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A 3-D simulation tool for hydrogen detonation during severe accident and its application

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ABSTRACT

A 3-D simulation tool (DEST, Detonation Simulation tool) for hydrogen detonation during severe accident has been developed. The compressible three-dimensional Euler equations in Cartesian coordinate system are solved by a second-order additive semi-implicit Runge–Kutta method with 5th weighted essentially non-oscillatory scheme (WENO) and Steger-warming flux vector splitting approach handling the convection flux. The multi-blocking patching method is used to handle the flow problem of complex geometry. Afterward, the hydrodynamics solver is tested by applying DEST to the classical shock tube problems, and the results show that hydrodynamics solver can capture the shock wave correctly and give a detailed description of shock wave even if the gradient of pressure, density or velocity is large. Then two detonation experimental tests of RUT facility are simulated by DEST, and the comparisons between the predicted results and experimental data show a reasonably good agreement. Furthermore, DEST is applied to a hypothetical detonation in two connected compartments of containment. The predicted results show that the maximum pressure and temperature always occur at the corner of the compartment. The influence of ignition position is analyzed and the results show that the pressure tended to be larger when the mixture is ignited at a farther location. The DEST can be used to analyze the pressure and temperature load during detonation process under severe accident and has guidance on the strategy of hydrogen mitigation.

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1. Introduction

The nuclear reactor safety analysis is one of the most important issues in the nuclear power plant design, construction and operation. In the early years, the research mainly focused on the design basis accident analysis. Numerous scientific results had emerged up, some of which has been successfully used in the safety analysis of nuclear plant (Su et al., 2013). After the Three Mile Island accident, severe accident research began to attract researcher's attention. Many experimental and theoretical researches on severe accident have been carried out after that.

A severe accident is an incident starting from the melting of the reactor core and ending with the release of fission products to the environment. According to the development process, severe accident can be divided into two stages: in-vessel accident progression and ex-vessel accident progression (Zhang et al., 2015). During the in-vessel accident progression, the core melts and the chemical reaction between the Zr and steam cause the production of hydrogen. The hydrogen will flow into the containment through the break of the primary circuit boundary. After the failure of RPV (reactor pressure vessel), the molten core drops to the cavity and reacts with the concrete, which leads to the formation of hydrogen. Research has showed that the zirconium-water reaction and molten core-concrete interaction (MCCI) are the main source of hydrogen during the nuclear power plant accident (Bachellerie et al., 2003). If the hydrogen concentration in the local space reaches to the flammability limit or detonation limit, the combustion or explosion may happen. The pressure and temperature loads of these processes will threaten the integrity of the containment. Throughout the history of nuclear reactor development, hydrogen explosion occurred in the TMI accident (Sehgal, 2012) and Fukushima accident (Ohnishi, 2011). Especially during Fukushima accident, the pressure load of hydrogen explosion destroyed the reactor building. Therefore, the research of hydrogen explosion is of great importance and significance.

Large amount of experimental study on hydrogen explosion has been carried by researchers all over the world. The flame acceleration (FA), deflagration, deflagration to detonation transition (DDT) and detonation have been investigated by many experiments.

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Some criteria for FA (σ-criteria) and DDT (λ-criteria) were proposed according to the experimental data (Dorofeev, 1996; Dorofeev et al., 2001). These criteria provide the theoretical foundations for the judgement of the explosion stages and have been successfully applied to the code development. Besides, the deflagration and detonation in small scale and middle scale facility have been studied by lots of researchers. The data of pressure and temperature during deflagration was got and used for the verification of hydrogen explosion analysis code (Breitung et al., 2005). However, there are some restrictions and limitations for experimental research. The most important is that engineering-level hydrogen explosion experiment has safety risk and high costs. Numerical simulation provides an effective approach to solve this problem. One can analyze the characteristics of hydrogen explosion in containment by simulation tools which have been verified by experimental data

Many CFD tools have been developed to simulate hydrogen explosion during severe accident of nuclear power plant, such as COM3D and DET3D (Bielert et al., 2001) However, none of these tools could simulate the whole stage of hydrogen explosion, including deflagration, DDT and detonation. There are two reasons: (a) the controlling mechanisms of different stages are different, and (b) the detailed transition mechanism from deflagration to detonation is still unknown. Hence, different stages of hydrogen explosion are simulated by different tools. In the hydrogen explosion analysis during severe accident, the deflagration can be simulated by tools like REACFLOW, COM3D and ANSYS CFX, because some detailed turbulence models are concerned in these tools. The occurrence of DDT is judged by the λ-criteria and the detonation is simulated by tools such as DET3D and secondary development of TONUS.

