

RBD-FAST BASED SENSITIVITY AND UNCERTAINTY ANALYSIS ON A COMPUTATIONAL HYDROGEN RECOMBINER TEST CASE

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ABSTRACT

Deflagration-to-Detonation Transition Ratio (DDTR) is an important parameter in measuring the hazard of hydrogen detonation at given thermodynamic conditions. It's among the major tasks to evaluate DDTR in the study of hydrogen safety in a nuclear containment. With CFD tools, detailed distribution of thermodynamic parameters at each instant can be simulated with considerable reliability. Then DDTR can be estimated using related CFD output. For stochastic or epistemic reasons, uncertainty always exists in input parameters during computations. This lack of accuracy can finally be reflected in the uncertainty of computation results, e.g. DDTR in our consideration. The analysis of the influence of the input uncertainty is therefore a key step to understand the model's response on the output and possibly to improve the accuracy. The increase of computational power makes it possible to perform statistics-based sensitivity and uncertainty (SU) analysis on CFD simulations. This paper aims at presenting some ideas on the procedure in safety analysis on hydrogen in nuclear containment. A hydrogen recombiner case is constructed and simulated with CFD method. DDTR at each instant is computed using a semi-empirical method. RBD-FAST based SU analysis is performed on the result.

Key words: Hydrogen safety; Computational Fluid Dynamics; Deflagration-to-Detonation Transition Ratio; Random Balanced Design-Fourier Amplitude Sensitivity Test

1. INTRODUCTION

During a severe accident in nuclear power plant, hydrogen, mainly produced from zirconium-water reaction, can leak into the atmosphere of containment. The hazard of hydrogen explosion menaces the integrity of containment, as the case in Fukushima Daiichi nuclear disaster. Deflagration-to-Detonation Transition Ratio (DDTR) tells whether the possibility of detonation can be ruled out ($DDTR < 1$) or not ($DDTR > 1$)^[1]. Thus the precise prediction of DDTR at each instant is an important task in the safety analysis of the hydrogen in a nuclear containment.

The value of DDTR can be estimated given the distribution of thermodynamic parameters, including temperature, pressure and concentrations of the components^[2], which can be simulated using whether lumped-parameter or CFD codes. Simulation cases requires a set of input data. For stochastic or epistemic reasons, however, the input data for the boundary conditions, initial conditions and physical models cannot always be determined with precision.^[3] This lack of accuracy can significantly impair the precision of model output. Uncertainty analysis is to quantify the uncertainty of the output while sensitivity analysis is to determine the influence of the input uncertainty on the output. Therefore, uncertainty and sensitivity (SU) analysis is a key step to understand the model behavior and possibly to improve the accuracy.

This paper is aimed at designing a 3-step procedure of hydrogen safety analysis in containment. First, CFD simulation is performed on hydrogen behavior using specialized modules such as catalyst hydrogen recombiner model. Second, the possibility of detonation and its destructiveness are evaluated with chemical-dynamical codes using the distribution of thermodynamic parameters provided by the CFD output. At last, input uncertainty is considered and SU analysis is performed to show the uncertainty of output and its sensitivity to the input parameters.

In order to demonstrate the idea of the study, a hydrogen recombiner test case is constructed and

simulated using CFD method. Then DDTR at each instant is predicted using a semi-theoretical semi-empirical method. At last, an uncertainty of 5% is assumed to some key input parameters and a random balanced design Fourier amplitude sensitivity test (RBD-FAST) method is applied to make SU analysis on the test case. The results of the SU analysis are presented and discussed.

2. DEFLAGRATION-TO-DETONATION TRANSITION RATIO

DDTR at a given instant, t , is defined as,

$$DDTR(t) = \frac{D(t)}{7\lambda(t)} \quad (1)$$

where $D(t)$ - characteristic geometrical size of the flammable gaseous cloud, m; $\lambda(t)$ - detonation cell width, m.

For general geometries, D can be estimated as the cubic root of the total volume of the flammable gaseous cloud. For wet hydrogen-air mixtures, the term “flammable” requires the volume fractions of steam and hydrogen to meet the demand^[4],

$$\begin{cases} X_{H_2O} < 60\%, \\ X_{H_2} \geq 4\% + \max \left[0, \frac{8}{30} (X_{H_2O} - 30\%) \right] \end{cases} \quad (2)$$

In order to determine the border of the flammable cloud, detailed distribution of the concentration of each component is required. This made it necessary to apply CFD method for the simulations. The volume of the cloud then can be calculated by summing up the volume of the mesh cells which meet the demand in Eq.(2).

