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MULTI-DIMENSIONAL SIMULATION OF HYDROGEN MIXING AND TRANSPORT IN THE CONTAINMENT USING CFD CODES

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ABSTRACT

Oxidation of the metallic components of the reactor core and the interaction of core/concrete will produce hydrogen under severe accident. Hydrogen combustion in the containment building may threaten the integrity of the containment. It is important to predict hydrogen transport and mixing in the containment, in order to determine whether the mixture can locally reach flammability limits. GASFLOW and FLUENT are two CFD codes available to analyze hydrogen mixing and transport in the containment. The main goal of the investigation is to assess the capability of the GASFLOW code to predict hydrogen concentration distributions and velocity fields for a variety of physical conditions. The assessment relied on the comparison with the results obtained using the commercial computational fluid dynamics code FLUENT. FLUENT calculation results with standard $k-\varepsilon$ model and laminar model showed nearly the same hydrogen concentration distributions. But in the much coarser grid in GASFLOW, large differences exist between the turbulence and laminar simulation. Calculation using laminar flow assumption in the investigated grid is very misleading, and the effects of turbulence and mass diffusion can not be neglected in the present GASFLOW grid.

Keywords: severe accident, hydrogen mixing and transport, NPP, CFD

1. INTRODUCTION

Large amounts of hydrogen could be generated and released into the containment during the course of severe accidents in water-cooled nuclear power plants (NPPs). The formation of

hydrogen inevitably accompanies any core degradation process. Gas transport and mixing within the containment free volume are important thermal hydraulic phenomena in severe accident analysis. It poses a particular threat to the containment because it may lead to a dangerous combustion load if it remains unmitigated for nearly all anticipated severe accident sequences. So it is particularly important that CFD codes are able to predict hydrogen transport and mixing in the containment, in order to determine whether the mixture can locally reach flammability limits [1].

Mixing is an intra-compartment process, whereas transport is an inter-compartment process. Mixing is a process where separate fluids with distinguishable characteristics tend to come together to form a fluid with a single characteristic. When hydrogen is injected into a mixture of air and steam, the incoming gas stream mixes with the surrounding atmosphere. If the mixing process proceeds to completion, a uniform composition of hydrogen, air, and steam will be created. Transport is a process where fluids or aerosols move from one defined region to another. Transport usually refers to movement between compartments, such as convection loops that develop between a series of coupled compartments or the flow of liquids between various compartments [2].

In this paper, hydrogen mixing and transport in the large scale containment of Daya Bay NPP during large LOCA sequence are simulated using CFD codes GASFLOW and FLUENT. Local hydrogen, steam, and air concentration are investigated so as to determine where hydrogen combustion risk may occur. The calculation results between GASFLOW and FLUENT are also compared.

2. CODES DESCRIPTION

2.1 Computer Codes for Hydrogen Behavior Analysis

Computer codes for analysis of thermal hydraulic behavior and hydrogen distribution in a reactor containment are either lumped-parameter codes, field codes or a combination of both.

2.1.1 Lumped-Parameter Codes

Lumped parameter codes are based on the fundamental assumption that within a chosen control volume, spatial differences of thermal hydraulic variables, like fluid density, concentration, and temperature, are neglected. The time-dependent behavior is represented by conservation equations that describe containment transport processes.

The lumped parameter codes have a relatively fast-running on a variety of platforms, such as mainframes, PCs, and workstations. The main disadvantages of lumped parameter codes are that they can't predict some of the details of local gas mixing, and molecular/turbulent diffusion model is generally lacking.

Lumped parameter codes include: CONTAIN (SNL/NRC, USA), MELCOR (SNL/NRC, USA) , GOTHIC(NAI/EPRI, USA), FUMO (DCMN Pisa University, Italy), MAAP (EPRI/FAI), RALOC (GRS, Germany), FIPLOC (GRS, Germany), WAVCO (Siemens/KWU, Germany), etc.

2.1.2 Field Codes

In field codes, spatial variation of flow parameters is locally taken into account and a momentum equation is solved at a number of discrete points that represent a finite control volume. Conservation equations for mass, energy, and momentum are developed on the basis of partial differential equations where trends in spatial variations of parameters are calculated inside a control volume. One significant difference, comparing to a lumped-parameter code, is that the momentum equation in a field code is a multidimensional equation, considering transfers from the connected control volumes and accounting for the advection of momentum between volumes.

The field codes can predict local steam–gas concentrations that could be important in determining the spatial progression of certain hydrogen combustion events and the details related to an evaluation of hydrogen mitigation strategies. But because of complex containment geometrical model and relatively larger quantities of grids, the field codes always have protracted input set-up time and long computational time.

Field codes include: GASFLOW (FZK, Germany, and LANL/NRC, USA), INSPAT/CV (NUPEC, Japan), CFX-F3D, FLUENT, etc.

2.1.3 Combination of Lumped Parameter Codes and Field Codes

The combination of both types of codes, such as TONUS (IPSN, France), can combine the advantages of each of them. The lumped parameter code is used to analyze an accident in a more global way, while the field code is employed to analyze special phenomena over limited periods.

2.2 CFD codes GASFLOW and FLUENT

2.2.1 GASFLOW

The 3-D-field code, GASFLOW version 2.1 is a joint development of Forschungszentrum Karlsruhe and Los Alamos National Laboratory for the simulation of steam and hydrogen distribution and combustion under severe accident conditions in nuclear reactor containments. GASFLOW gives a solution of the compressible 3-D Navier–Stokes equations and has been validated by analyzing experiments that simulate the relevant aspects and integral sequences of such accidents and related experiments[3]. An analysis with GASFLOW will result in a prediction of (1) the gas composition and discrete particle distribution in space and time throughout the facility and (2) the resulting pressure and temperature loadings on the walls and internal structures with or without combustion. A major application of GASFLOW is for predicting the transport, mixing, and combustion of hydrogen and other gases in nuclear reactor containments and other facilities. It has been applied to situations involving transporting and distributing combustible gas mixtures. It has been used to study gas dynamic behavior (1) in low-speed, buoyancy-driven flows, as well as sonic flows or diffusion dominated flows; and (2) during chemically reacting flows, including deflagrations. The effects of controlling such

mixtures by safety systems can be analyzed.

