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CODE PACKAGE FOR ASSESSING THE POTENTIAL FOR DDT IN A POST-ACCIDENT NUCLEAR CONTAINMENT

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1 Introduction

The consequence of a potential hydrogen burn is a safety issue for nuclear containment [1,2]. There are two modes of hydrogen burn: deflagration and detonation. Direct initiation of detonation is very unlikely inside a containment building, since it requires high-energy ignition sources such as solid explosives. However, a detonation may occur via a transition from a deflagration. Deflagration to Detonation Transition (DDT) refers to the abrupt change in the mode of combustion from deflagration to detonation in the absence of a high-energy source. The magnitude of the shock waves associated with atmospheric H_2-air detonations are of the order of 15 atm (1.5 MPa). Such a strong blast wave may pose a threat to containment integrity. To assess the potential threat of a hydrogen burn in a post-accident containment, it is necessary to evaluate the potential or likelihood of a DDT under various accident scenarios.

The scenario of transition to detonation usually consists of a continuous acceleration of an initially slow flame to a critical speed at which the mechanism of propagation of the reaction front suddenly changes from a diffusion-controlled to a kinetically controlled process, auto-ignition via shock heating [3-5]. Experimental observations suggest that flame acceleration is an essential step in DDT. Detailed mechanistic models capable of predicting flame acceleration and subsequently transition to detonation have not yet been developed. To analyze the potential for DDT in a post-accident containment, analysts have to rely on a set of experimentally determined criteria as a guide. The paper describes a computer code package that uses these criteria to assess the potential for DDT under various accident scenarios. Sections 2 to 5 of this paper describe the theory of these criteria. Section 6 and 7 describe the application of this code.

2 Flame Acceleration and Transition to Detonation

A freely propagating flame strongly influences the flow conditions ahead of it. Its burning rate is then influenced by these flow conditions when it moves ahead into these regions [6-9]. When obstructions are present in the path of a propagating flame, turbulence will be generated as the unburnt gas flow (induced by the thermal expansion of the burnt gases) passes over these obstructions. The structure of this turbulence usually consists of large eddies characterized by the size of the obstruction [3]. As the flame front advances into this turbulent flow field, the initially smooth flame surface will be distorted. The distorted flame will now consume unburnt gas over a larger surface area, leading to an increase in the rate of heat release (i.e., a higher flame speed). This increase in the flame speed caused by turbulence increases the volumetric burning rate, resulting in a larger flow velocity of the unburnt mixture ahead of the flame. This in turn increases the turbulence, leading to an even higher burning rate. Thus, a positive feedback mechanism, coupling the flow velocity and the burning rate, is established. The interaction between the fluid dynamics and the combustion process can lead to a highly unstable situation, which may result in continuous flame acceleration to choking velocity or transition to detonation [3]. For a situation where the gas mixture is ignited by a weak ignition source such an electrical spark or a hot surface, the flame acceleration process is the controlling step in the transition to detonation.

2.1 Run-up Distance for DDT

The run-up distance (also commonly referred to as the transition distance or the induction distance) is defined as the distance between the ignition point and the location of DDT. This run-up distance is not an intrinsic property of the mixture; it depends on the size of the duct, the level of confinement of the surrounding walls, as well as the obstacle configuration used in the experiments [7]. The run-up distance, although not an intrinsic property of the mixture, can have significant implications in safety analysis. If it is possible to determine the minimum run-up distance for a certain mixture, this distance represents the critical cloud size required for DDT to occur. DDT can be precluded if the combustible cloud is smaller than this critical size. The challenge is to determine this minimum run-up distance.

Chan [10] reported the run-up distances for H_2-air-steam mixtures in a 28 cm diameter duct filled with obstacles. These results are summarized in Fig. 1. These experiments were performed in an apparatus which was designed to produce the highest rate of flame acceleration. It has been demonstrated that obstacles with a blockage ratio of 0.4 and spaced one tube diameter apart produce the highest rate of flame acceleration (block ratio = blocked area / total cross sectional area) [11]. Therefore, the results from these experiments, data shown in Figure 1, represent the shortest run-up distances of these mixtures.