λ is the average width of the cell structures behind detonation wave at given conditions^[5]. Due to the limitation of the knowledge on detonation phenomenon, the value of λ can only be estimated using empirical or semi-empirical correlations. An OCDE/NEA report^[6] recommends 2 methods to compute λ , of which the one with wider adaptability is applied in this paper. It is supposed that λ is highly correlated to a characteristic reaction zone width, δ , and the ratio λ/δ is a function of 2 dimensionless parameters, i.e., a dimensionless effective chemical activation energy $E_a/R/T_{ps}$, and a dimensionless temperature of the gas mixture, T_{vn}/T_0 , where E_a is the activation energy of the reaction, R is the gas constant, T_{ps} is the post-shock temperature of the gas, T_{vn} is the von-Neumann temperature and T_0 is the initial temperature of the gas^[7]. With a large amount of experimental data, a correlation of $\lambda/\delta = f(E_a/R/T_{ps}, T_{vn}/T_0)$ is built using different analytical correlation and least squares fitting,

$$\lg(\lambda/\delta) = Y(aY - b) + X[cX - d + (e - fY)Y] + g \ln Y + h \ln X + Y(i/X - jY/X^k) - l \quad (3)$$

where, $X = E_a/R/T_{ps}$ and $Y = T_{vn}/T_0$. Little letters $a \sim l$ are regression parameters, of which the values are given in [7].

In this paper, thermodynamic conditions of the flammable gaseous cloud, including temperature, pressure and concentrations of components, are at first preconditioned into δ , $E_a/R/T_{ps}$ and T_{vn}/T_0 , using an open-source chemical-dynamics code, Cantera^[8]. Then the value of λ is computed with Eq.(3).

3. CONSTRUCTION OF A HYDROGEN RECOMBINER CASE

For the reason that this paper is mostly aimed at the demonstration of a study methodology, a simple computational test case is constructed. It is assumed that in a confined vessel of which the sketch is shown in Figure. 1, a SIEMENS FR-90/1-150 hydrogen recombiner is located on the central axis. As initial condition, the vessel is filled with hydrogen-air mixture. Hydrogen distributes in a stratification zone in the upper part of the vessel. The distribution of hydrogen in upright direction is shown in Figure. 2. The initial temperature and pressure inside the vessel are respectively 20°C and 1 atm. The temperature of the wall remains 20°C during the whole computation. A constant heat transfer coefficient (5W/m²/°C)

is assumed to the heat exchange between the gas and the wall. For the sake of simplification, steam condensation is not considered in computation.

The simulation is performed with an in-house CFD code, HYDRAGON, of which the validity has been proved by practical utilizations^{[9]–[12]}. Hexahedral meshes with different refinements (10×10×24, 20×20×48 and 40×40×96) are compared during grid sensitivity analysis and the medium mesh is selected for the geometry. Low Mach number model^[13] is applied to ensure the accuracy in simulating the behavior of hydrogen. Standard $k-\varepsilon$ model is used to consider the turbulence. Buoyancy is considered in both fluid governing equations and turbulence model. SIEMENS hydrogen recombiners are described with a “0D” model^[14], which computes the consumption rate of hydrogen using Eq.(4).

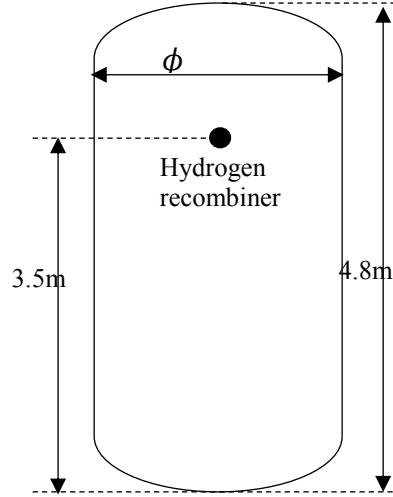


Figure. 1 Sketch of the vessel

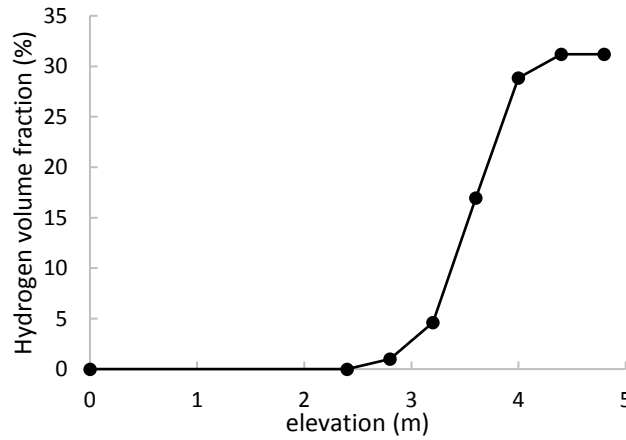


Figure. 2 Distribution of hydrogen at different elevations

$$\begin{cases} \frac{dm_{H_2}}{dt} = 0, \text{ if } X < X_{H_2, \min} \\ \frac{dm_{H_2}}{dt} = -10^{-3} \times \eta \times (A \times 10^{-5} \times p + B) \tanh[100 \times (X - X_{H_2, \min})] \end{cases} \quad (4)$$

where, $X = \min(X_{H_2}, 2X_{O_2}, 0.08)$, $X_{H_2, \min} = 0.005$

X - volume fraction, 1; p – pressure, Pa; η - recombiner output parameter. η allows to take into account the decrease of the efficiency of the recombiner for the weak concentrations of oxygen,

$$\begin{cases} \eta = 1, \text{ if } X_{H_2} < X_{O_2} \\ \eta = 0.6, \text{ if } X_{H_2} \geq X_{O_2} \end{cases}$$

where A and B are parameters provided by SIEMENS. For the FR90/1-150 the values are respectively

$0.48 \times 10^{-3} \text{ kg/s/bar}$ and $0.58 \times 10^{-3} \text{ kg/s}$.

