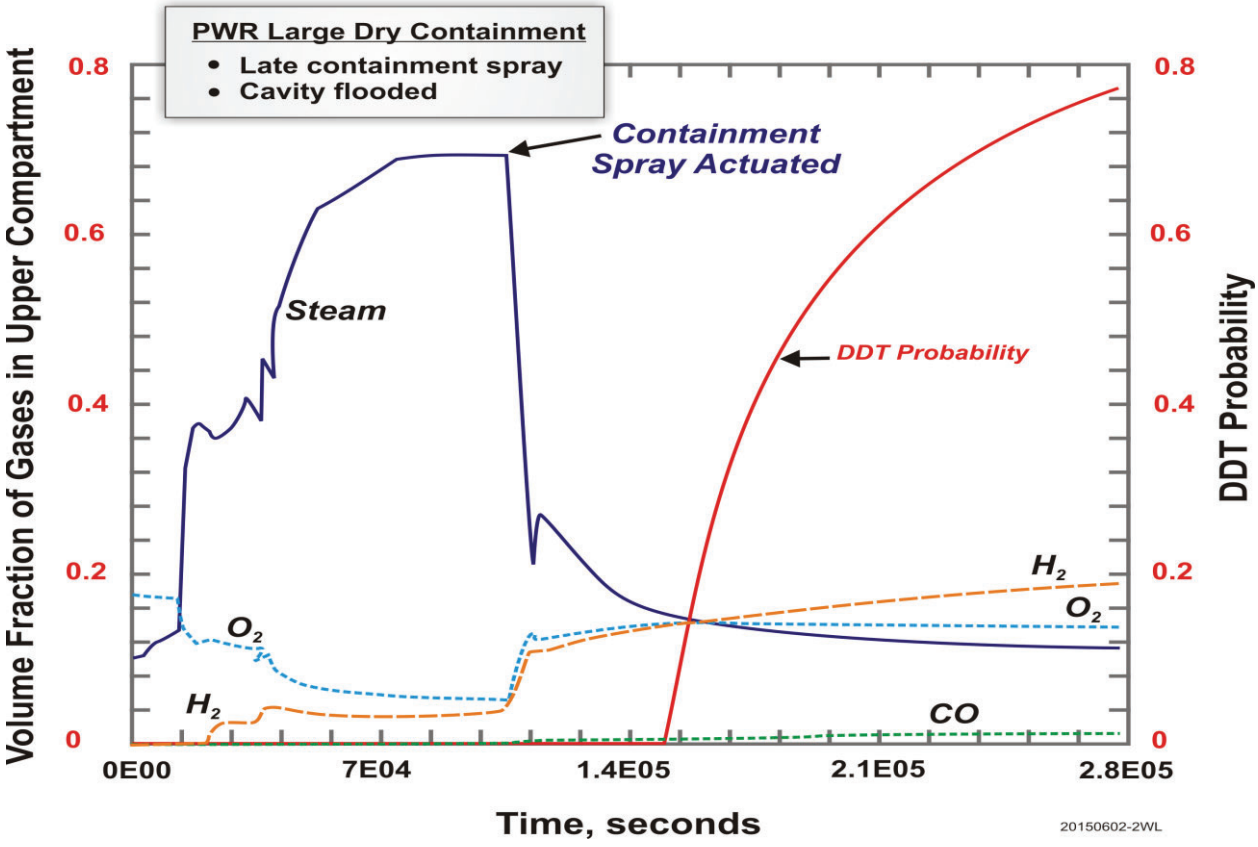

Figure 3: DDT Probability of Severe Accident Sequence in Example PWR with Flooded Cavity due to Late Containment Spray Actuation

