Proceedings of ICONE 23:
23th International Conference on Nuclear Engineering
May 17-21, 2015, Chiba, Japan

ICONE23-1655

DEVELOPMENT OF HYDROGEN BEHAVIOR SIMULATION CODE SYSTEM –OUTLINE OF CODE SYSTEM AND VALIDATION USING EXISTING DATA-

Atsuhiko TERADA
JAEA, 4002 Narita-cho, Oarai-machi, Ibaraki, JAPAN 311-1393
Phone:029-267-4141, Fax:029-266-7608
e-mail:terada.atsuhiko@jaea.go.jp

Masaaki MATSUMOTO
Mitsubishi Research Institute Inc, 6-9-3 Higashiueno, Taitou-ku, Tokyo, JAPAN 110-0015
Phone:03-5246-2553, Fax:03-5246-2537
e-mail:nakajima.norihiro@jaea.go.jp

Hitoshi SUGIYAMA
Utsunomiya University, 7-1-2 Yotou, Utsunomiya, Tochigi, JAPAN 321-8585
Phone:028-689-6031, Fax:028-689-6031
e-mail:sugiyama@cc.utsunomiya-u.ac.jp

Yu KAMIJI
JAEA, 4002 Narita-cho, Oarai-machi, Ibaraki, JAPAN 311-1393
Phone:029-267-4141, Fax:029-266-7608
e-mail:kamiji.yu@jaea.go.jp

Satoshi KADOWAKI
Nagaoka University of Technology, 1603-1 Kamitomioka, Nagaoka, Niigata, JAPAN 940-2188
Phone:0258-47-9719, Fax:0258-47-9770
e-mail:kadowaki@mech.nagaokaut.ac.jp

Ryutaro HINO
JAEA, 4002 Narita-cho, Oarai-machi, Ibaraki, JAPAN 311-1393
Phone:029-266-7154, Fax:029-266-7608
e-mail:hino.ryutaro@jaea.go.jp

Keywords: Hydrogen, Simulation, general-purpose commercial code, Open source code, Code system, validation

ABSTRACT

In the Fukushima Daiichi Nuclear Power Station (NPS) accident, hydrogen was generated by oxidation reaction of the cladding and water etc,., then leaked into the NPS building, and finally led to occurrence of hydrogen explosion in the building. This resulted in serious damage to the environment. To improve the safety performance of the NPS, especially on the hydrogen safety under severe accident conditions, a simulation code system has been developed to analyze hydrogen behaviors including diffusion, combustion, explosion and structural integrity evaluation. This developing system consists of CFD and FEM tools in order to support various hydrogen user groups of students, researchers and engineers. Preliminary calculated results obtained with above mentioned

Copyright © 2015 by JSME

tools, damage of piping induced by hydrogen combustion, agreed well with existing test data.

1. INTRODUCTION

The accident of the Fukushima Daiichi Nuclear Power Station (NPS) made deepen our awareness on nuclear safety, especially nuclear hydrogen safety. At the severe accident (SA), a large quantity of high temperature steam and chemical substances are released with flammable gas mixed with hydrogen. It is necessary to predict hydrogen distribution in NPS, combustion risk, and its effects (TECDOC I.,2011). In the world, research organizations and companies have been made and/or improved special analysis codes on hydrogen behavior such as diffusion, convection, combustion and explosion in order to evaluate hydrogen safety and propose hydrogen safety technologies (OECD/NEA I.,2008.,2014).

This paper introduces development status of a simulation code system on hydrogen behavior to contribute SA analyses, preliminary validation using the system, and simulation results of fluid-structure interaction under hydrogen combustion.