Moreover, the reaction $\text{H}_2 + (1/2)\text{O}_2 \rightarrow \text{H}_2\text{O}$ is exothermic. The released heat is 122 MJ/kgH_2 .

With the simulation results, the domain of the flammable gaseous cloud can be determined by comparing the concentrations of components in each mesh cell and the criterion in Eq.(2). According to the CFD results, the temporal variations of average pressure, mass average temperature and average volume fractions of hydrogen and steam in the cloud are summarized in Figure. 3 and Figure. 4.

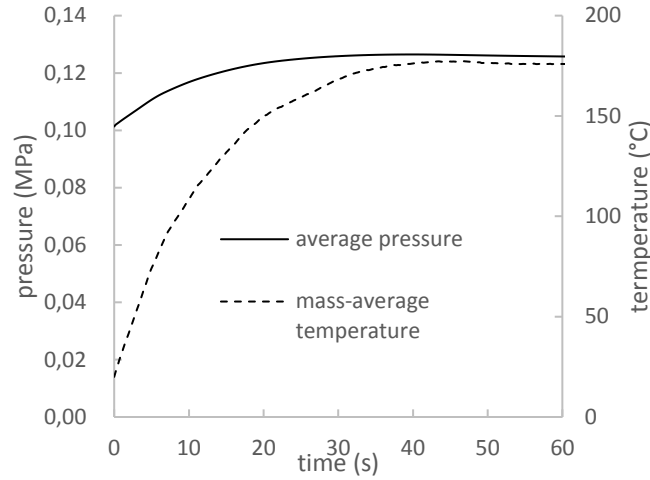


Figure. 3 Average pressure and mass average temperature v.s. time in the flammable cloud

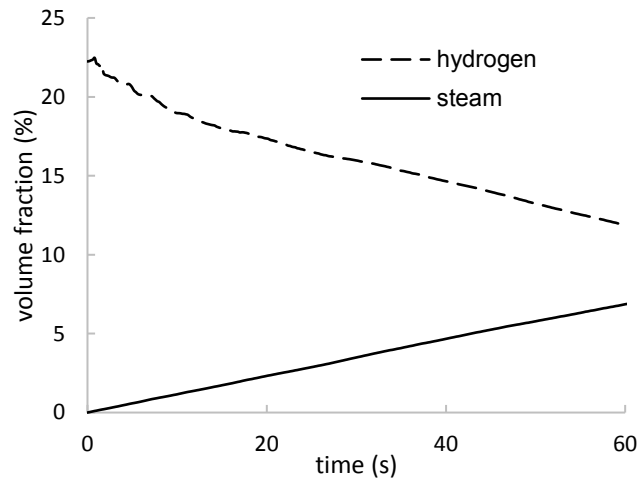


Figure. 4 Average volume fraction of hydrogen and steam v.s. time in the flammable cloud

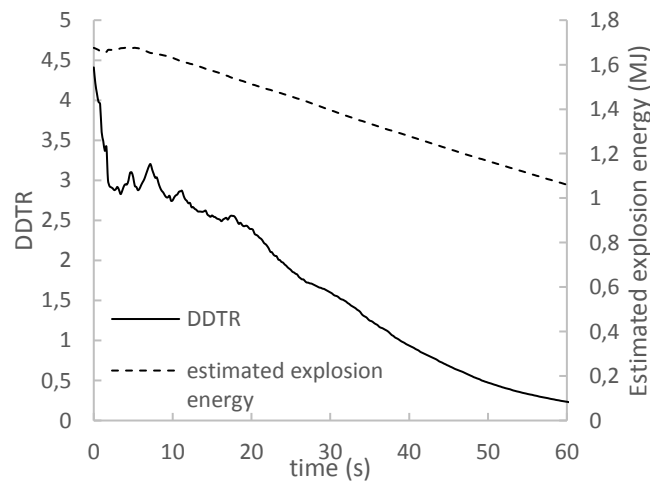


Figure. 5 DDTR and estimated maximum explosion energy of the flammable cloud v.s. time

Using the data presented in Figure. 3 and Figure. 4, DDTR of the flammable cloud is computed. The temporal variation of DDTR is described in Figure. 5. It can be found that at the beginning, DDTR is as high as 4.5, meaning a great possibility of hydrogen detonation. With the application of catalyst recombiner, hydrogen is consumed by reaction with oxygen, leading to the decrease of DDTR. However, during the first 20 seconds, oscillation happens to DDTR. This is a result of the competition between the effect of the increase of temperature as well as pressure and the effect of the decrease of hydrogen concentration. The oscillation vanishes when pressure and temperature trends to be steady, as a result of the removal of heat through the wall. The possibility of hydrogen detonation can be ruled out when $DDTR < 1$.

Along with DDTR, an estimated maximum explosion energy, Q_{max} , is also presented in Figure. 5. It is a simple summation of the energy that can be released by H_2-O_2 reaction in the cloud, assuming that the hydrogen in the cloud can be consumed thoroughly and simultaneously during an explosion. The ideal reaction may not happen practically but the parameter can provide a preliminary estimation for the destructiveness of hydrogen detonation. It can be found in Figure. 5 that the value of Q_{max} decreases continuously with the consumption of hydrogen. Meanwhile, it can be observed that, in the first 8s, the behavior of Q_{max} (almost stable) in Figure. 5 does not follow the behavior of the decreasing hydrogen volume fraction in Figure. 4. It is possibly a result of the recombiner-induced convection that enhanced the mixing of gas in the upper space, leading to some initially unflammable cells satisfying the demand in Eq.(2). The assumption should be investigated in future study.