2.2.2 FLUENT

FLUENT is a state-of-the-art computer program for modeling fluid flow and heat transfer in complex geometries. FLUENT provides complete mesh flexibility, solving your flow problems with unstructured meshes that can be generated about complex geometries with relative ease. [4]

The FLUENT solver has the following modeling capabilities:

·flows in 2D or 3D geometries using unstructured solution-adaptive triangular/tetrahedral, quadrilateral/hexahedral, or mixed (hybrid) grids that include prisms (wedges) or pyramids.
·incompressible or compressible flows
·steady-state or transient analysis
·inviscid, laminar, and turbulent flows
·convective heat transfer, including natural or forced convection
·coupled conduction/convective heat transfer
·chemical species mixing and reaction, including combustion sub models and surface deposition reaction models
·arbitrary volumetric sources of heat, mass, momentum, turbulence, and chemical species
·phase-change models
·multiphase flows, including cavitation
·free-surface flows with complex surface shapes

3. CONTAINMENT GEOMETRICAL MODELS AND PHYSICAL CONDITIONS

3.1 Geometrical Models for FLUENT and GASFLOW

The geometrical configuration studied in this paper is a simplified enclosure with all the main features of a PWR containment. The geometry is a 64 meters high cylinder with a radius of 20 meters，as Figure 1 shown. Two internal cylindrical walls with 18 m and 6 m radius and 10 radial walls divide the internal space of the containment into several rooms: three steam generator (SG) rooms, three pump rooms and one pressurizer room, as shown in Fig 2. The SG rooms are open at the top, allowing a free circulation of gas between the rooms and the dome, while the other four rooms are closed by the ceiling. Some openings have been included in the geometry between the SG rooms and the pump rooms, between the radial rooms and the external annular rooms. The total free gas volume in the containment is 50,648 m^3 (the original volume of the empty cylinder was 74,634 m^3). GASFLOW simulates the containment in 3-D cylinder meshes with 31,968 cells (18r, 37theta, 48z), and FLUENT simulates in unstructured meshes with 424,879 cells. The average cell volumes are 2.3 m^3 and 0.176 m^3 for GASFLOW and FLUENT, respectively.