2. SIMULATION CODE SYSTEM

2.1 System diagram

Based on the phenomenal progress scenario, this system is consisted of following three analysis phases: (i) diffusion analysis of leaked flammable gas, (ii) Combustion analyses under deflagration or detonation, (iii) structural analysis against detonation and deflagration. Figure 1 shows the system diagram. In these phases, key models are summarized as follows:

(i) Diffusion analysis of leaked flammable gas

To carry out diffusion analysis of leaked hydrogen gas, it is necessary to consider local density and temperature changes which generate local buoyancy flow. These changes are promoted mainly by steam condensation. Condensation model and buoyancy turbulence model (Kato, N. et al., 2015) are incorporated in this phase.

(ii) Combustion analyses

Diffusion analysis results are used as initial conditions of this phase, and then combustion analyses including explosive analyses are conducted to obtain a flame speed, a blast pressure under deflagration or detonation along an ignition scenario (ignition time, ignition place etc.). The flame speed and the blast pressure are affected by diffusion spaces and obstacles such as pipings and apparatuses in the space. Flame acceleration model (Katsumi,T. et al.,2014) and turbulence combustion model are incorporated to this phase.

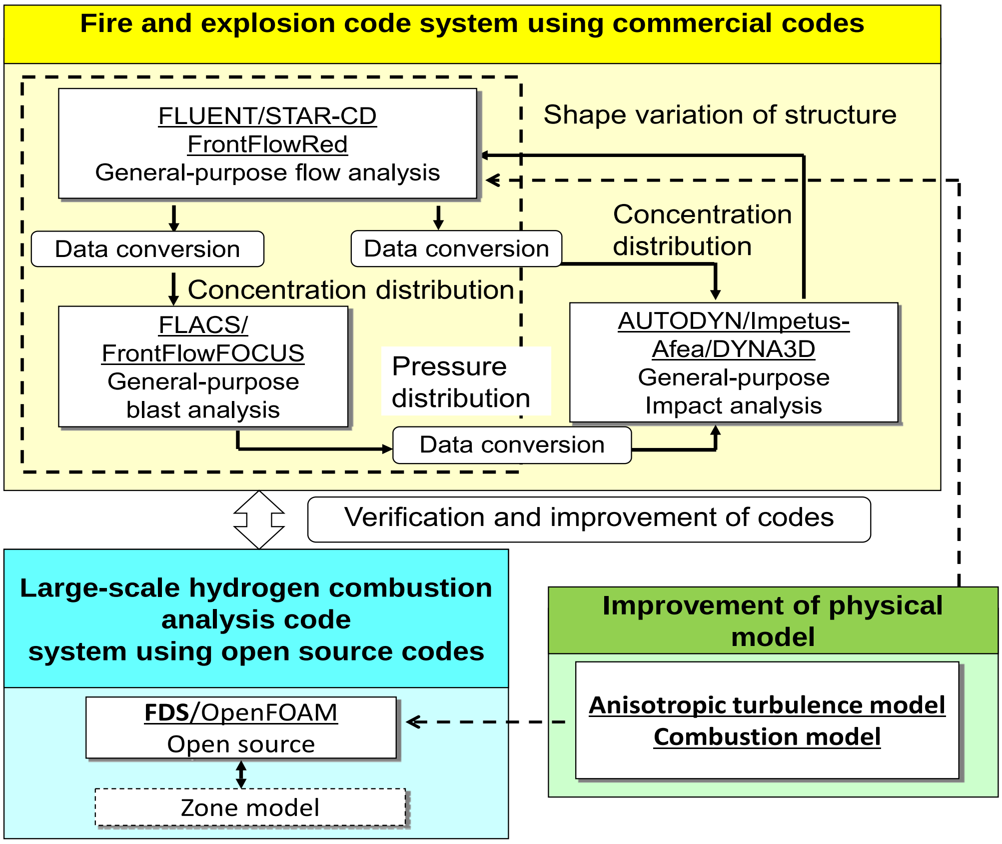


Fig.1 Simulation code system

(iii) Structural analysis against deflagration or detonation

Blast pressure obtained in combustion analyses is used as an initial condition of this phase. Effect investigation (combustion and explosive effects) is conducted to obtain stress distribution. Then, stress loaded to NPS structures such as steel-reinforced concrete walls and a steel-made container is analyzed to confirm its deformation or destruction of these structures.