4. RBD-FAST BASED SENSITIVITY & UNCERTAINTY ANALYSIS

4.1. Introduction to RBD-FAST

The methods for sensitivity and uncertainty analysis are based on either deterministic or statistical procedures^[15]. Due to the complexity and nonlinearity of fluid system, it is impractical to perform deterministic SU analysis methods on CFD simulations. On the other hand, however, statistics-based SU analysis methods require repeated computations for a large amount of samples. The number of samples varies from tens to thousands according to different methods applied. Considering the computation effort needed for a single run of CFD simulation for a complicated system, even the roughest statistical SU analysis method can sometimes demand unaffordable amount of computational time and resources.

In order to cut down the computational cost, nonparametric statistical methods are applied in SU analysis in earlier studies^{[16][17]}. Tolerance limits with a certain degree of confidence are treated as the quantity of uncertainty, while Spearman's correlation coefficient (SCC) or Pearson's correlation coefficient (PCC) between input parameter and output variable is used as the measurement of sensitivity. With such methods, merely hundreds of samples are required to produce an evaluation of uncertainty and sensitivity. However, mathematically, SCC or PCC is a parameter quantifying the monotonic correlation between two sets of data^[18]. Therefore, theoretically, it is not able to measure the aptitude of output variation due to input error, thus the coefficient cannot fully reflect the dependency of the output on the input, i.e., the sensitivity.

The increase of the computational power has made it feasible for large scale parallel computations. Thus it is possible to apply finer methods to make SU analysis for CFD simulations. Random balance design Fourier aptitude sensitivity test (RBD-FAST) is an SU analysis method developed from analysis of variance and Fourier transform^[19]. This method computes the 1st-order sensitivity by deciding the contribution of the variance caused by a given input parameter to the whole variance of the output. The definition of sensitivity is,

$$S_{Y|X} = \frac{\text{var}[E(Y|X)]}{\text{var}(Y)} \quad (5)$$

where Y - output variable; X - input parameter; $E(Y|X)$ - conditional expectation of Y at given X ; var – variance; $S_{Y|X}$ - sensitivity of Y on X .

In order to introduce the procedure in performing RBD-FAST, at first a computer model $Y = f(x_1, x_2, \dots, x_N)$ is considered, where N is the number of independent parameters and the domain of independent

parameters is the hypercube,

$$\Omega_n = \{x \mid x_i^{\min} < x_i < x_i^{\max}, i = 1, \dots, N\}$$

where x_i^{\min} and x_i^{\max} are the minimum and maximum possible values of x_i . To produce a set of samples of x_i , a search function is introduced to explore the space Ω_n ,

$$x_i = F_i^{-1} \left(\frac{1}{2} + \frac{1}{\pi} \arcsin(\sin(\omega s)) \right), s = -\pi + \frac{2\pi j}{M}, j = 1, \dots, M \quad (6)$$

where M - total number of samples; ω - characteristic frequency for x_i (which can be set to 1 in RBD-FAST); F_i^{-1} - inverse cumulative distribution function (ICDF)^[20] for x_i . With Eq.(6), M samples can be generated for each x_i . X_i is defined as the sample sequence of x_i ,

$$X_i = [x_{i1}, x_{i2}, \dots, x_{iM}] \quad (7)$$

Then we randomly reorder the M units in X_i and get,

$$X_i^{(r)} = [x_{i1}^{(r)}, x_{i2}^{(r)}, \dots, x_{im}^{(r)}, \dots, x_{iM}^{(r)}] \quad (8)$$

where m - sample order after reordering. (r) stands for reorder. Random reordering is performed N times for each x_i . The model is then run on the reordered parameter values to get the model output,

$$Y_m = f(x_{1m}^{(r)}, x_{2m}^{(r)}, \dots, x_{Nm}^{(r)}), m = 1, 2, \dots, M \quad (9)$$

Finally, for a specific parameter of interest, x_i , on the model output values according to the original sample order (i.e., order before applying the random reordering in Eq.(7)), the FAST analysis is applied by calculating the spectrum of the fast Fourier transform,

$$\begin{aligned} \Lambda_k &= \frac{1}{M} (A_k^2 + B_k^2), k = 1, 2, \dots, M \\ A_k &= \frac{2}{M} \sum_{j=1}^M Y_j \cos\left(\frac{-2\pi(j-1)(k-1)}{M}\right) \\ B_k &= \frac{2}{M} \sum_{j=1}^M Y_j \sin\left(\frac{-2\pi(j-1)(k-1)}{M}\right) \end{aligned} \quad (10)$$

Then the partial variance in model output arising from the uncertainty of parameter x_i , V_i , can be estimated with Eq.(11), where L is an order number which is usually set to 4~6. The total variance, V , can be estimated with Eq.(12)

$$V_i = 2 \sum_{k=2}^L \Lambda_k \quad (11)$$

$$V = \sum_{k=2}^M \Lambda_k \quad (12)$$

The ratio V_i/V measures the contribution of parameter x_i to the total variance of response variable Y . This ratio is also termed the first-order sensitivity,

$$S_{Y|x_i} = V_i / V \quad (13)$$

In earlier investigations on RBD-FAST, the error from the theoretical value of sensitivity increases as sensitivity decreases and the error decreases as sample number increases. It is shown that when the sample number is larger than 1000, the error can be less than 5% for sensitivities larger than 0.1.^[19] Such a feature of RBD-FAST meets our demand as the primary task of sensitivity analysis in this paper is to screen out the input parameters of which the uncertainty has higher influence on the output.