These results suggest that the run-up distance is inversely proportional to the laminar burning velocity of the corresponding mixture [12]. In this series of experiments, no DDT was observed for mixtures of 30% or more steam by volume. The run-up distance derived from these experiments can be used to estimate of the critical (or minimum) cloud size required for DDT.

2.2 Scaling Parameters for DDT

The initiation of a detonation can be divided into two separate phases: 1) the creation of conditions for the onset of detonation and 2) the actual formation of the detonation wave itself. Processes in the first phase are scale dependent. They depend on the specific initial and boundary conditions of the problem. The actual formation of the detonation, on the other hand, appears to be more or less universal. It is from this first phase of onset of detonation that a scale limitation (a criterion for DDT) can be derived.

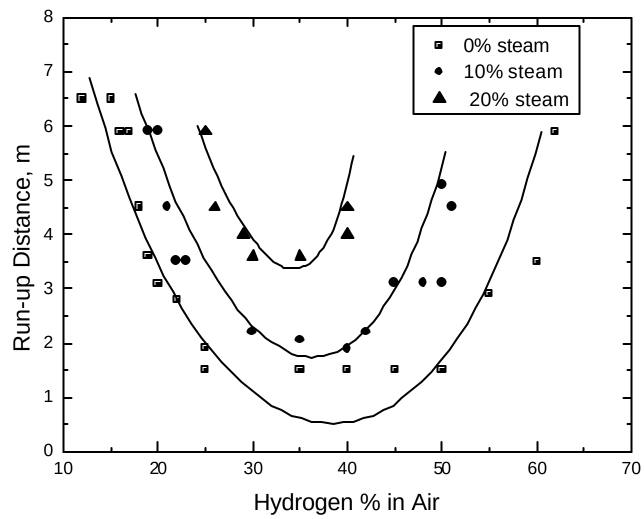


Figure 1. The Run-up Distance for Various H_2-air-steam Mixtures in a 28 cm Diameter Duct Filled with Obstacles (B.R. = 0.31) [10]

In order to formulate a criterion for onset of detonations, a definition of characteristic geometrical sizes L of an enclosure is necessary. The size L should be a macroscopic size of a sensitized mixture where a detonation wave might originate and develop. Dorofeev [14,15] has shown (Fig. 2 and Fig. 3) that the criterion for onset of detonation equires $L > 7\lambda$, where λ is the detonation cell size. This result suggests that a criterion $L = 7\lambda$ can be used as a conservative estimate for one of the necessary condition for DDT. Based on this observation, it is helpful to define a DDT Index, ϕ_{DDT}, for assessing the likelihood of a DDT. The DDT Index is the ratio of the two length scales L and L_m, where L is the dimension of the detonable cloud and L_m is the critical cloud size taken as 7λ. The value of the DDT Index indicates the possibility of a DDT. A DDT is possible for $\phi_{DDT} > 1$ and a DDT is highly unlikely or impossible for $\phi_{DDT} < 1$. The likelihood decreases as the ϕ_{DDT} value decreases.

3 Criteria for Flame Acceleration and Transition to Detonation

3.1 Criteria for DDT (the λ criteria)

The above methods were determined from tests with uniform mixtures. If the gas mixture is not uniformly mixed inside the containment building or a sub-compartment, the gas mixture inside this detonable cloud is not likely to be uniformly mixed either. To properly assess the likelihood of a DDT for an imperfectly mixed gas cloud, it is necessary to evaluate the DDT Index, ϕ_{DDT}, inside the cloud such that the DDT Index discussed earlier still applies.