2.2 Outline of code system

The code system consists of fire and explosion code system using general purpose commercial codes and large-scale hydrogen combustion analysis code system using open source codes and database. An input database for hydrogen generation is calculated result data of complex radiolysis, SA codes (MAAP etc.). Physical model and apparatus model for hydrogen safety improves based on experimental data and knowhow stored from now.

Also, fire and explosion code system consists of three phenomena, hydrogen diffusion, combustion, effect investigation (explosive effect). In this system, users simulate the hydrogen concentration in the vessel and building by using FLUENT (http://ansys.jp/products/fluid/fluent/) and FrontFlowRed (http://www.nufd.jp/product/nufd_frontflowred.html). Based on the concentration distribution, users simulate combustion status such as overpressure on the wall and blast propagation by FLACS (http://www.gexcon.com/flacs-software)and FrontFlowFOCUS(http://www.advancesoft.jp/product/index.html). Based on the pressure distribution, users simulate the stress distribution on the vessel and building wall by AUTODYN (http://ansys.jp/products/explicit/autodyn/), DYNA3D(http://www.oecd-nea.org/tools/abstract/detail/ests0138) and ImpetusAfea (http://impetus-afea.com/). If the wall was broken and deformed, the shape of analytical model changes and users simulate flow diffusion analysis by FLUENT etc., again. The date mentioned above such as hydrogen concentration and pressure distribution is converted as input data of the codes using interfaces.

FLUENT, FLACS, AUTODYN etc. mentioned above are general-purpose commercial codes based on FEM or FVM methods and have been used for hydrogen behavior analysis. But these codes are high-cost and limit the improvement of codes. So, we have been proceeding to develop by the open source codes in parallel with by commercial codes.

The open source code system is prepared for various hydrogen users who would like to directly incorporate their own latest knowledges such as physical models and databases with the system. FDS (http://code.google.com/p/fds-smv/) and OpenFOAM (http://www.openfoam.com/) can be used for combustion analyses as well as diffusion analyses.

3. PRELIMINARY ANALYSIS

3.1 Hydrogen combustion analysis

Preliminary hydrogen combustion analyses were conducted using FrontFlowFOCUS under the conditions of ISP49 HD-tests (OECD/NEA I., 2011). Figure 2 shows the test vessel configuration of the THAI HD test in ISP49 HD-tests. A cylindrical combustion room of 60m^3 is 9.2m height and 3.2 m diameter. The outer surface temperature of the room was controlled by thermal oil. The initial test conditions were as follows:

- pressure : 1.5bar
- temperature: 90℃
- volume fraction (H_2) at HD22: 10%
- volume fraction (steam) at HD22: 25%
- volume fraction (H_2) at HD23: 12%
- volume fraction (steam) at HD23: 25%

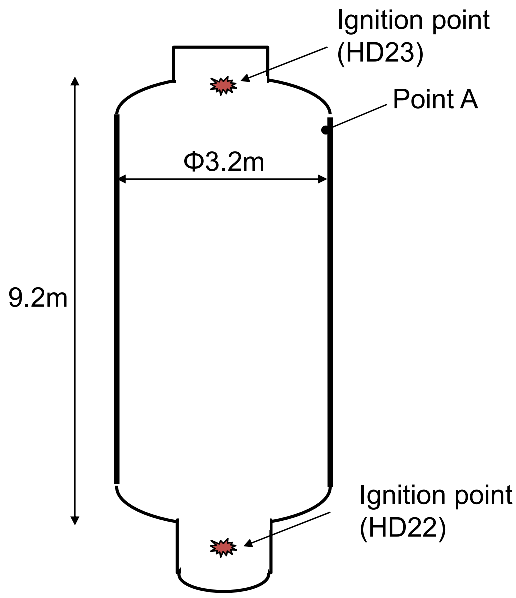


Fig.2 Test vessel configuration of THAI HD-tests (OECD/NEA I., 2011)

HD22 test was the flame propagation to upward after ignition at the bottom, and HD23 test the flame propagation to downward after ignition at the top. Combustion speed was made slow by steam, so that combustion phenomena are in the slow deflagration.