4.2. Selection of input and output parameters to be analyzed

In the hydrogen recombiner case, 6 parameters listed in Table 1 are selected as input parameters with uncertainty. The distribution types of the uncertainties of all the 6 parameters are assumed Gaussian and the standard deviations are assumed to be 5% of their nominal values. The total sample number is 1000 and the samples are generated in the way proposed by RBD-FAST. DDTR and Q_{\max} are selected as the output variable to be analyzed. The computations are performed on the high performance computation (HPC) platform in Tsinghua University. The cluster has 740 nodes, each of which is composed with 2 Intel Xeon X5670 CPU (6-core processor). It means theoretically the 1000 sample cases can be computed simultaneously without the consideration of queuing. And it takes a core about 4 hours to accomplish the computation of a sample case.

Table 1. Input parameters with uncertainty and their nominal values

Symbol	Parameter name	Nominal value
x_1	Wall temperature, T_w	20°C
x_2	Wall heat transfer coefficient, h_w	5J/m ² /°C
x_3	Initial temperature, T_0	20°C
x_4	Initial hydrogen volume fraction coefficient, α^*	1
x_5	Recombiner performance parameter, A	0.48×10^{-3} kg/s/bar
x_6	Recombiner performance parameter, B	0.58×10^{-3} kg/s

*The initial hydrogen distribution stratified. When sampling the initial hydrogen volume fraction, the coefficient, α , is sampled and multiplied by the nominal fraction in each layer to get the actual fraction.

4.3. Uncertainty analysis

The upper and lower bounds of the variation of DDTR due to the uncertainty of input parameters are shown in Figure. 6. “Nominal value” is the DDTR output when all the parameters in Table 1 are set to their nominal values. “Mean value” is the arithmetic average of DDTR in all 1000 sample results. It can be found that the curve of the nominal value coincides with that of the mean value. The upper or lower bound is formed, respectively, with the maximum or minimum values of DDTR among 1000 sample results at each instant. Thus all the time-variation curves of DDTR are between the two bound curves. The distribution histograms of DDTR at 0s, 30s and 60s are presented in Figure. 8. It can be found that the assumed distributions of input parameters lead to skewed Gaussian distributions of DDTR output at each instant. Figure. 6 and Figure. 8 together come to a conclusion that the uncertainty of DDTR is high at the beginning of the computation. Then the uncertainty becomes lower and lower as DDTR decreases.

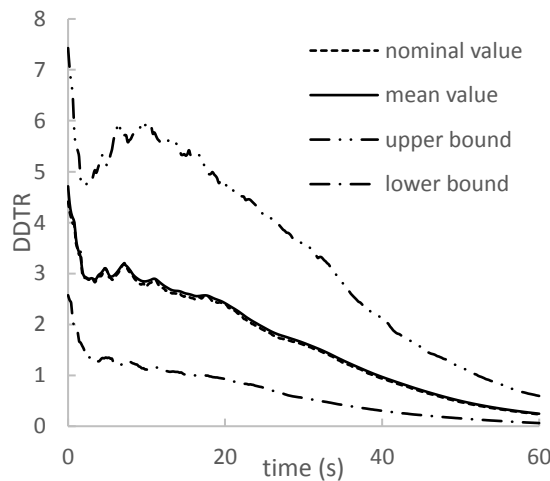


Figure. 6 Temporal variation of upper and lower bounds for DDTR

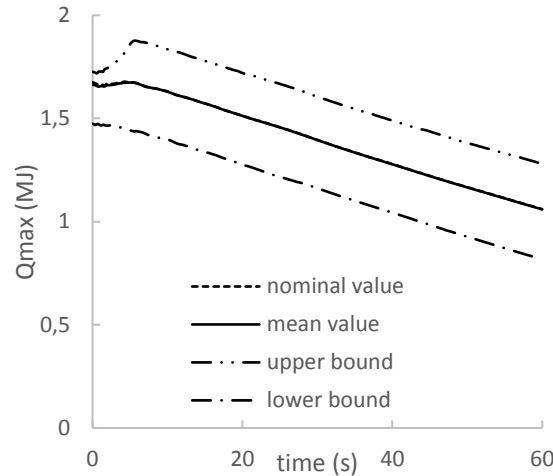


Figure. 7 Temporal variation of upper and lower bounds for Q_{\max}

Figure. 7 presents the upper and lower bounds for Q_{\max} while Figure. 9 shows its distribution histogram at 3 given instants. It can be found that, during the first 6 seconds, the maximum value of Q_{\max} increases with time and the nominal curve as well as the mean curve is far from the center between the two bounds. Such phenomenon agrees with the fact that the distribution of Q_{\max} is quite skewed at 0s in Figure. 9. Then, unlike the conclusions about DDTR, the uncertainty of Q_{\max} almost remains constant during the rest of the simulation, although the value of Q_{\max} decreases continuously with time. Meanwhile, the normality of the distribution of Q_{\max} is better than that of DDTR at 30s and 60s.