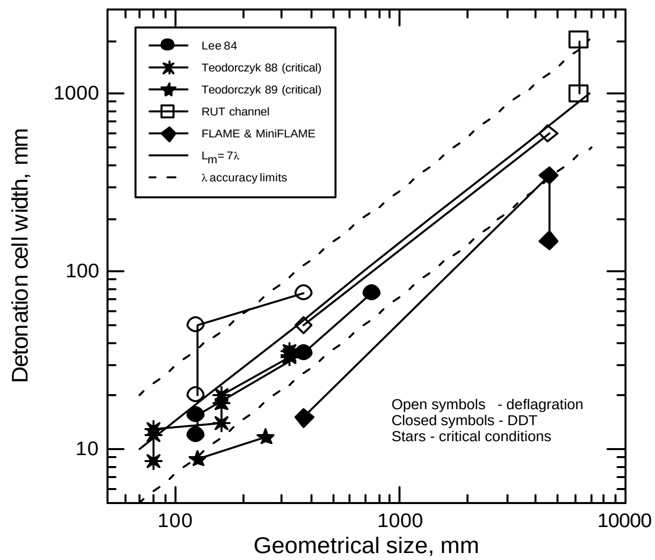


Figure 2. DDT Conditions in Channels (tubes) at Normal Initial Temperature [14].

For a non-uniform combustible cloud, it is difficult to directly apply the criteria for detonation onset that are based on detonation cell size λ. It is necessary, at least, to define what λ value should be used as a representative chemical length scale. One approach is to use the average cell size in a combustible cloud. Due to nonlinear behavior of the cell size on concentration, λ of an averaged composition <C> is usually smaller than the average cell size <λ>. Thus, the former (cell size of an average mixture) gives more conservative estimates for L/λ criterion.

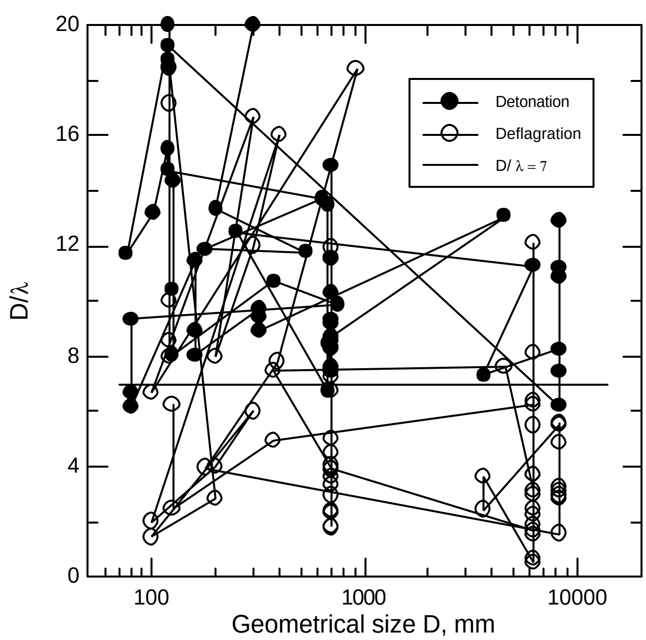


Figure 3. Summary of DDT Conditions in D/l , where D is the Characteristic Dimension of a Room [14].

If the gas concentration distribution is known, one can start from the cloud boundary with determination of a normal size (e.g. $L = V^{1/3}$) and the averaged cell size, and test the $L/7\lambda$ criterion for the cloud. This procedure can be repeated going into a smaller and more sensitive cloud. If at a certain stage the DDT Index is found to be bigger than 1, this means detonation is potentially possible inside this part of mixture if L is larger than the minimum run-up distance for the averaged mixture.

To apply the DDT Index requires identifying the envelopes for various hydrogen concentrations, calculating the volume of each envelope and determining the DDT Index for each envelope. DDT can be ruled out if the DDT Index is below unity for each envelope.