Copyright © 2015 by JSME

In the analysis, a pre-mixture combustion model considering the flame acceleration caused by hydraulic instability of the flame front surface (Tomizuka, T. et al., 2013). In order to consider the acceleration due to turbulence of the flame in real scale to use the following artificial reaction model (1).

$$\frac{\partial(\rho c)}{\partial t}+\frac{\partial(\rho c u_j)}{\partial x_j}=\dot{\rho}_B \qquad (1)$$

$$\begin{aligned}\dot{\rho}_B &= \rho S_T|\nabla c| \quad & 0\le c<1\\ \dot{\rho}_B &= 0 & c\ge 1\end{aligned} \qquad (2)$$

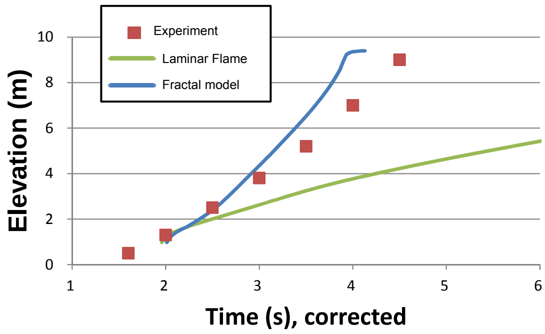
Here, St is the burning speed. St have been introduced with fractal flame propagation model. This model is expressed by the following equation.

$$S_T=\max\left\{S_L,\frac{3}{2}c_g\left(\frac{\rho_u}{\rho_b}\right)\frac{S_L^2}{\sqrt{\kappa}}t^{1/2}\right\} \qquad (3)$$

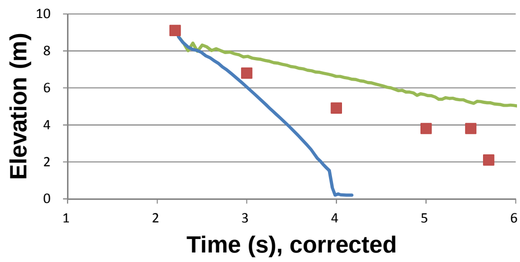
Here, this model (3) includes expansion rate of the gas (ρ_u / ρ_b), laminar combustion speed (S_L) and thermal diffusivity (κ) in the physical properties of the flammable gas, model constant Cg.In this combustion model, the flame progresses in a laminar combustion speed (S_L) and is accelerated in the S_T if S_T by Fractal flame propagation model exceeds the S_L. In this preliminary analysis, it is assumed the laminar burning velocity 1m/s, the thermal diffusivity: were the κ = 3.2 × 10^{-5} model constants Cg = 1.6 × 10^{-3} (Tomizuka, T. et al., 2013).

Figure 3 shows calculated results of a vertical motion of the flame front (flame propagation speed), and Fig. 4 pressure transient at Point A (Fig.2).

The flame propagation speed and pressure increase trends almost agree with test data of HD22. As for HD23, calculated results could not predict the test data. This would be improved by introducing an appropriate flame propagation acceleration model considering the space scale effect as well as a detailed thermal property database of the reactant composition such as GRI-Mech (http://combustion.berkeley.edu/gri-mech/).