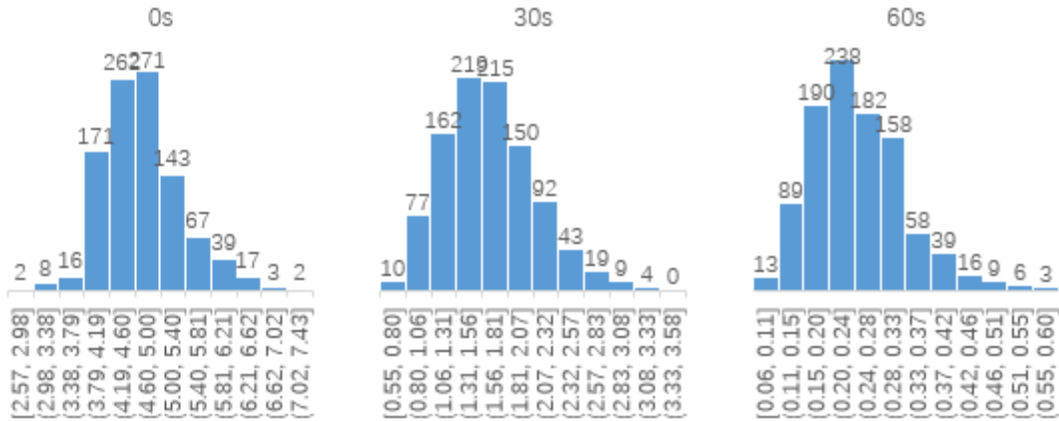


Figure. 8 Distribution of DDTR at given instants. The unity of the x-axis is 1.

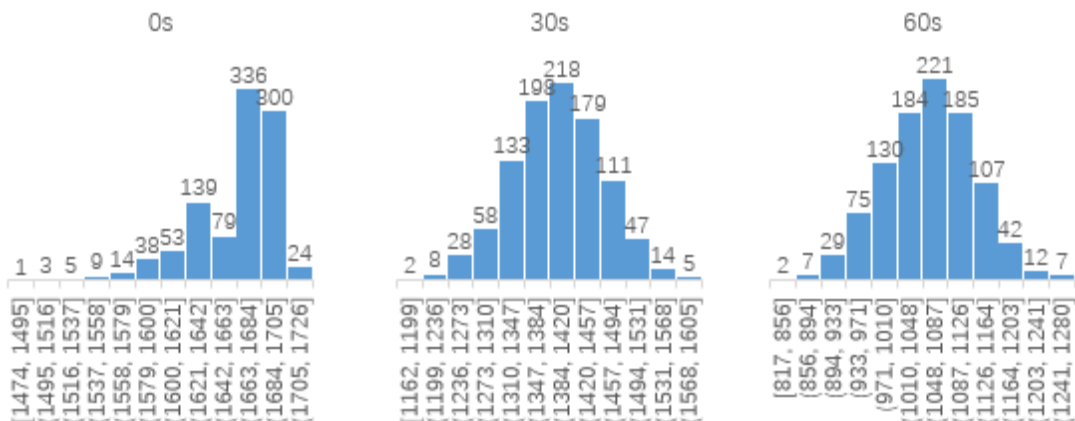


Figure. 9 Distribution of Q_{\max} at given instants. The unity of the x-axis is MJ.

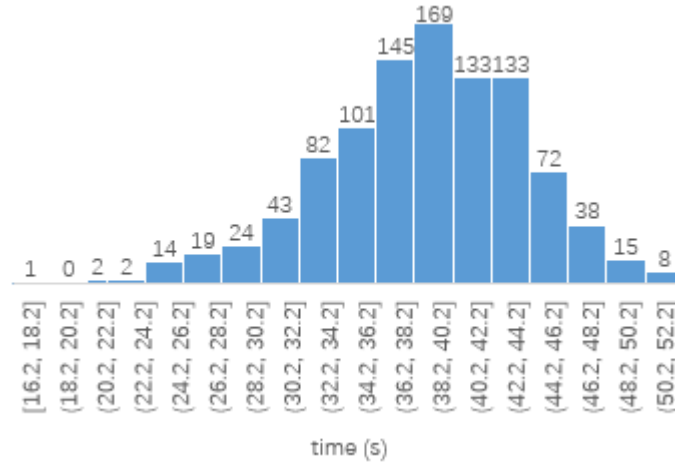


Figure. 10 Distribution of the time need for DDTR to fall below 1

Another concerned issue in hydrogen analysis is the time needed, when safety measures are taken, for DDTR to fall below 1 where the possibility of detonation can be ruled out. In this case, the average value is 38.7s, the standard error is 5.2s and its distribution is described in Figure. 10.