It should be noted that these solutions for a non-uniform mixture can be applied only as estimates. Although they are based on the DDT correlation from uniform mixtures, no direct experiments are available to verify them. It should also be noted that a DDT Index greater than 1.0 only indicates that DDT is possible, a necessary condition for DDT. It is not a sufficient condition.

3.2 Criteria for Flame Acceleration (the σ criteria)

The mechanism for flame acceleration is dominated by the product expansion in the burned gas. To develop the criteria for flame acceleration, it is important to estimate whether the flame is able to accelerate under given conditions resulting in fast turbulent combustion regimes (like “sonic” or “choked” flames). If these conditions are not met, flame acceleration can eventually result in a benign combustion and even flame quenching.

A series of tests was made recently to study systematically the effects of scale and mixture properties on the behavior of turbulent flames in obstructed areas [12, 13]. A set of parameters was chosen which can influence the flame-flow-flame feedback in obstructed area. It was found that whether a flame can reach supersonic velocities via flame acceleration depends on the expansion ratio (density of the unburned gas to the density of the burned gas), σ, and the Zeldovich number, β. The Zeldovich number is defined as

$$\beta = E_a(T_b-T_u)/(RT_b^2),$$

where E_a is the effective activation energy,
T_u is the initial unburned gas temperature of the mixture,
T_b is the burned gas temperature, and
R is the gas constant.

These two parameters appeared to be those defining the eventual flame velocity. It was found that with $\beta(Le-1) < -2$, (where Le is the Lewis number of the mixture, a ratio of the thermal diffusivity to molecular diffusivity) the borderline between slow and fast combustion regimes changes with the critical expansion ratio $\sigma*$ in the range of 2 to 3.75. For $\beta(Le-1) > -2$, the value of $\sigma*$ ranges from 3.5 to 4.

For mixtures typical for nuclear containment atmosphere (H_2-air-steam), hydrogen-lean mixtures are generally characterized by $\beta(Le-1) < -2$ and hydrogen-rich mixtures by $\beta(Le-1) > -2$. For H_2-lean mixtures, the eventual outcome of flame acceleration is expected to depend on β, and hence on initial temperature. For gas mixtures near room temperature (~ 300K), σ* is close to 3.75. For gas mixtures at 400K and 500K, σ* equals to 2.8 and 2.25, respectively. For hydrogen rich mixtures, the critical expansion ratio is not a strong function of temperature and has a value of 3.75.

The results of the previous consideration enable the construction of a combustion regime map for a particular set of thermodynamic conditions. The key parameters in this map are the amount of hydrogen and steam in the mixture. Figure 4 illustrates that within the flammable regime, there is a narrow region of mixtures for which only slow flame are possible. Inside of this region, fast flames can appear once the expansion ratio, σ, is large than the minimum values described earlier. Also included in this figure are the flammability limits, DDT limits and the detonation limits.