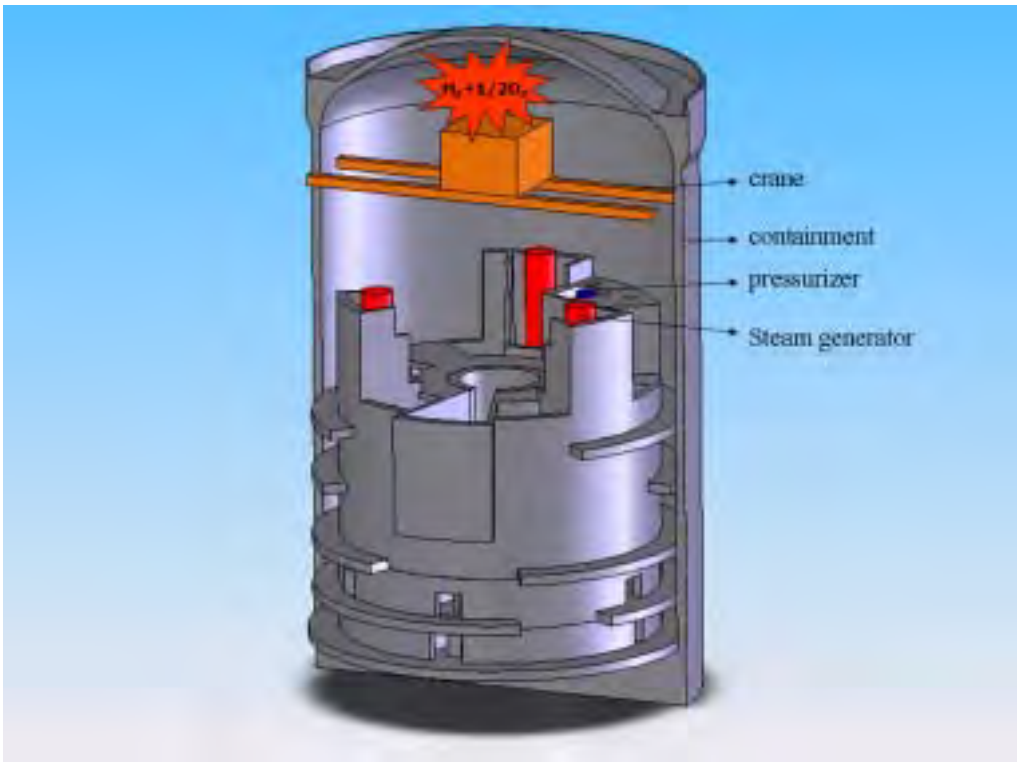


Fig.1 Geometrical Model of the Containment of PWR NPP

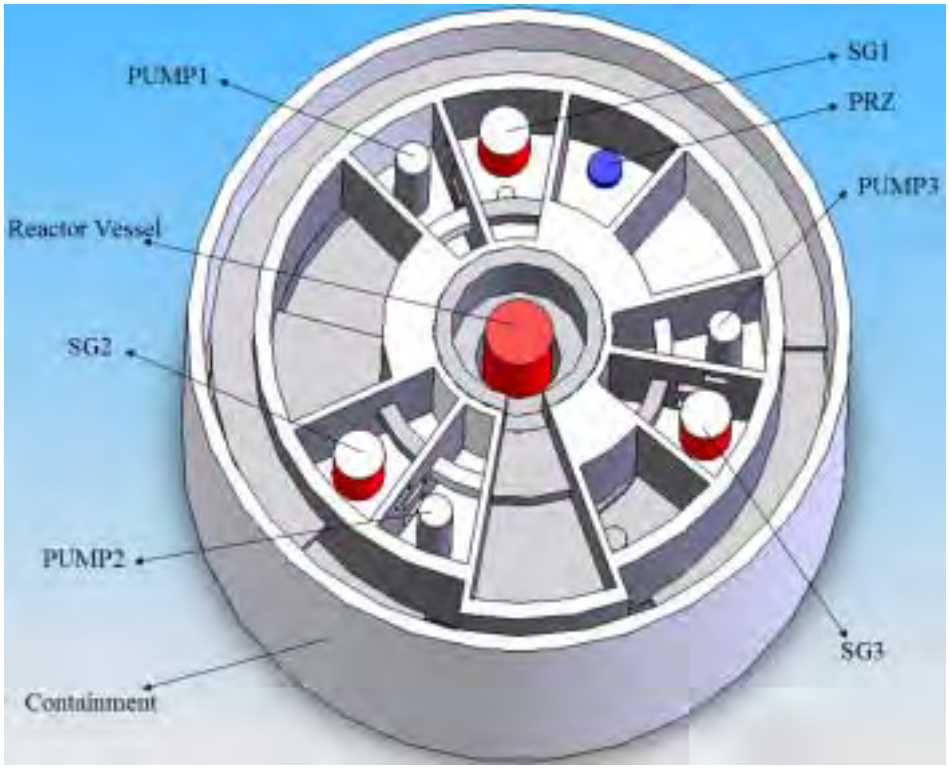


Fig.2 19 Points that Record Local Hydrogen Concentration

3.2 Boundary Conditions and Physical Models

3.2.1 Basic Assumptions and Boundary Conditions

The hypothetic severe accident sequence of large LOCA is investigated in this paper, and the leak, whose diameter is 0.8m, is at the cool leg in the steam generator room. The initial condition of pressure and temperature in the containment is assumed to be homogenous, 2bar and 383k, respectively. The mass flow rate of the gas mixture from the inlet is constant at 2kg/s, and the volume fraction of hydrogen and steam are 50%, respectively. At 500s, the 500 kg of hydrogen presents in the containment of a French 1,000MWe PWR could yield a mean 11.1% H2 volume fraction in a dry atmosphere.

The reaction of hydrogen and oxygen is not considered in order to investigate local hydrogen concentration without mitigation measures. Condensation of the steam on the walls is not considered because steam is assumed as to be super heated in the simulation. Under these assumptions, local hydrogen and steam concentration are only controlled by the fluid dynamics.

3.2.2 Basic Numerical Models

3.2.2.1 Standard $k-\varepsilon$ Model

The standard $k-\varepsilon$ model is a semi-empirical model based on model transport equations for the turbulence kinetic energy (k) and its dissipation rate (ε). The model transport equation for k is derived from the exact equation, while the model transport equation for ε was obtained using physical reasoning and bears little resemblance to its mathematically exact counterpart.

The turbulence kinetic energy, k, and its rate of dissipation, ε, are obtained from the following transport equations:

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}[(\mu+\frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial x_j}]+G_k+G_b-\rho\varepsilon-Y_M+S_k \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon)+\frac{\partial}{\partial x_i}(\rho \varepsilon u_i)=\frac{\partial}{\partial x_j}[(\mu+\frac{\mu_t}{\sigma_\varepsilon})\frac{\partial \varepsilon}{\partial x_j}]+C_{1\varepsilon}\frac{\varepsilon}{k}(G_k+C_{3\varepsilon}G_b)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}+S_\varepsilon \quad (2)$$

In these equations, G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients. G_b is the generation of turbulence kinetic energy due to buoyancy. Y_M represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate. $C_{1\varepsilon}$, $C_{2\varepsilon}$ and $C_{3\varepsilon}$ are constants. σ_k and σ_ε are the turbulent Prandtl numbers for k and ε, respectively. S_k and S_ε are user-defined source terms.

The turbulent viscosity, μ_t, is computed by combining k and ε as follows:

$$\mu_t=\rho C_\mu\frac{k^2}{\varepsilon} \quad (3)$$

where C_μ is a constant.

The model constants $C_{1\varepsilon}, C_{2\varepsilon}$, C_μ, k and ε, have the following default values:

$C_{1\varepsilon}$=1.44, $C_{2\varepsilon}$=1.92, C_μ=0.09, σ_k=1.0, σ_ε=1.3

3.2.2.2 Species Transport Model

When conservation equations for chemical species are solved, FLUENT predicts the local mass fraction of each species, Y_i, through the solution of a convection-diffusion equation for the *i*th species. This conservation equation takes the following general form:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \bullet (\rho \vec{v} Y_i) = -\nabla \bullet \vec{J}_i + R_i + S_i \quad (4)$$

where R_i is the net rate of production by chemical reaction and S_i is the rate of creation by addition from the dispersed phase plus any user-defined sources. In turbulent flows, FLUENT computes the mass diffusion in the following form:

$$\vec{J}_i = -(\rho D_{i,m} + \frac{\mu_t}{Sc_t})\nabla Y_i \quad (5)$$

where Sc_t is the turbulent Schmidt number.