4.4. Sensitivity analysis

The sensitivity of DDTR and Q_{\max} on different input parameters are presented in Figure. 11. The correspondences between $x_1 \sim x_6$ in the legend and the 6 parameters are listed in Table 1. It can be found in the two graphs that in this test case, only the uncertainty of the initial hydrogen distribution (x_4) has significant influence on the variation of DDTR and Q_{\max} . What's more, the influence of this parameter decrease gradually with time. The sensitivities of the other 5 parameters are all less than 0.1. According to the introduction in 4.1, for RBD-FAST, when the sample number is not larger than 1000, the value of sensitivity is reliable only when it is larger than 0.1. One thing can be sure is, however, that the influence of the uncertainties of the other 5 parameters on these two output variables are negligible. The sensitivity analysis comes to a conclusion that, within the scope of this test case, the uncertainties of DDTR and Q_{\max} are produced mainly due to the uncertainty of the initial hydrogen distribution.

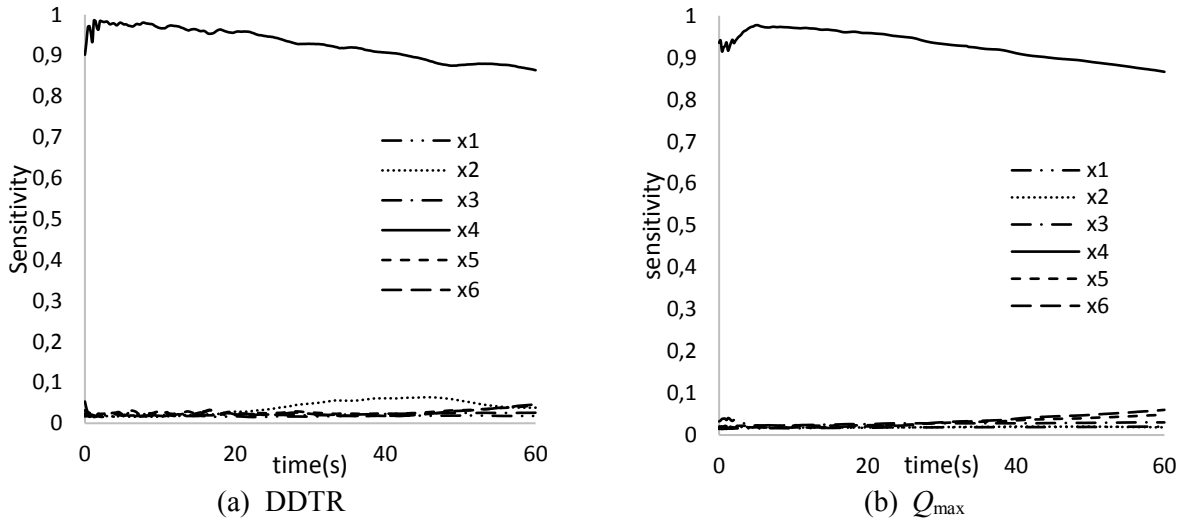


Figure. 11 Sensitivity of DDTR and Q_{\max} on different input parameters

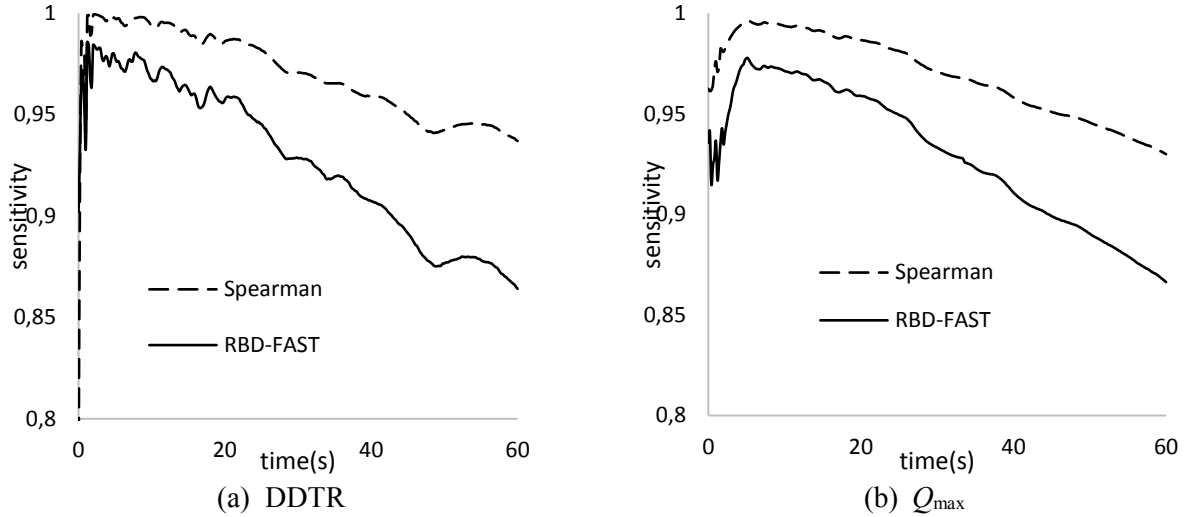


Figure. 12 Comparison of the sensitivity of DDTR and Q_{\max} between SCC and RBD-FAST

Spearman's correlation coefficient (SCC) between the initial hydrogen volume fraction coefficient and the DDTR and Q_{\max} output is also calculated for the 1000 samples. It is compared to the sensitivity defined in RBD-FAST, as presented in Figure. 12. The curves of sensitivity computed defined in the two methods show similar variation trend. But the sensitivity defined by RBD-FAST is generally lower than SCC. In order to measure the variation of the sensitivity, a sensitivity variation ratio is defined as the ratio between the actual sensitivity and the maximum sensitivity ever observed during computation. It can be found in Figure. 13 that the variation of the sensitivity by RBD-FAST is stronger than that of SCC except for DDTR at 0 second where SCC has a very low value (0.76).

