CFD Letters www.cfdl.issres.net Vol. 3 (1) – March 2011

Application of RANS and LES Based CFD to Predict the Short and Long Term Distribution and Mixing of Hydrogen in a Large Enclosure

Pavan K Sharma[c], B. Gera, R. K. Singh

Reactor Safety Division, Bhabha Atomic Research Centre
Trombay, Mumbai 400085, INDIA

Received: 26/10/2010 – Revised 17/01/2011 – Accepted 19/01/2011

Abstract

The paper presents CFD simulations from Reynolds Average Navier Stokes (RANS) and Large Eddy Simulation (LES) based approach of hydrogen release and dispersion inside the large enclosure and comparison with experimental data. The experiment was reported by HySafe Network of Excellence partners, consisting of a 1 g/s vertical hydrogen release for 240 s from an orifice of 20 mm diameter into a rectangular room of dimensions 7.2X2.88X3.78 m in length, height and width respectively. Two small openings were provided at the front and bottom side of the room. During the test hydrogen concentration time histories were measured at few positions in the room, for a period up to 5160 s after the end of release, covering both the release and the subsequent diffusion phases The CFD simulations were performed using a) a 3D transient in-house developed RANS CFD code b) LES based Fire Dynamics Simulator (FDS). Initially when the jet is injected the turbulence intensity is high, but later on the problem is diffusion dominated. Therefore suitable approaches were used to simulate the problem. Initially k-ε High Re number model with standard wall function and buoyancy modification was used and subsequently the transport was modelled as laminar in RANS based approach. The default LES based scheme adopted for LES based computations. The gas mixture was treated as weakly compressible and gravity force was also considered. The results obtained by computations have a good agreement with experiment particularly for LES based calculation. The performed simulation provides useful insight regarding performance of CFD code to simulate hydrogen transport problem and this capability can be further utilized to simulate the hydrogen transport in the real containment geometries.

Keywords: hydrogen distribution; RANS; LES; validation; turbulence.

1. Introduction

The reliable knowledge of the temporal and spatial distribution of hydrogen within reactor containment after an accident is an important issue for its safety assessment. Following the accident at Three-Mile-Island (TMI) in 1979 in USA, the reactor systems all over the world were and are

[c] Corresponding Author: Pavan K. Sharma
Email: pksharma@barc.gov.in Telephone: +91-22-25595158 Fax: +91-22-25505151
 PII: S2180-1363(11)3118-X

still being reviewed for safety against releases of hydrogen under various postulated accident scenarios. Substantial amount of hydrogen is produced by a variety of sources inside containment following severe accident events that lead to degraded fuel cooling and/or high steam content in the containment building. Hydrogen is produced primarily from steam-zirconium (fuel clad) reaction and other sources i.e. radiolysis of water, corrosion of metals and from core concrete interaction. Hydrogen generated in this way is distributed under the effect of forced flow from release and buoyancy into different compartment of containment. Hydrogen in air has the potential for uncontrolled combustion that may cause serious damage to the containment structure due to global burning or explosion. Moreover hydrogen can locally explode in a sub compartment and may damage safety-related equipments. Hydrogen is known to have very low density (about one fourteenth that of air) and wide flammability limit (4-74 % v/v). These unique characteristics imply that hydrogen could disperse extremely fast at an accidental release and combust easily at the presence of an ignition source. A sound understanding of dispersion, stratification and diffusion of released hydrogen during severe accidents is, therefore, of practical importance and use to better understand the possibility of ignition, combustion and explosion of such releases within the context of containment safety.

However, most of the code used for such analysis are based on lumped parameter approach and provide information about average concentration in one compartment. The containment of Indian Pressurised Heavy Water Reactor (IPHWR) has sufficient large volume to accommodate the hydrogen generated well below the flammability limit, but there are chances that hydrogen concentration may increase locally because of complex geometry and flow path restrictions in a sub compartment and may reach to flammability range. Recent uses of computational techniques have shown significant improvements towards modelling such phenomenon in complex geometry. CFD has widely been accepted as a practical tool for such type of hydrogen distribution analysis. CFD has been successfully applied to safety analysis of various engineering system. It has been shown by several users that numerical simulations can reproduce such phenomenon accurately. But to rely on these results, these codes/models must be validated against suitable data. Since it is difficult to model the complex containment geometries it is the simplest approach to start with some standard available case to validate the CFD codes.