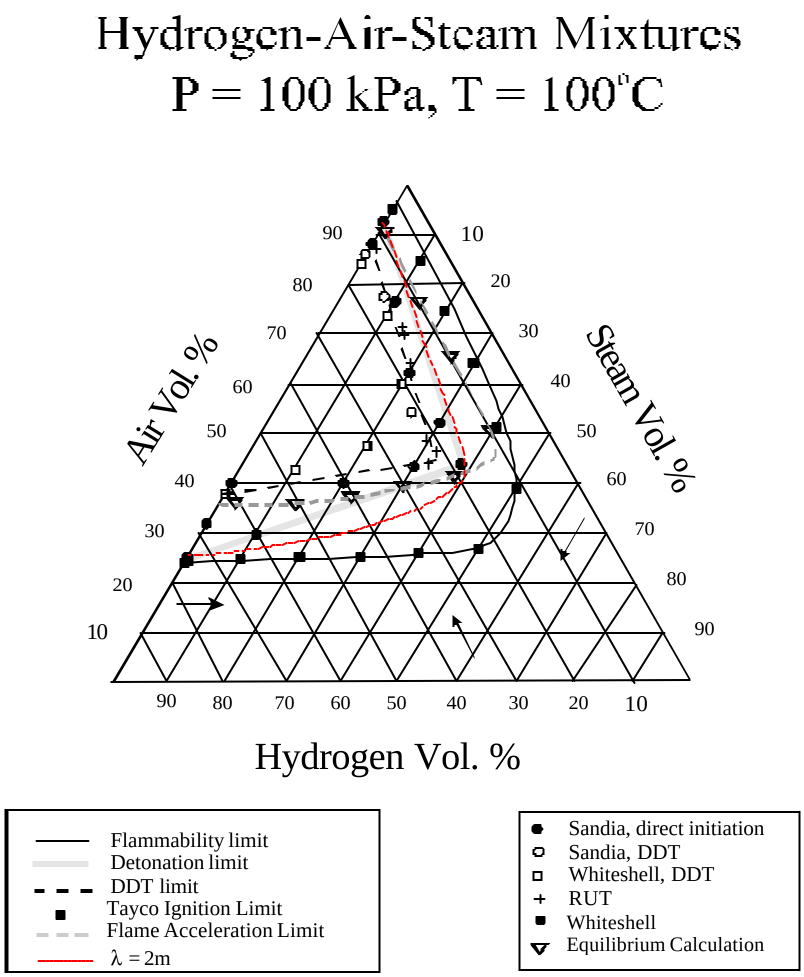


Figure 4. Combustion Regimes for Hydrogen-Air-Steam Mixtures at P_i = 100 kPa and T_i = 100C

4 Methodology for calculating DDT Index and DDT Potential

To assess the potential hazard of a hydrogen burn inside a containment building after a reactor accident, it is necessary to calculate the gas distribution within the containment following a postulated accident. A computational code such as GOTHIC can be used to perform the calculation.

To determine L, one needs to select a reference hydrogen concentration. If a reference hydrogen concentration is selected to be 10% (6%, 8%, 12% etc.), the volume of all the cells that have a hydrogen concentration equal to or higher than 10% can be determined. This gas cloud (with all cell $H_2\% > 10\%$) can be of any shape. The hydraulic diameter of this non-spherical cloud is the diameter of a sphere that has the same volume of this gas cloud. The equivalent hydrogen concentration of this cloud is the average hydrogen concentration inside this cloud. The equivalent $H_2\%$ is always higher than 10%. The detonation cell size of the equivalent mixture is used to calculate L_m ($L_m = 7\lambda$).

Because it has been established that DDT cannot occur if the cloud size is less than the minimum run-up distance for DDT, a "DDT Potential" can also be defined as a second criteria for DDT. A DDT Potential, $\gamma_{DDT} = L/L_{DDT}$, can also be calculated for each cloud, where L is the hydraulic diameter of the combustible gas cloud and L_{DDT} is the run-up distance for DDT. DDT is possible only when γ_{DDT} is larger than unity.

5 Methodology for calculating FA Index and FA Potential

The Flame Acceleration Index (FA Index) is the ratio of σ of the equivalent mixture (obtained from the reference data set) to σ^*, where $\sigma = \rho_u/\rho_b$ is the expansion ratio (density of unburned gas to the density of the burned gas) and σ^* is the critical expansion ratio which depends on the mixture composition and its initial temperature. It should be noted that the critical expansion ratio is independent of the steam concentration because the effect of diluents (in all tests with He, Ar, N_2, H_2O and CO_2) could be condensed into one common value. The critical expansion can be evaluated using the following correlation.