4. ANALYSIS RESULTS

The main goal of the investigation is to assess the capability of the GASFLOW code to predict hydrogen concentration distributions and velocity fields for a variety of physical conditions. The assessment relied on the comparison with the results obtained using the commercial computational fluid dynamics code FLUENT [5]. The assessment of the GASFLOW code was based on the following aspects:

· assessment of the implementation and performance of the $k-\varepsilon$ model, because a much coarser mesh of GASFLOW than that of FLUENT is used;

· assessment of the results with $k-\varepsilon$ turbulence model and without turbulence model using the code GASFLOW;

· assessment of the results with $k-\varepsilon$ turbulence model and laminar model using the code FLUENT.

Four cases were selected to complete the assessment, as table 1 shown.

Table.1 Four cases to assess GASFLOW calculation capability

case	code	Flow model	Mass and energy diffusion	Momentum diffusion
1	FLUENT	Turbulence($k-\varepsilon$)	yes	yes
2	FLUENT	laminar	no	no
3	GASFLOW	Turbulence($k-\varepsilon$)	yes	yes
4	GASFLOW	laminar	no	no

4.1 Hydrogen Concentration and Velocity Field

The released gas mixture of steam and hydrogen form a buoyant jet that rises through the steam generator tower above the source. The momentum of the ejected material dissipates fast

after steam and hydrogen are released into the steam generator room. The gas mixture rises through the opening of the steam generator room to the dome. The velocity field of the mixtures, the calculation result of case 1 at 500s, is shown in Fig. 3.

As Fig.4 shown, hydrogen cloud, which is assumed not to be reacted with oxygen, transports and stratifies in the upper of the containment at 100s, 200s, 400s, and 500s.

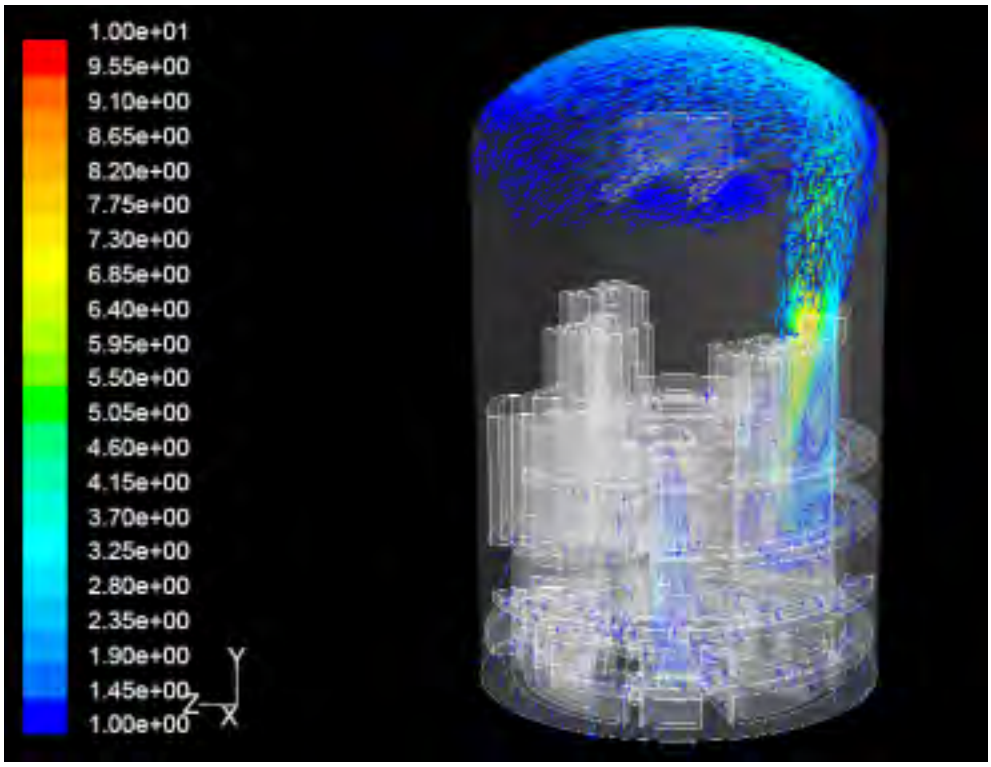


Fig.3 Velocity Field of the Mixtures of Case 1

Hydrogen accumulates in the dome at first. With hydrogen mass in the containment increasing, hydrogen begins to stratify. After 500s, all hydrogen from the jet is mixed inside the stratified cloud. If the hydrogen cloud exists in a dry atmosphere without steam, this cloud would stay stratified for a long time. Steam condensation on the structures will locally increase the gas density and start a secondary downward-directed flow that brings the hydrogen from the stratified region down into the lower part of the containment [6].

Hydrogen distributions at 200s of the four cases above are compared, as Fig.5 shown. At 200s, there was about 200kg hydrogen in the containment. Calculation results with standard $k-\varepsilon$ model and laminar model using FLUENT code show in case1 and case2 in Fig.5. They show nearly the same hydrogen concentration distributions, which indicate that turbulence simulation has minor effects in the investigated grid. To further study turbulence flow and vortex formations in the containment, finer grid is needed. GASFLOW results with standard $k-\varepsilon$ model and laminar model were shown in case 3 and case 4 in Fig.5. They show large difference in the hydrogen concentration distributions. With $k-\varepsilon$ model and diffusion model used in case3, hydrogen distribution is nearly the same as the results of FLUENT. But local hydrogen volume fraction is 8% at the dome region, which is lower than the volume fraction of 12% calculated in FLUENT. Without consideration of turbulence and diffusion in case4, hydrogen rises directly to the dome, and then accumulates in the dome. The highest

hydrogen volume fraction in the dome is 26%, and hydrogen concentration in the dome region is obviously higher than the other region in the containment. Calculation using laminar flow assumption in the investigated grid will be very misleading, and the results of case 4 are not acceptable. It indicates that the investigated grid in GASFLOW is not so fine that the effect of turbulence simulation can be neglected.