In the present work LES based FDS and 3D in-house CFD code has been used to calculate the distribution of hydrogen from a release orifice in a large enclosure. The geometry has been used as used by the Experiments performed by HySafe Network of Excellence partners Zhang et al. [1]. The exercise was performed within an enclosure with two openings located just above the floor level for code and model benchmarking in areas relevant to hydrogen safety. The experiment was performed with the main objective for establishing a framework for validation of codes and models for simulation of problems relevant to hydrogen safety. The experiment reported in Zhang et al. [1] was modelled using CFD code. Cross comparison was made between the results of CFD predictions and the experimental data, in terms of the hydrogen volume fraction at various locations. Venetsanos et al. [2] have presented an inter-code comparison exercise of CFD code capabilities for the same problem. Various authors have presented results of various CFD code with different turbulence model and different approaches (grid size, time step and convective scheme etc.). Few general remarks have been presented based on this exercise. Standard k-ε model with standard wall function along with turbulent Schmidt number 0.7 combined with a smaller time step and higher order convective scheme adopted to capture the release phase and use of laminar approach adopted during diffusion phase in present modelling Zhang et al. [1].

2. Physical Problem

CFD computations have been performed for the enclosure geometry used by HySafe Network of Excellence partners Zhang et al. [1] for their experiments. The code has been used to predict the

hydrogen concentration inside the enclosure and comparison with available data. The enclosure is rectangular in shape with average dimensions 7.2 X 2.88 X 3.78 m in length (x-direction), height (y-direction) and width (z-direction) respectively. The enclosure was built in a rock; all the side walls, floor and ceiling were at constant temperature during experiment. The release orifice has a diameter of 20 mm, located at 0.265 m above the floor. Two openings with a diameter of 5 cm are located at 5 cm above the floor. The release mass flow rate is 1 g/s, which gives an equivalent exit velocity of around 39.2 m/s. Measurements were made for hydrogen volume fraction using 16 concentration sensors, located on the plane X=0 as shown in the coordinate system in figure 1, the precise location of the sensors is given in table 1. The hydrogen was released for 240 s and measurements were conducted upto 5160 s after release.

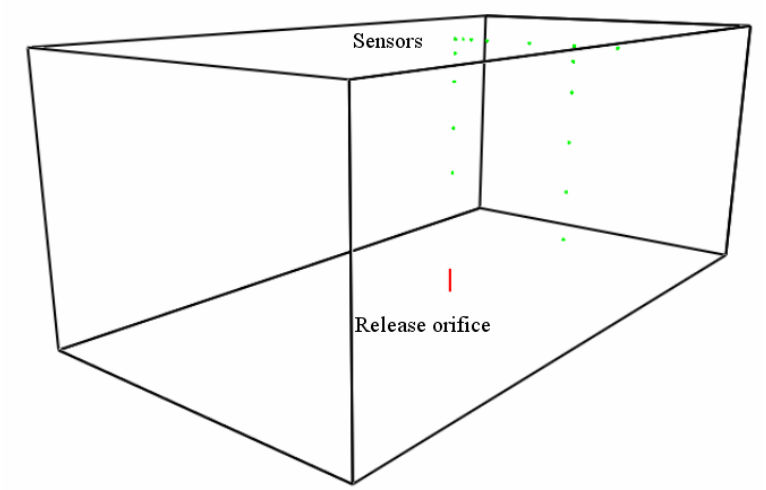

Figure 1. Simplified geometry for CFD computation

TABLE1: LOCATION OF SENSORS

Sensors	X(m)	Y(m)	Z(m)
1	0	2.83	0
2	0	2.83	0.1
3	0	2.83	0.2
4	0	2.83	0.4
5	0	2.83	0.9
6	0	2.83	1.85
7	0	2.83	1.4
8	0	2.68	1.4
9	0	2.38	1.4
10	0	1.88	1.4
11	0	1.38	1.4
12	0	0.88	1.4
13	0	2.68	0
14	0	2.38	0
15	0	1.88	0
16	0	1.38	0