$\sigma^* = 3.75$ for $X_{H2} =$ or $> 2X_{O2}$, X is the gas pressure ratio or vol. %

$\sigma^* = 3.75 - 0.0115(T-25) + 0.00002(T-25)^2$ for $X_{H2} < 2X_{O2}$, T is average temperature of the gas cloud in ^oC

Similar to the "DDT Potential", a "FA Potential" can also be defined as a second criteria for supersonic flame. The FA Potential, ϕ_{FA}, is an indication for the potential for flame acceleration to supersonic velocities such that $\phi_{FA} = L/L_{SF}$, where L is the hydraulic diameter of a combustible gas cloud and L_{SF} is the run-up distance for a supersonic flame. Flame acceleration to supersonic velocity is possible only for $\phi_{FA} > 1$. The methodology for determining the FA Potential, γ_{FA}, is similar to that for determining the DDT Potential. The hydraulic diameter and the equivalent hydrogen concentration for the combustible gas cloud are determined the same way as above. From the reference data set, run-up distances for DDT and for supersonic flame can be determined for the equivalent mixture.

6 DDTINDEX Program

A computer code called DDTINDEX has been developed to perform the assessment of the likelihood of DDT and creation of a supersonic flame inside a post-accident nuclear containment. DDTINDEX takes the hydrogen and steam distribution output from a CFD code such as GOTHIC and determines the DDT Index, DDT Potential, FA Index and FA Potential for various regions. If these parameters are less than 1 everywhere in the containment, DDT and supersonic flames can be precluded. It should be noted that computer codes such as GOTHIC assume a uniform distribution of gas within each grid cell. This means that DDT and FA indices cannot be calculated for regions smaller than the resolution the grid spacing used in the simulation. To avoid these difficulties, it is important to employ fine grid resolution in regions that have large hydrogen concentration gradients.

The above parameters are calculated for each cell inside a gas cloud. The gas cloud is determined by default threshold values or threshold values supplied by the user.
DDTINDEX may only be applied to hydrogen cases, as interpolation tables only exist for hydrogen. DDTINDEX can potentially be used for other gasses, but they are not being considered here.

6.1 Capabilities and Features

The following list briefly describes the capabilities and features of the DDTINDEX program:

- The four indices used to determine if DDT or a supersonic flame is possible are calculated.
- The error and warning messages generated are printed to an output file.
- User can enter input to the program via flags in the command line or via the configuration file.
- Users can select the amount of information in the output files.
- The output from GOTHIC 6.1 or previous versions of GOTHIC may be used.
- The interpolation tables or look up tables can be changed to meet the needs of the problem being analyzed.

6.2 Limitations and Restrictions

The following is a list of the limitations and restrictions for the DDTINDEX program:

- If the GOTHIC simulation had blocked cells or blocked walls there is no mechanism to transfer this information to DDTINDEX. Because the blocked cells will have a small amount of H_2, a PERL script, was created to set the indices to 0 after running DDTINDEX.
- The results may not be conservative in certain situations:
    - When only the six cells touching the cell being examined are used to determine whether the cell is in the current cloud.
    - When calculating the hydraulic diameter, a spherical cloud is assumed. The hydraulic diameter for a long cloud in a narrow chamber will not be calculated correctly.
    - When large mesh sizes are used. Computer codes such as GOTHIC assume a uniform distribution of gas within each cell of the grid. This means that DDT indices cannot be

calculated for sub-volumes finer than the resolution the grid used in the simulation. Therefore DDT Index calculations may not be always conservative. To avoid these difficulties it is important to have a fine grid resolution in areas of large gradients in the gas concentration.

- The output from a CFD code must be extracted in the following columns: X, Y, and Z coordinates, steam (H_20), $H_{2,}$ and temperature.
- The maximum grid size that may be used is 50x50x50.

The current version of DDTINDEX (V1.1a) consists of the main program DDTINDEX.EXE and a few auxiliary programs for generating the reference data set.