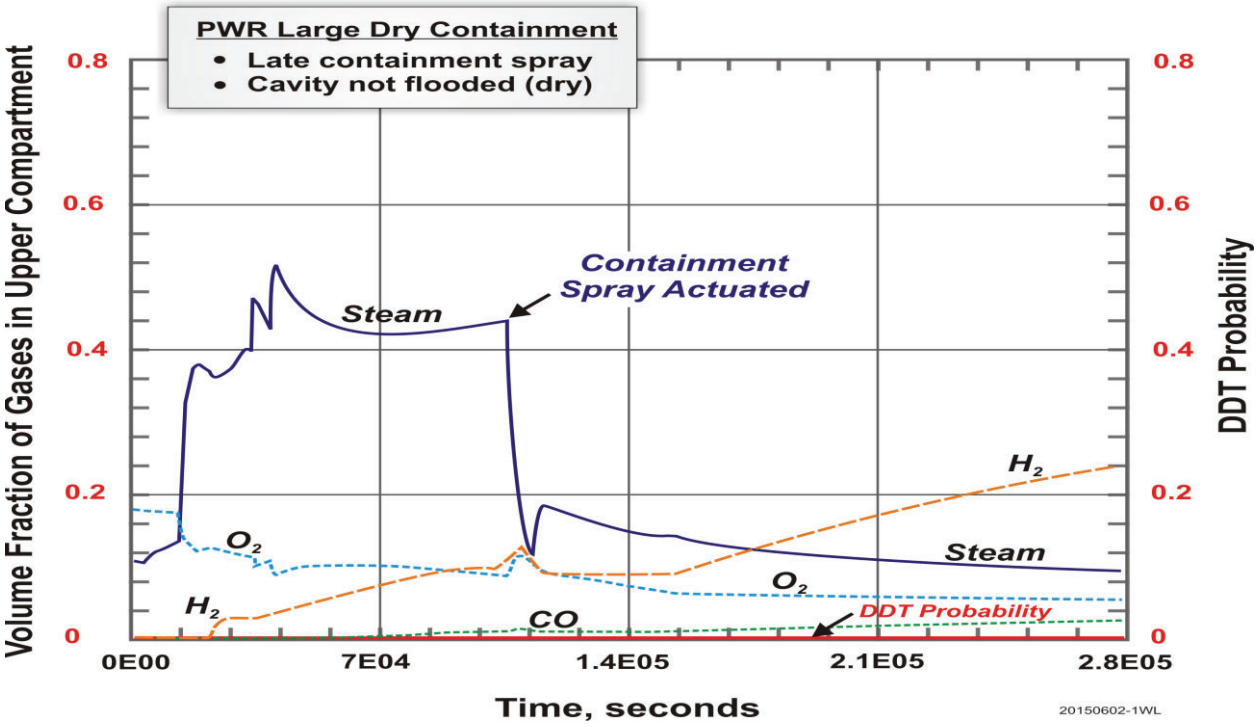

Figure 4: DDT Probability of Severe Accident Sequence in Example PWR with Late Containment Spray actuated but Cavity remained Dry