3. Mathematical Model of Hydrogen Transport for RANS based In-house Developed Code

The computer code has been developed in order to predict the 3D behaviour of the hydrogen distribution in a large enclosure following the hydrogen released from an orifice. The 3D time

dependent Navier-Stokes equation with the species transport was solved by using Patankar's SIMPLE algorithm [3]. To model the mixture behaviour of hydrogen and air, a continuum approach was used, where only one velocity field is defined using the average density of gas mixture. The independent behaviour of hydrogen was considered using transport equation. In the present CFD model, the initial hydrogen injection period has been modelled with High Re k-ε model with standard wall function and buoyancy modification. The k-ε model was chosen because it has been thoroughly validated, handles buoyancy effects and has minimum computational requirement. The simplified geometry shown in figure 1 has been modelled by Cartesian structured mesh. The governing conservation equation for mass, momentum, species transport, turbulent kinetic energy and dissipation rate has been solved in 3D space. The governing equations are as follows:

$$\frac{\partial(\rho\phi)}{\partial t} + div(\rho\vec{U}\phi) = div(\Gamma_{\phi} grad(\phi)) + S_{\phi} \tag{1}$$

For continuity $\Phi = 1$ and $S_\Phi=0$. For X-momentum $\Phi = u$ and $\Gamma_\Phi=\mu_{eff} =\mu+\mu_t$ and

$$S_{\phi} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}(\mu_{eff}\frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\mu_{eff}\frac{\partial v}{\partial x}) + \frac{\partial}{\partial z}(\mu_{eff}\frac{\partial w}{\partial x}) \tag{2}$$

For Y-momentum $\Phi = v$ and $\Gamma_\Phi= \mu_{eff} =\mu+\mu_t$ and

$$S_{\phi} = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x}(\mu_{eff}\frac{\partial u}{\partial y}) + \frac{\partial}{\partial y}(\mu_{eff}\frac{\partial v}{\partial y}) + \frac{\partial}{\partial z}(\mu_{eff}\frac{\partial w}{\partial y}) + \rho g \tag{3}$$

For Z-momentum $\Phi = w$ and $\Gamma_\Phi= \mu_{eff} =\mu+\mu_t$ and

$$S_{\phi} = -\frac{\partial p}{\partial z} + \frac{\partial}{\partial x}(\mu_{eff}\frac{\partial u}{\partial z}) + \frac{\partial}{\partial y}(\mu_{eff}\frac{\partial v}{\partial z}) + \frac{\partial}{\partial z}(\mu_{eff}\frac{\partial w}{\partial z}) \tag{4}$$

For Species transport $\Phi = Y$ and $\Gamma_\Phi=\rho D+\mu_t/Sc_t$ and $S_\Phi=0$ and for the k-ε model the turbulent viscosity is modelled as:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{5}$$

For Turbulent kinetic energy $\Phi = k$ and $\Gamma_\Phi=\mu+ \mu_t/Pr_k$ and

$$S_{\phi} = G_k + G_B - \rho\varepsilon \tag{6}$$

For Turbulent Dissipation rate $\Phi = \varepsilon$ and $\Gamma_\Phi=\mu+ \mu_t/Pr_\varepsilon$ and

$$S_{\phi} = (\varepsilon/k)(C_1 G_k - C_2\rho\varepsilon + C_3 G_B) \tag{7}$$

Where Pr_k, Pr_ε, C_1, C_2 and C_μ are empirical coefficients whose standard values were taken from Launder and Spalding [4] and

$$G_k = \mu_t(2((\frac{\partial u}{\partial x})^2 + (\frac{\partial v}{\partial y})^2 + (\frac{\partial w}{\partial z})^2) + (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})^2 + (\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x})^2 + (\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y})^2) \tag{8}$$

And the term G_B has been modelled by Simple Gradient Diffusion Hypothesis (SGDH)

$$G_B = -\frac{\mu_t}{Pr_T}\frac{1}{\rho^2}\frac{\partial\rho}{\partial y}(\frac{\partial p}{\partial y} + \rho_\infty g) \tag{9}$$

In the equation (9) it has been assumed that the pressure gradient is negligible. Assuming the pressure gradient negligible is reasonable due to the fact that the plume velocity is relatively low creating low pressure gradients. In equation (7) representing the transport equation of ε; Viollet [5] has adopted the following procedure for determining the value of C_3 based on the sign of G_B; the

term denoting the buoyancy production of turbulence. If $G_B > 0$; $C_3 = C_1 = 1.44$ and $C_3 = 0$ if $G_B<0$. The sign of G_B is related to the stability of flow. If $G_B > 0$; the flow is unstable since $\partial\rho/\partial y > 0$ and, if $G_B<0$; the flow is stable $\partial\rho/\partial y < 0$. Where $C_1 = 1.44$; $C_2 = 1.92$; $C_3 = 1.44$ ($G_B > 0$); $C_3 = 0$ ($G_B<0$); $C_\mu = 0.09$; $Pr_k=1.0$; $Pr_\varepsilon=1.30$; $Sc_t=0.7$. Inclusion of the production term due to buoyancy in the k-ε model was first proposed by Rodi [6].