6.3 Application to Nuclear Containment

In certain reactor accidents, hydrogen can be formed and released into the containment building. Development of a supersonic flame or DDT is a concern because of the resulting pressure loads. Even with ignitors and hydrogen recombiners being used by various reactor designs to mitigate the impact of hydrogen, safety analysts still need to determine the potential impact of a hydrogen burn inside containment. DDTINDEX is a computer program that can assist analysts to assess the potential for the creation of a supersonic flame via flame acceleration
DDTINDEX, this program was used to analyze a po
accident involves a reactor outlet header break in the
heated water is ejected into the containment building
hydrogen. For such an accident, as much as 100 kg
machine room. This may pose a threat to the integrity

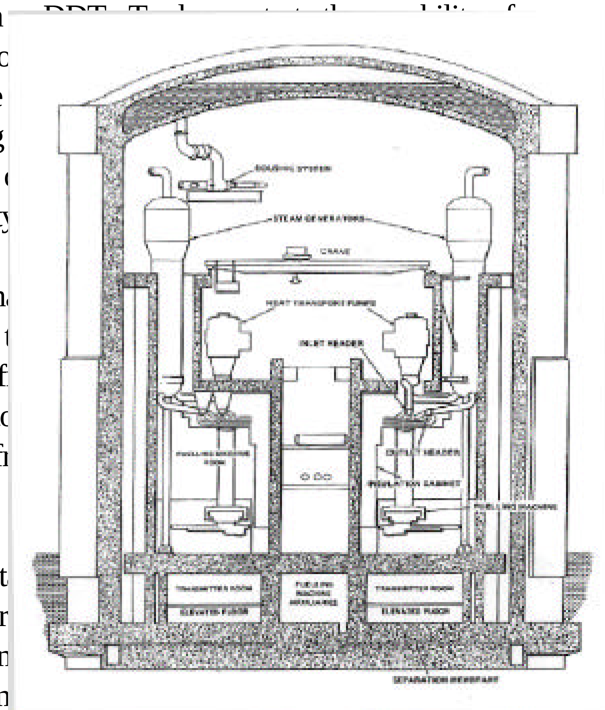
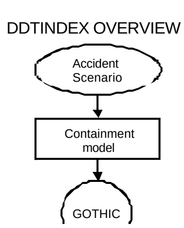


Figure 6. A Schematic of a CANDU 6 Reactor Containment

DDTINDEX is not a program that can be used to an
another computer code such as GOTHIC to analyze
containment building following an accident. Results f
assessing the potential for a slow burn to develop into
software package is also needed to view the output fr
shown in Fig. 5.

Figure 6 is an illustration of a CANDU 6 reactor cont
the steam generator enclosure, containing the reactor
distributed parameter model or 3-D model. The dom
parameter model. The rest of the containment was m
fuelling machine room, a 3242m^3 volume, was model
cells x 5 cells x 26 cells) ranging in size from 1.5m^3 to
header break was simulated by releasing hydrogen at
major equipment such as steam generators were modeled with null cells. For this example, a hydrogen control system that included local air coolers, fans, and ignitors was activated.



the simulation are shown in Fig. 7. At the peak of the
ration in the vicinity of the broken header (the cell at

which hydrogen was injected) reaches a maximum value of about 15%. The hydrogen concentration at 2m above the break is about 10%. Further away from the break, the hydrogen concentration is even lower. Most of the hydrogen and steam are carried upwards into the dome region and diluted to a concentration below the flammability limit. In this simulation,
the released hydrogen becomes well mixed through out the containment building after 2000 seconds into the accident. As shown by the graphs for DDT Index, DDT Potential, FA Index, and FA Potential, hydrogen concentrations within the containment are below the combustible limit except the region in the vicinity of the broken header. The DDT Index for the cell at the break is 1.36 and the FA Index for the same cell is 1.27. The DDT Index including the 3 cells with the next highest hydrogen concentration is 0.37. It should be noted that these indices represent the necessary but not sufficient conditions for flame acceleration and DDT. For the cell at the break, DDT Potential and FA Potential are calculated to be 0.29 and 0.32, respectively, indicating the cloud size is not sufficient for a flame to accelerate to supersonic speeds or trigger a DDT. Therefore, a local supersonic flame and DDT within the cloud are not possible and can be precluded in the safety analysis.