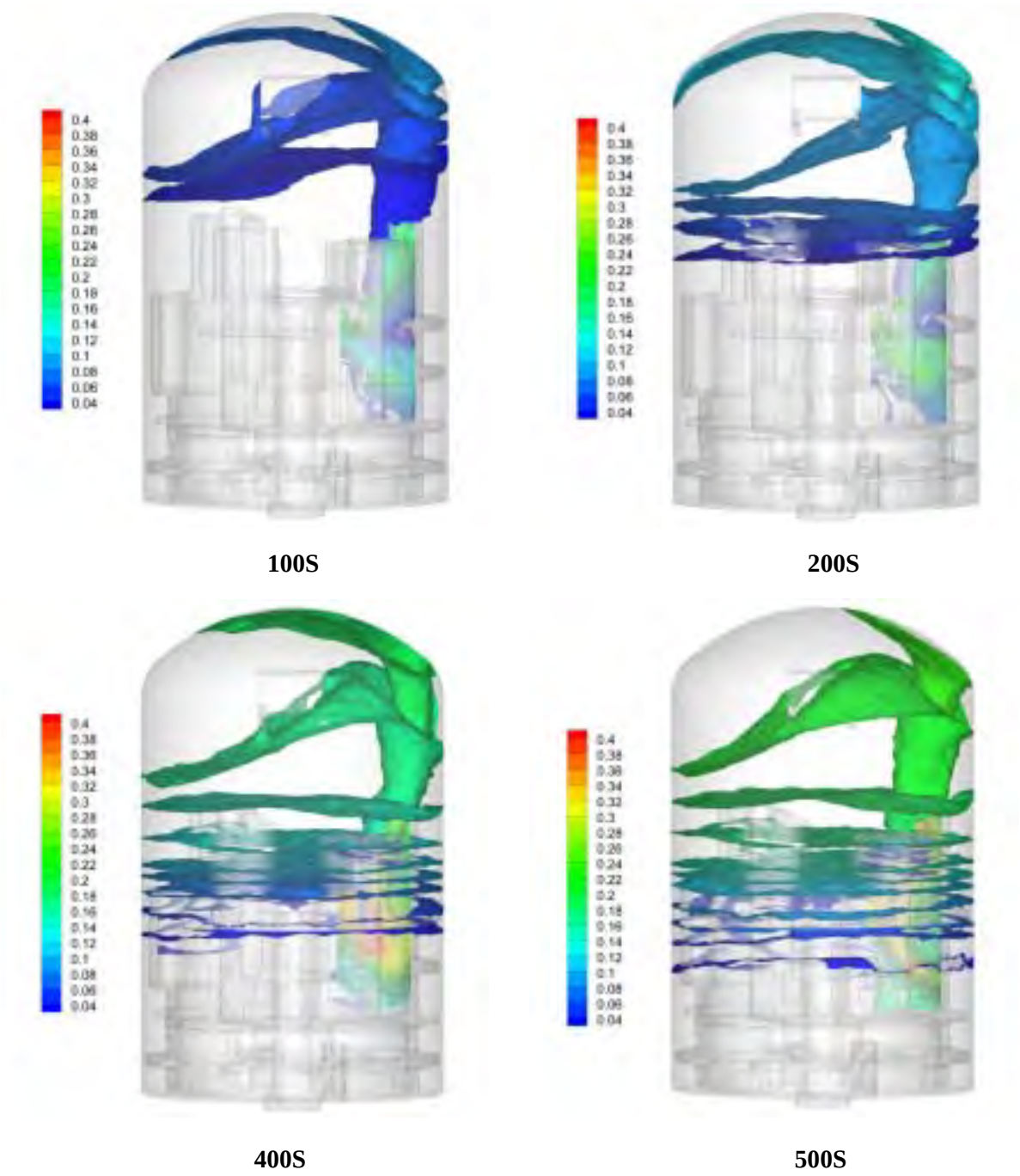
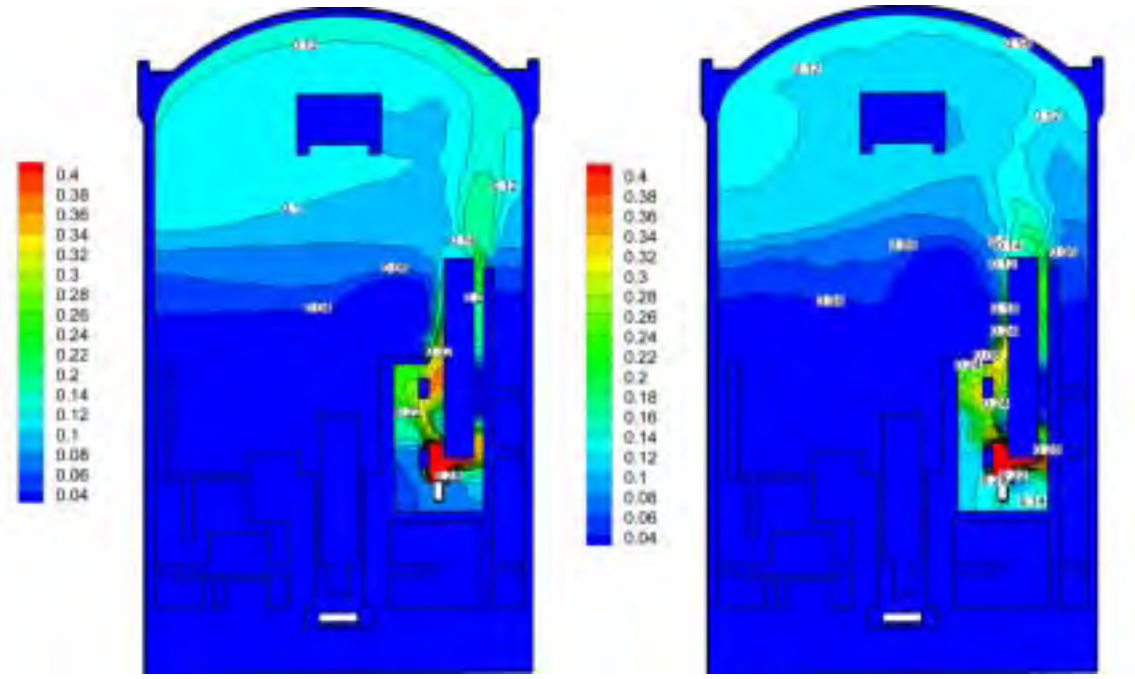