The hydrogen behavior analysis strategy during severe accident is shown in Fig. 1. When a severe accident happens, the source is calculated by severe accident system analysis programs like MAAP and MELCOR. Then the source can be taken as the input of the distribution simulation tools to get the distribution of hydrogen, steam and other gases in the containment. According to the hydrogen concentration and ignition condition, the induced stage of explosion can be determined. σ-criteria and λ-criteria are used to judge the stage of explosion. Different stages of explosion can be simulated by different tools and the calculated pressure load and temperature load are output to ABAQUS for structure response analysis. As a part of hydrogen behavior, hydrogen detonation should be studied in detail for two reasons: (a) the existing hydrogen mitigation system could not exclude the possibility of detonation, and (b) the load during this process is so huge that it may threaten the integrity of the containment. However, we have no access to the detonation simulation tools like DET3D for the moment. In order to study the detonation process and to meet the domestic demand of software autonomous scheduling, a 3-D hydrogen detonation simulation is developed.

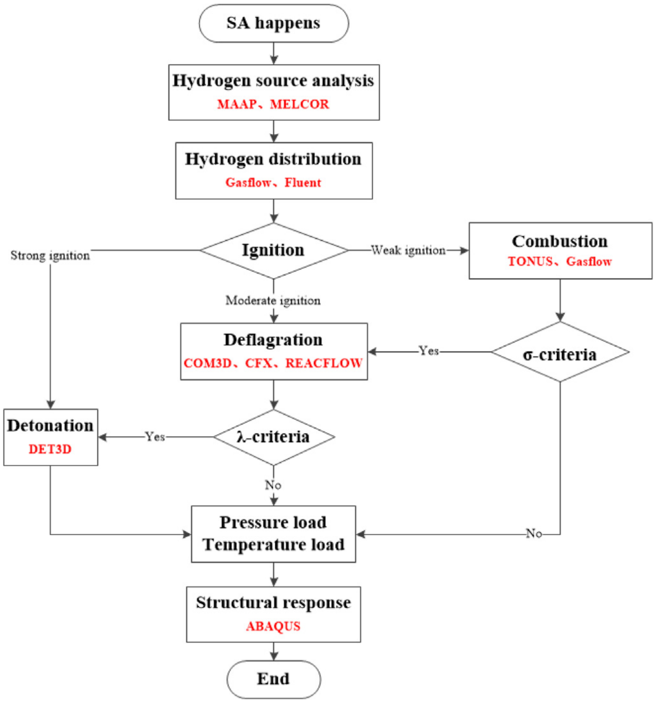

Fig. 1. Hydrogen behavior analysis strategy during severe accident (Breitung et al., 2000).

In the present study, a 3-D hydrogen detonation simulation tool, DEST, is developed. There are three main aims for the DEST development: (a) to analyze the pressure and temperature load during detonation process under severe accident; (b) to provide initial condition for the subsequent structure analysis; (c) to fill the blank of hydrogen detonation simulation tool in our research team.

2. Mathematical formulation of DEST

2.1. Governing equations

For the detonation process, the detonation propagates followed by the reaction zone and it is maintained by the energy from chemical reaction (Kuo, 1986). The mechanism of detonation is quite different from that of deflagration, because the turbulence is not the dominant effects in this process. Hence, the turbulence effects can be ignored. Assuming the system consisting of n gaseous components is under thermal equilibrium and the viscosity, turbulence, molecular diffusion and heat conduction can be neglected, the three-dimensional governing equations in Cartesian coordinate system are as follows,

$$\frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial x}+\frac{\partial G(U)}{\partial y}+\frac{\partial H(U)}{\partial z}=S(U) \tag{1}$$

where U is the vector of the conserved variables, $F(U)$, $G(U)$ and $H(U)$ are the convective flux vectors in x, y and z direction, respectively. $S(U)$ is the vector of the source terms. The vectors can be written as

$$U=\begin{pmatrix}\rho_1\\ \vdots\\ \rho_n\\ \rho u\\ \rho v\\ \rho w\\ E\end{pmatrix} S(U)=\begin{pmatrix}\varpi_1\\ \vdots\\ \varpi_n\\ \rho f_x\\ \rho f_y\\ \rho f_z\\ \rho u f_x+\rho v f_y+\rho w f_z\end{pmatrix}$$

$$F(U)=\begin{pmatrix}\rho_1 u\\ \vdots\\ \rho_n u\\ \rho u^2+p\\ \rho u v\\ \rho u w\\ (E+p)u\end{pmatrix} G(U)=\begin{pmatrix}\rho_1 v\\ \vdots\\ \rho_n v\\ \rho u v\\ \rho v^2+p\\ \rho v w\\ (E+p)v\end{pmatrix} H(U)=\begin{pmatrix}\rho_1 w\\ \vdots\\ \rho_n w\\ \rho u w\\ \rho v w\\ \rho w^2+p\\ (E+p)w\end{pmatrix}$$

where ρ_i is the i-th component density, kg/m^3, and n is the number of components. ρ is the mixture density, $\rho=\sum_{i=1}^{n}\rho_i$, kg/m^3. u, v and w are the velocity in three spatial dimensions, m/s. p donates the

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