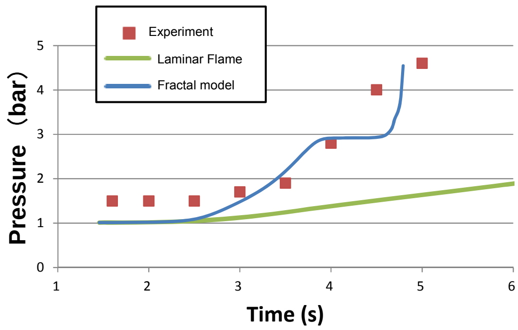


(a) HD22

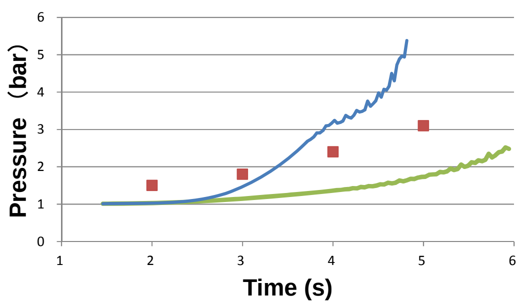


(b) HD23

Fig.3 Vertical motion of flame



(a) HD22



(b) HD23

Fig.4 Pressure transient at point A

3. 2 Fluid-structure interaction analysis

Preliminary analysis on fluid-structure interaction was conducted to confirm a data conversion between combustion and structural analysis codes using the existing data detonation wave propagation in a closed piping (TENPES, 2007). FrontFlowFOCUS was used for combustion analysis and Dyna3D for structural analysis.

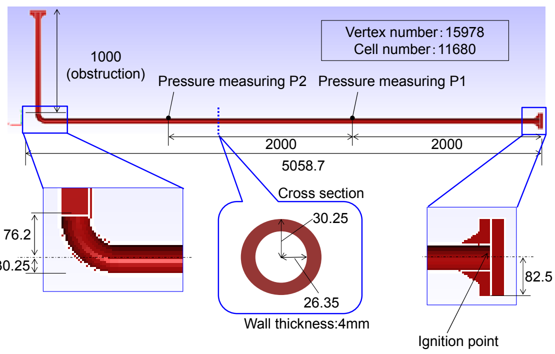
Figure 5 shows analytical models for combustion and structural analyses. Caluculated conditions are as follows:

[combustion analysis]

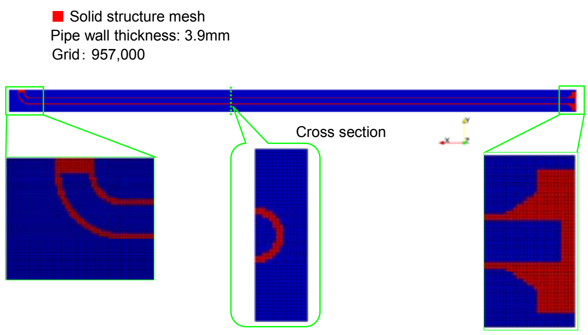
- time step Δt : 1.0×10^{-7} [s]
- initial pressure : 3.5 [MPa]
- initial temperature : 15 [℃]
- time integration method : explicit method
- detonation spped: ZND model caluculated (S. Kao and J. E. Shepherd, 2008)

[structural analysis]

- time step Δt: 1.0×10^{-7} [s]
- pipe material model : elastic perfectly plastic material
- Young ratio : 206 [GPa]
- Poisson ratio : 0.29 (elastic area)
- yield stress : 300 [MPa]
- time integration method : explicit



(a) Structural analytical model



(b) Combustion analytical model

Fig.5 Analytical model

In the analysis, hydrogen mixture gas was filled in the pipe initially. After ignition at the end of the pipe, the detonation wave propagated toward to the elbow. At last, the piping expands outward by the detonation wave as seen in Fig.6. Figure 7 shows the comparison of time-resolved pressure trends between test and analysis. The calculated pressure trends agree well with the test data, though analysis results overestimate peak pressures. This would be improved by pipe deformation in detail which will affect the detonation wave propagation. Also, analysis results predicted the detonation wave reflection at the closed end of the elbow, which provides impact load to damage the pipe wall.