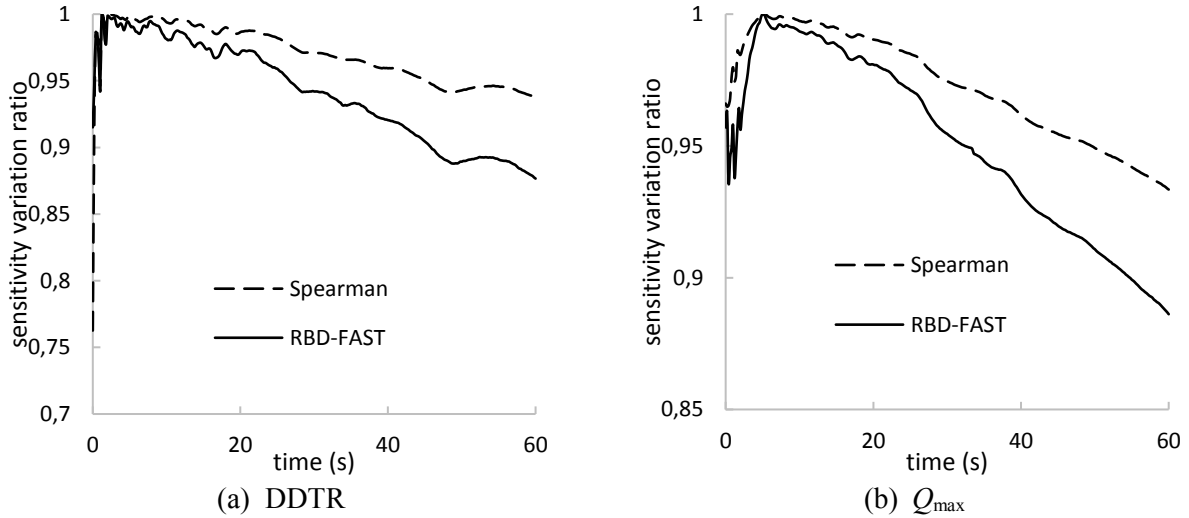


Figure. 13 Comparison of sensitivity variation ratio of DDTR and Q_{\max} between SCC and RBD-FAST

5. DISCUSSION

The first thing to be discussed is the validity of the method to compute detonation cell width and then to compute DDTR. Whether the criterion is valid for a uniform or non-uniform distributed hydrogen cloud depends on the experimental data used to establish the correlation. If the correlation is built from mean physical features of the clouds, then the CFD output has to be averaged in space before computing detonation cell width for certain clouds. To the authors' knowledge, mean physical properties are used to build Eq.(3) referring to [11]. Meanwhile, detonation probability depends not only on thermodynamic parameters but also very strongly on the geometry where the flammable cloud is found. Different expressions for characteristic size have been established for cloud in different simple geometrical structures, e.g. cuboid or cylindrical rooms. However, at present, precise computation of characteristic

size for cloud in arbitrary geometry is not yet available and a universal approximation as the cubic root of the total volume of the cloud is a compromise for complex geometries in CFD simulations.

The second thing is on uncertainty and sensitivity analysis. It should be stressed that the conclusions drawn from a case are only valid within the scope of the case itself. In the test case in this paper, only the uncertainty of initial hydrogen distribution has significant influence on the 2 output variables. It is possible that the 2 output variables were sensitive to other input parameters that are not discussed here. Meanwhile, the uncertainty of the other 5 parameters may have more contributions to the uncertainty other output variables. What's more, the dependency between output uncertainty and input uncertainty may be thoroughly changed for different conditions including the geometry condition, initial condition and boundary condition. For a given case, SU analysis is performed on concerned parameters. The conclusions of SU analysis are valid to a specific condition but they should be expanded very carefully. The third thing is the validity of SCC in measuring sensitivity. In this simple case, only one input parameter is screened out in sensitivity test and the monotonicity between the output variables and this input parameter seems quite straightforward. SCC, although not as fine and not as sensitive, has comparable reference value to the RBD-FAST result here. However, for more complicated cases where the reliance of output uncertainty on input uncertainty is not monotonous, whether SCC can reflect sensitivity is still an issue to be further discussed.

6. CONCLUSION

In this paper, a 3-step study procedure is designed for hydrogen safety analysis in containment. The 3 steps are namely CFD simulation, DDTR computation and SU analysis. The operation of the procedure is demonstrated on a simple test case. Its feasibility is ensured by growing computation power of nowadays. The procedure can be used in evaluating hydrogen detonation risk in containment, finding the key factors that can affect the risk and providing references to taking necessary safety measures.

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