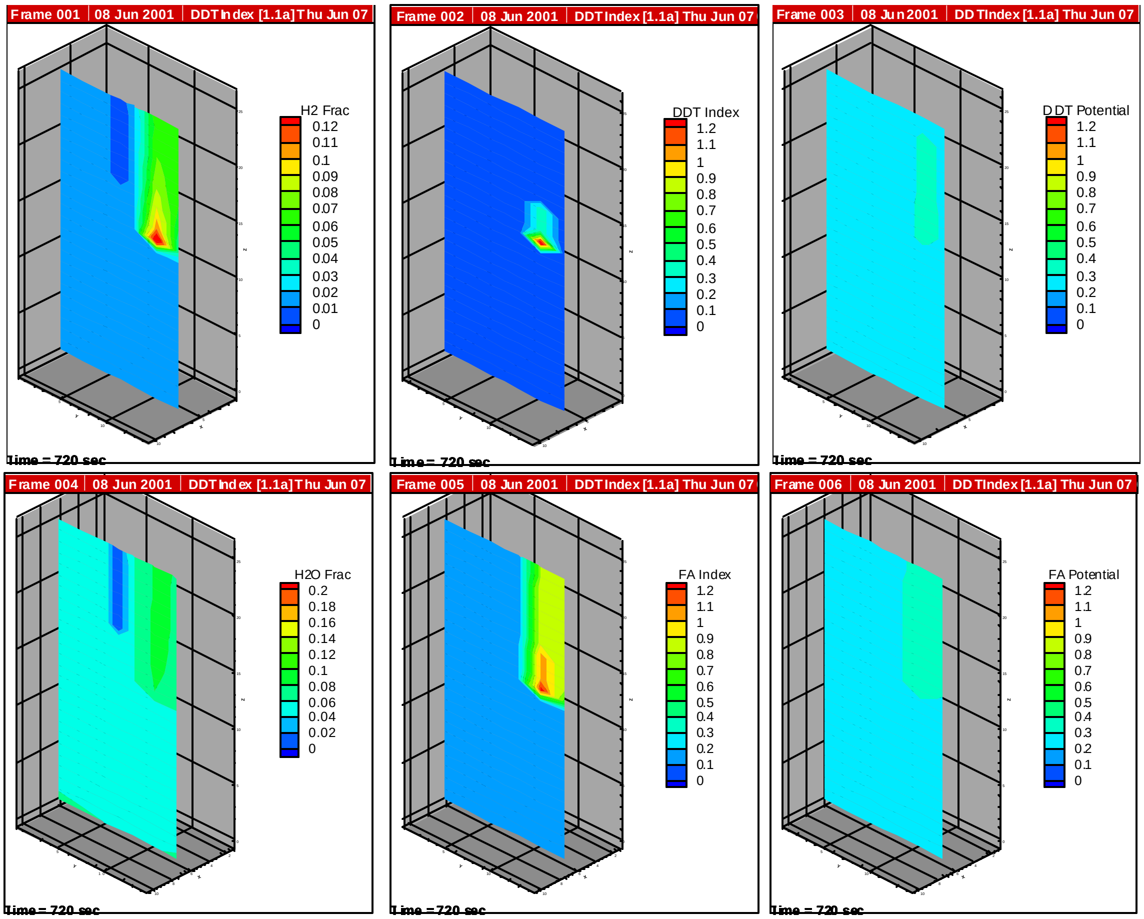


Figure 7. DDTINDEX Results for Reactor Header Break (hydrogen concentration, steam concentration, DDT Index, DDT Potential, FA Index and FA Potential)

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