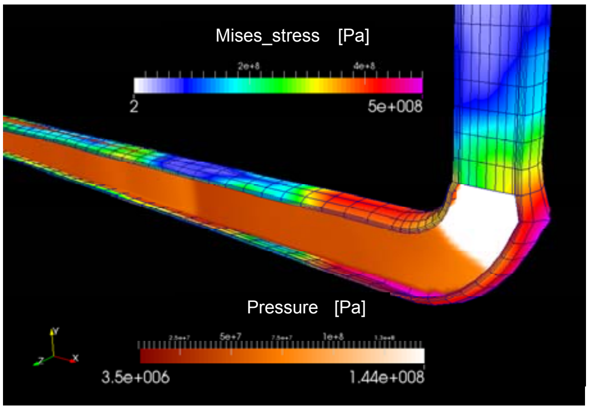


Fig. 6 Displacement and pressure distributions and deformation

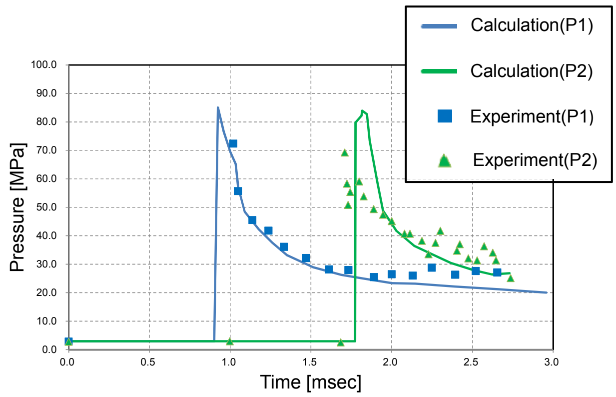


Fig. 7 Time trends of pressure at P1 and P2

4. CONCLUDING REMARKS

The simulation code system on hydrogen behavior is being developed to contribute SA analyses. Preliminary analysis using the system was conducted to validate its performance, especially in the field of combustion and explosion effects using a combustion and a structural analysis codes unified with an interface. This system will be improved step by step by verifying the codes using the existing database such as the OECD/NEA benchmark program etc. and our own dataset. We will provide the system to engineers, researchers and students in the near future.

NOMENCLATURE

c: reaction progree ration
u_j flow velocity
x_j: location of the xi-axis
t: time
κ : thermal diffusibity
S_T: turbulent combustion speed
S_L: laminar combustion speed
C_g: fractal model constant
ρ_u: unburned density
ρ_b: burned density

ACKNOWLEDEMENTS

We gratefully acknowledge Dr.Takayuki Tomizuka, Dr.Ichiro Nakamori, Mr. Keiji Suemitsu and others of AdovanceSoft Corporation for their valuable cooperation.

The present study was performed in the Advanced Nuclear Hydrogen Safety Research Program funded by Agency for Natural Resources and Energy of Ministry of Economy, Trade and Industry.

REFERENCES

Kato, N. et al., 2015, Proc. of 23th Int. Conf. Nucl. Eng., Tokyo, JAPAN, May 17-21, ICONE23-1069

Katsumi,T. et al., 2014, Proc. of 52th Symp. Combustion, Okayama, JAPAN, Dec 3-5.

TECDOC I.,2011., Tech,Rep.IAEA-TECDOC-1661.IAEA

OECD/NEA I.,2014. Tech, Rep. NEA/CSNI/R(2014)8

OECD/NEA I.,2008.,Tech,Rep. NEA/CSNI/R(2007) 13

OECD/NEA I.,2011.,Tech, Rep. NEA/CSNI/R(2011) 9

Tomizuka,T. et al., 2013, Int.J.Hydrogen Energy, Vol.38, pp5176-5180

TENPES, 2007, Design Guideline to prevent the pipe rupture accident due to combustion of radiolysis gas in BWR steam piping

S. Kao and J. E. Shepherd, 2008, GALCIT Report FM2006.007

Copyright © 2015 by JSME