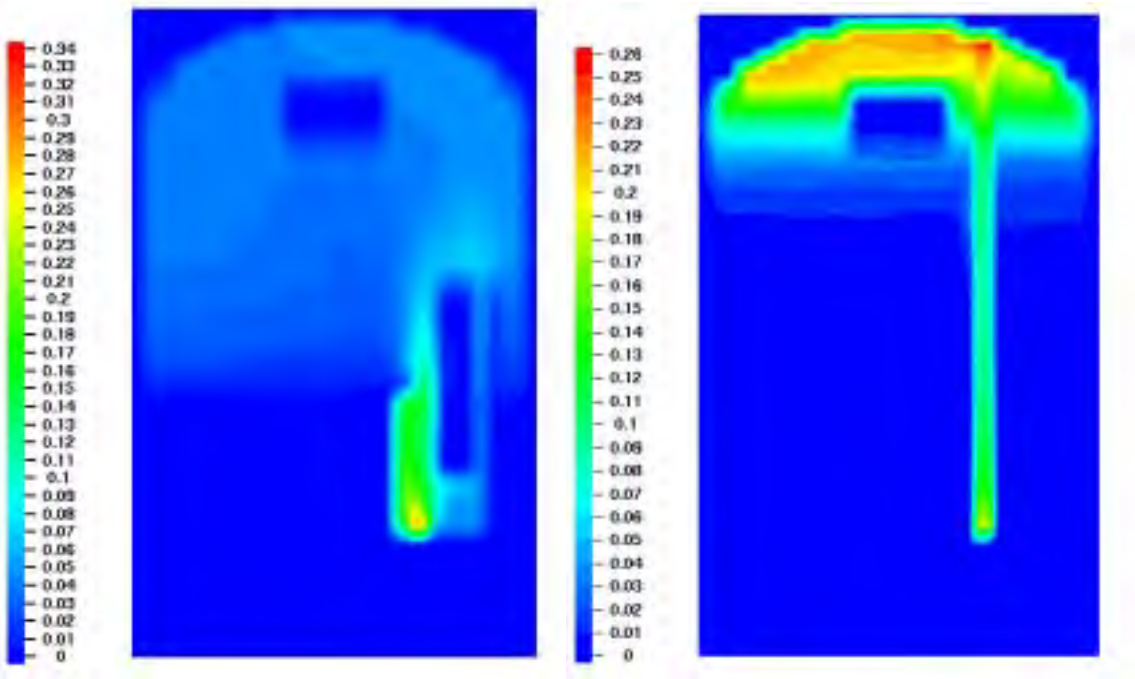