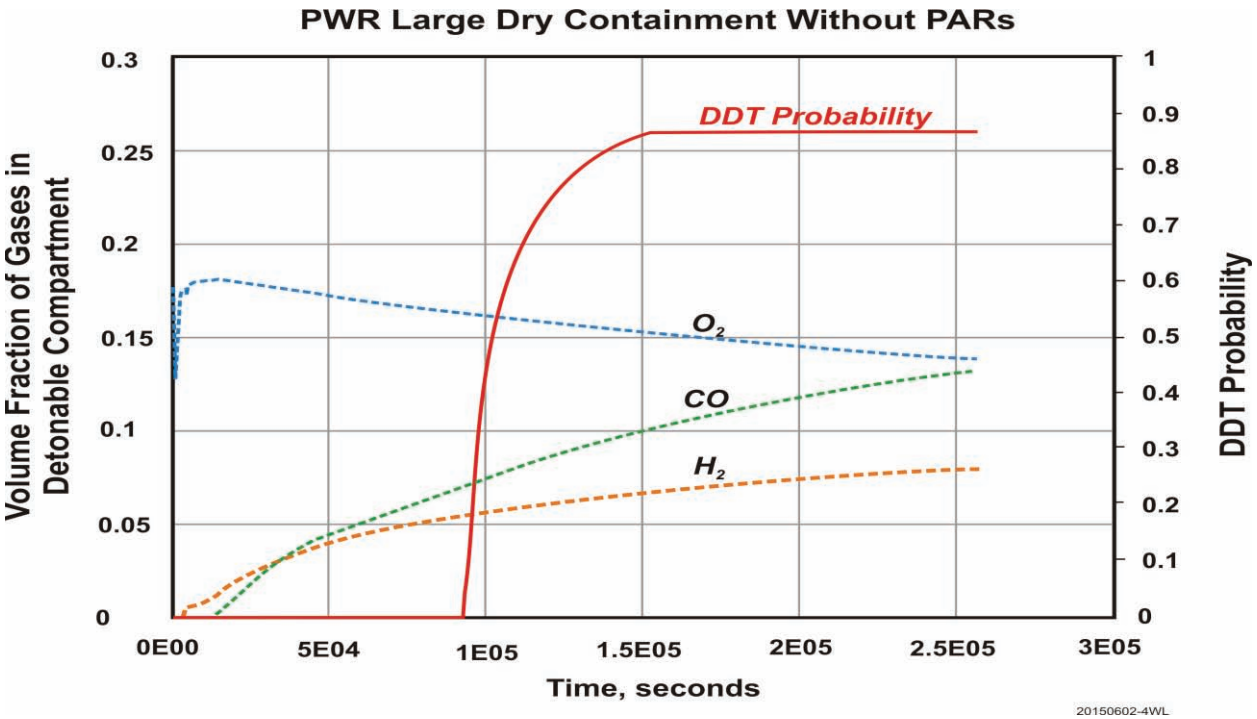

Figure 5: DDT Probability of Severe Accident Sequence in Example PWR without PARs

As another example, the proposed definition is applied to a simultaneous large LOCA and SBO accident in a larger PWR with a large dry containment. The accident leads to core melt, vessel failure and MCCI with limestone concrete in the cavity. In this case, a large amount of CO and lesser amount of H_2 are generated. The DDT probability was calculated and monitored for 3 days. The DDT probability peaks at a value of 0.866 as an ultimate result of a large amount of combustible gases generated from MCCI (Figure 5). The time when the peak value of 0.886 is attained corresponds to the time when the detonation cell width has increased beyond 2 m, the size over which DDT was never observed in any experiments [2]. It is used in this study as a detonation cell width cutoff criterion. The detonation cell width decreases and increases forming a U-shape during the time when DDT probability rises from zero to the peak value. The decrease in detonation cell width is due to an increase in combustible gas concentrations, while the increase is caused by an increase in containment pressure which increases about 0.8 bar to a total pressure of 5.5 bars during the time period.

However, when the plant is assumed to be equipped with a reasonable number of PARs commensurate with severe accident considerations (such as ~ 50 kg-mole/hr of combustible gas generation rate from MCCI), the calculated DDT probability turns out to be zero (Figure 6). In this example, CO is not modeled to be oxidized to CO_2 by PARs. If CO oxidation is modeled, CO concentration would be less than what is shown in Figure 6, and H_2 concentration would be higher.

It is well known that the hydrogen recombination rate of PARs is too slow to cope with the extremely fast zirconium alloy-steam reaction rate (say, ~0.3 kg/s or more) during the core melt process. This second example demonstrates that PARs has a potential to control combustible gases generated from the MCCI process to the levels where DDT is not possible. The generation rate of combustible gases from the MCCI process is not too fast and can be coped with by the recombination rates of PARs.