Fig.4 Hydrogen Cloud Transport and Stratification in the Containment at 100S, 200S, 400S, 500S



Case 1 **Case 2**



Case 3 **Case 4**

Fig.5 Hydrogen Volume fraction in the containment

4.2 Local Hydrogen Flammability

The local hydrogen, steam, and air volume fractions were recorded in 19 points during the simulation. Those points are identified in Fig.6 by the P1, P2, … and P19. As Fig.7 shown, local hydrogen volume fraction from 0s to 500s was recorded.

At the very beginning of the industrial development of pressurized water reactors (PWR), the possibility of an ignition of ternary mixtures containing hydrogen, air and water vapour was considered, and thoroughly described by Shapiro and Moffette[7][8]. They showed that, hydrogen being released with a large amount of steam from the primary circuit in case of a loss-of-coolant accident, the lower flammability limit of the mixture in the containment is significantly above the H2 = 4.1% limit in air (Fig. 8). The volume fraction of hydrogen, air and steam at 19 points of P1,…P19, is shown in Fig.9.

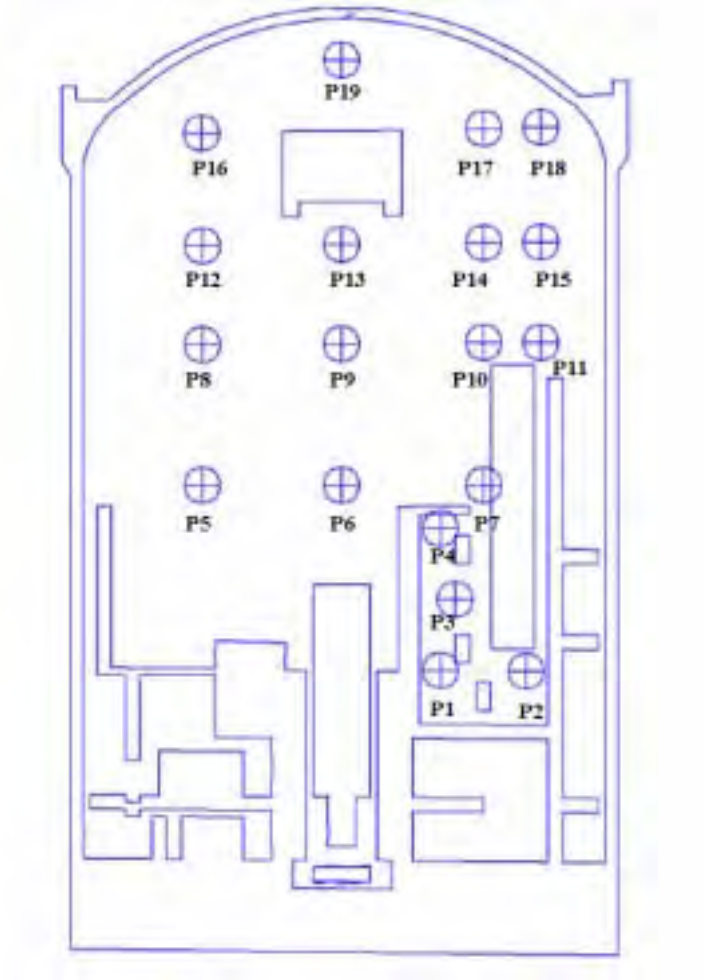


Fig.6 19 Points that Record Local Hydrogen Concentration

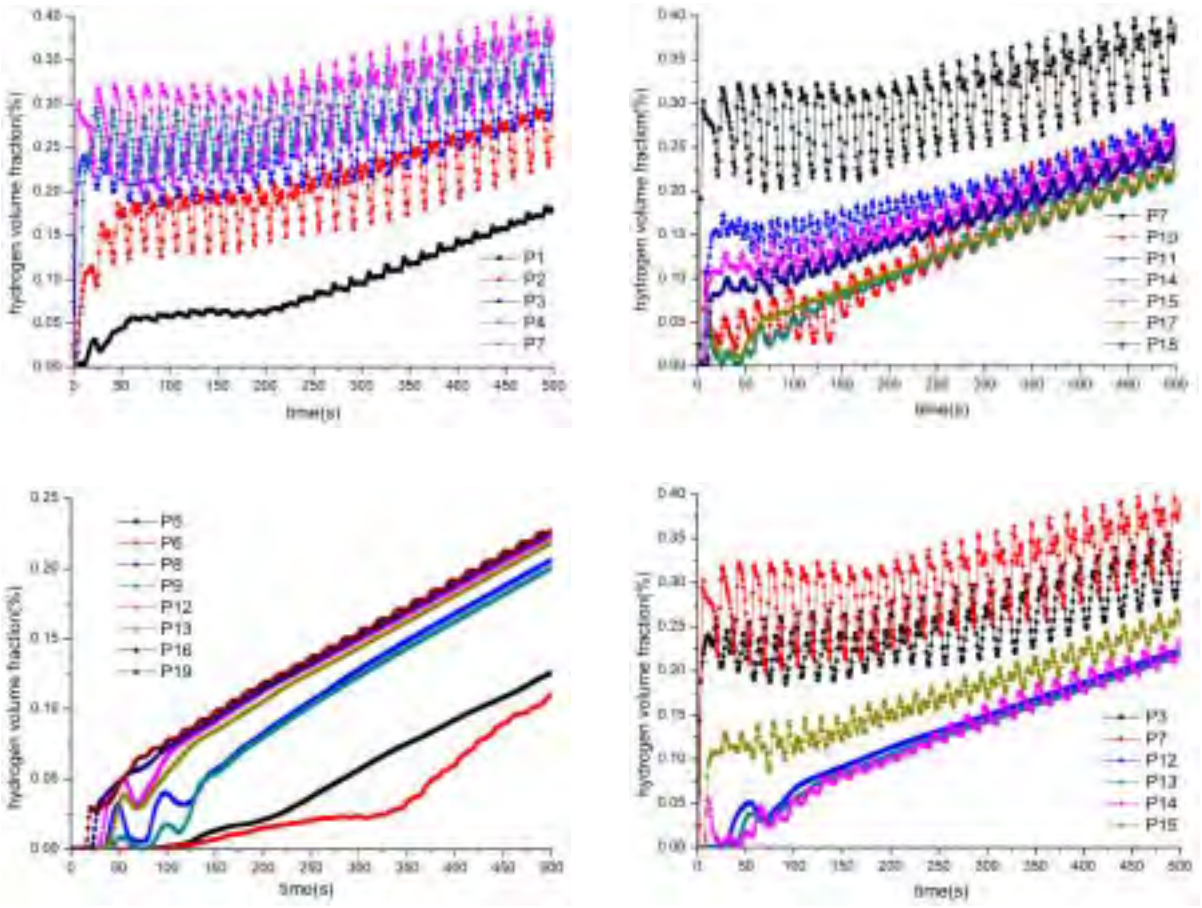


Fig.7 Local Hydrogen Concentration at 19 points from 0-500S

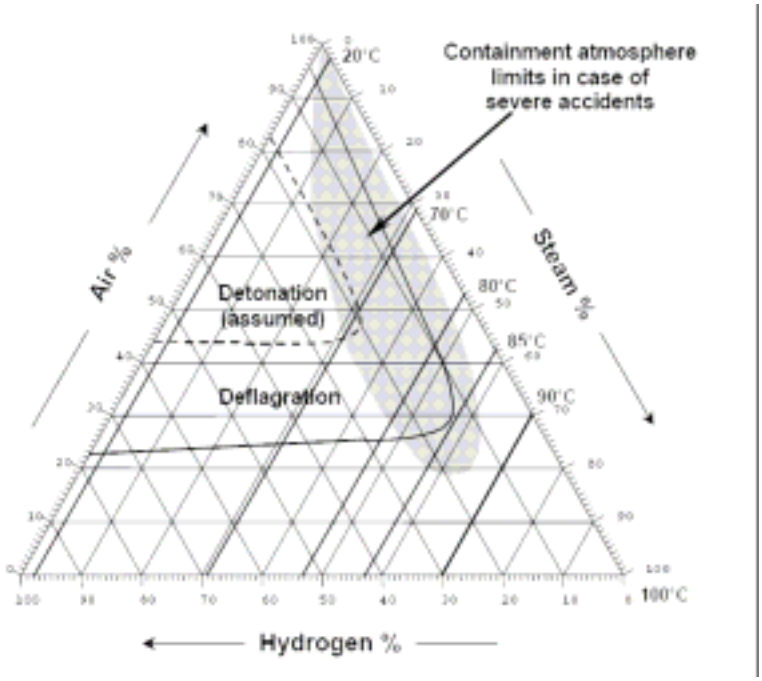


Fig.8 Flammability limits of hydrogen–air–steam mixtures

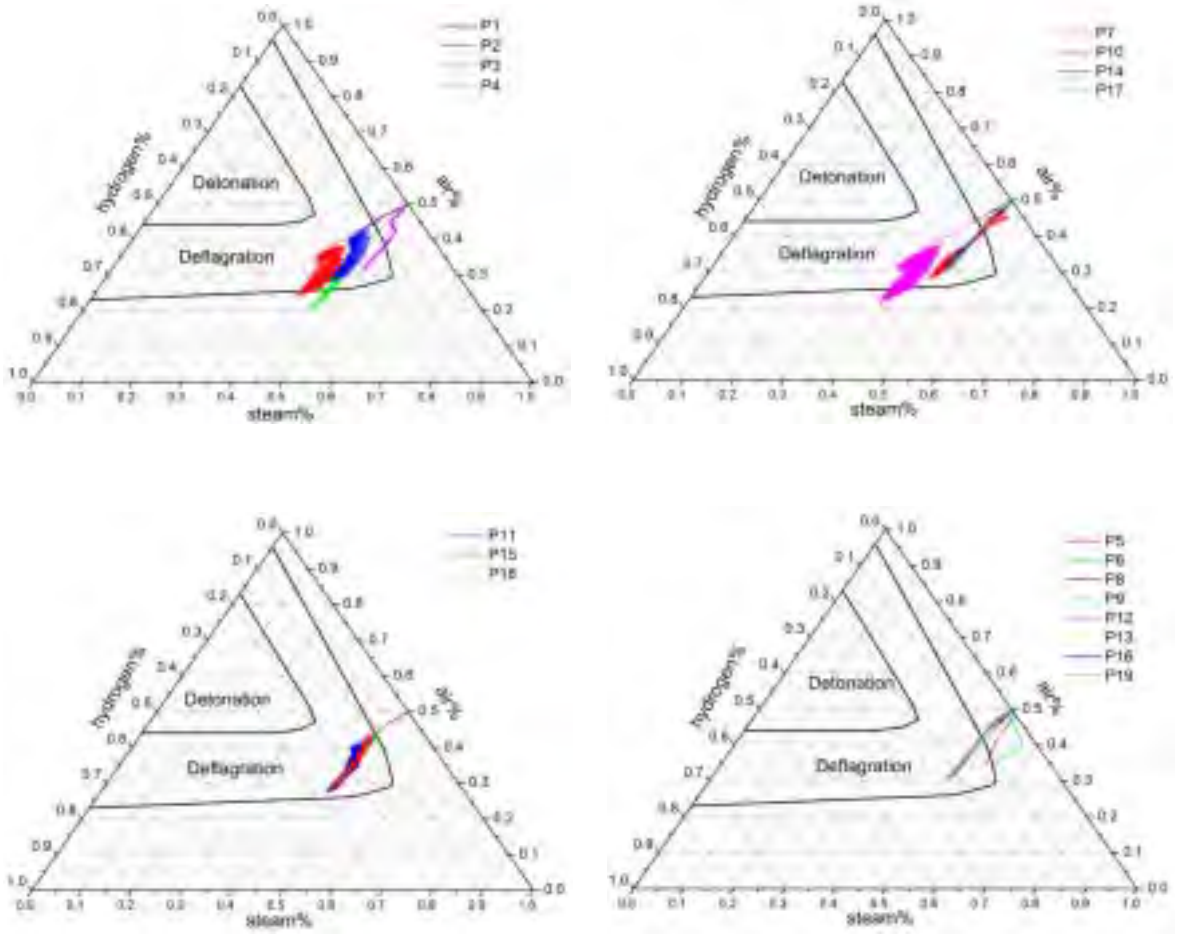


Fig.9 Local flammability of hydrogen–air–steam mixtures in 19 points

5. CONCLUSIONS

The discussed FLUENT and GASFLOW simulations of the large-break LOCA demonstrate hydrogen and steam injection in the containment. During the release phase with steam and hydrogen, the codes predict the transient formation of a buoyant jet that extends from the source up through the steam generator tower into the dome. Hydrogen accumulates in the dome region, and then begins to stratify with increasing of hydrogen mass in the containment. The hydrogen cloud would stay stratified for a long time, if steam condensation is assumed not to occur.

To assess the capability of the GASFLOW code to predict hydrogen concentration distributions and velocity fields for a variety of physical condition, four cases were selected. FLUENT calculation results with standard $k-\varepsilon$ model and laminar model showed nearly the same hydrogen concentration distributions, which indicate that turbulence simulation has minor effects in the investigated FLUENT grid. But in the much coarser grid in GASFLOW, large differences exist between the turbulence and laminar simulation. Calculation using

laminar flow assumption in the investigated grid in case4 is very misleading, and the effects of turbulence and mass diffusion can not be neglected in the present GASFLOW grid. To reduce the computational cost, grid in GASFLOW should be refined to simulate the flow with laminar model.

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