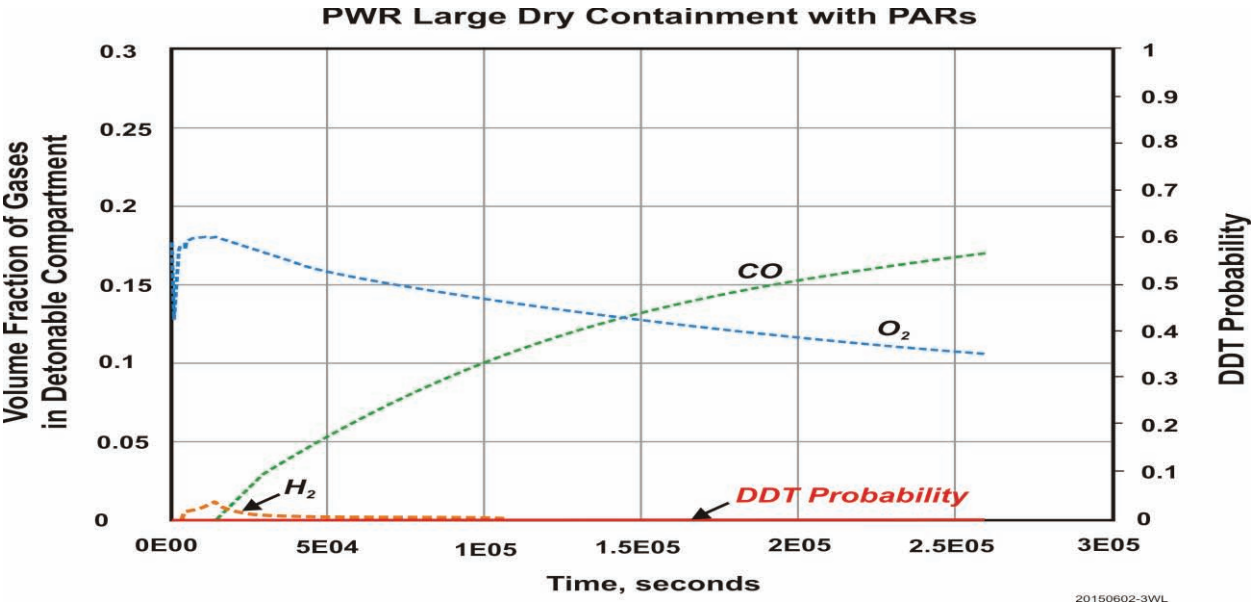

Figure 6: DDT Probability of Severe Accident Sequence in Example PWR with PARs

6. SUMMARY

The proposed definition of DDT probability in combination with realistic severe accident simulation is intended for two applications. First is the application in PSA level 2 assessments. In the past practice, the probability of DDT has been subject to qualitative engineering judgment and the overall results are likely inconsistent. The proposed definition is quantitative and objective and is entirely based on simulation of accident scenarios using a severe accident code that calculates the accident conditions as mechanistically as possible using the SOAR method to quantitatively calculate the DDT limits.

The second application of the proposed definition is to help assess the explosive conditions in the reactor building of unit 1 and unit 3 of Fukushima Daiichi reactors. The hydrogen explosion in unit 3 reactor building was very different from the explosion in unit 1. The explosion in unit 1 was directed horizontally from the top floor of the reactor building. Building roof and sidings were blown away by the explosion but concrete pillars remain intact with little damage. The explosions in the unit 3 were quite different and highly energetic. There appeared to be (from video recordings) at least two explosions. The first one was less energetic and directed horizontally (similar to that of unit 1). The second one was directed vertically with an almost perfect spherical fireball appearing above the building and shooting up very high into the sky. Large chunks of materials appeared to be carried up high with the fireball. Opposite to unit 1, the concrete pillars on the building top floor as seen from pictures were highly damaged. Several accident analyses using MAAP [17, 18], MELCOR and SAMPSON have been performed for unit 1 [19, 20, 21] and unit 3 [22, 23, 24, 25]. These analyses focus on the conditions of the reactors and the primary containments. Leakages to reactor buildings have not been part of the analyses yet. There are also still many uncertainties in the analyses before meaningful explosive conditions in the reactor buildings can be recreated.

The proposed definition can be used to objectively and quantitatively differentiate the DDT probability of different scenarios due to impacts of equipment availability or operator actions.

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