The domain was divided in 46X42X33 grid. The grid used for computation has chosen judiciously to make a compromise between accuracy and computational resource. The grid was made non-uniform with fine grid near the plume and coarser away from the plume near the wall. The release orifice was modelled as square with equivalent area and was resolved by 3X3 grid. The y^+ was in the range of 80-120 near the walls which is required to use standard wall function. For temporal discretization of the governing equations, the fully implicit scheme was employed. A time step of 0.05 s was defined for injection period which was increased to 1 s after 300 s. The time step was defined small enough to accurately predict the hydrogen concentration transients during injection period. At the orifice inlet boundary condition was used where known value of velocity, hydrogen mass fraction and turbulent quantities were specified. All the side boundaries have been modelled as adiabatic no-slip impermeable wall. The standard wall function has been used with the turbulence model. Initial conditions were used as u=0, v=0, w=0, k=0.001 and ε=0.002 to start the calculation.

The governing equations were discretized using Finite Volume Method. Equations were solved for 3D configuration for transient condition. The mixture density as a function of mass fraction was modelled as ideal gas law as follows.

$$\rho = \frac{p_{ref}}{R_u T \sum \frac{Y_i}{MW_i}} \tag{10}$$

Property like diffusion coefficient was assumed as a constant value of $7.5X10^{-5}$ m^2/s. Staggered scheme of solution was used in which fluid velocities were calculated at cell face and scalars such as pressure, hydrogen mass fraction and turbulent quantities were evaluated at cell centre. Power law scheme was utilized as differencing scheme for the convective terms for all equation, whereas the central difference scheme was used for the diffusive terms. The convergence criterion was set 10^{-5} based on overall mass residual.

4. Fire Dynamics Simulator

The main criticism levelled at the RANS approach targets the validity of the turbulence models employed to provide closure to the governing equation set. These turbulence models contain empirically determined parameters that can only be considered applicable for the specific flow cases where they have been validated. This narrows the range of validity for the RANS CFD approach. Large Eddy Simulation (LES) is a branch of Computational Fluid Dynamics (CFD). It differs from other CFD approaches, in that LES explicitly calculates the large-scale turbulent flow structures from first principles. The small-scale turbulent motion not calculated directly from the governing equations has its influence on the resolved flow field modelled. The simplest and most common form of SGS turbulence model used in LES is the Smagorinsky model [7] [8]. This is the default SGS model used in the FDS fire code. The Smagorinsky model uses the eddy viscosity approach to quantify the stresses that the turbulent velocity fluctuations place on the mean flow. In this modelling approach, the Reynolds stresses are assumed to relate to the local mean velocity gradient.

The present work has been carried out using the code FDS which have been extensively validated using salt water modelling experiments [9, 10], gravity current modelling [11, 12, 13],

isolated plumes [14, 15, 16, 17], buoyant plume in cross flow [18, 19] and by qualitative observations in above mentioned studies. The details of formulation of the equations and the choice of numerical algorithm available are contained in a companion document, called Fire Dynamics Simulator – User and Technical Reference Guide [20, 21]. A detailed systematic validation exercise for the FDS hydrodynamic model can be found in reference [22, 23, 24].

5. Results And Discussion

CFD analysis was performed for the hydrogen distribution inside a large enclosure. The predicted hydrogen mole fraction contours at various time instants are presented from Figure 2 to 5 by RANS and LES approaches. Qualitatively both the approaches predicted the buoyant jet impingement followed by hydrogen spread along the ceiling and subsequent descent downwards. After the hydrogen injection phase gets over, a stratified situation was predicted. The lower limit on the contour range corresponds to the lower flammability limit (4%). It can be seen that hydrogen jet rises because of initial momentum and buoyancy and impinges on the ceiling. A highly convective region is associated with hydrogen jet, where the ambient gas is entrained and mixes with the hydrogen. The hydrogen jet spreads along the ceilings, and further moves downwards upon impacting on the side walls.

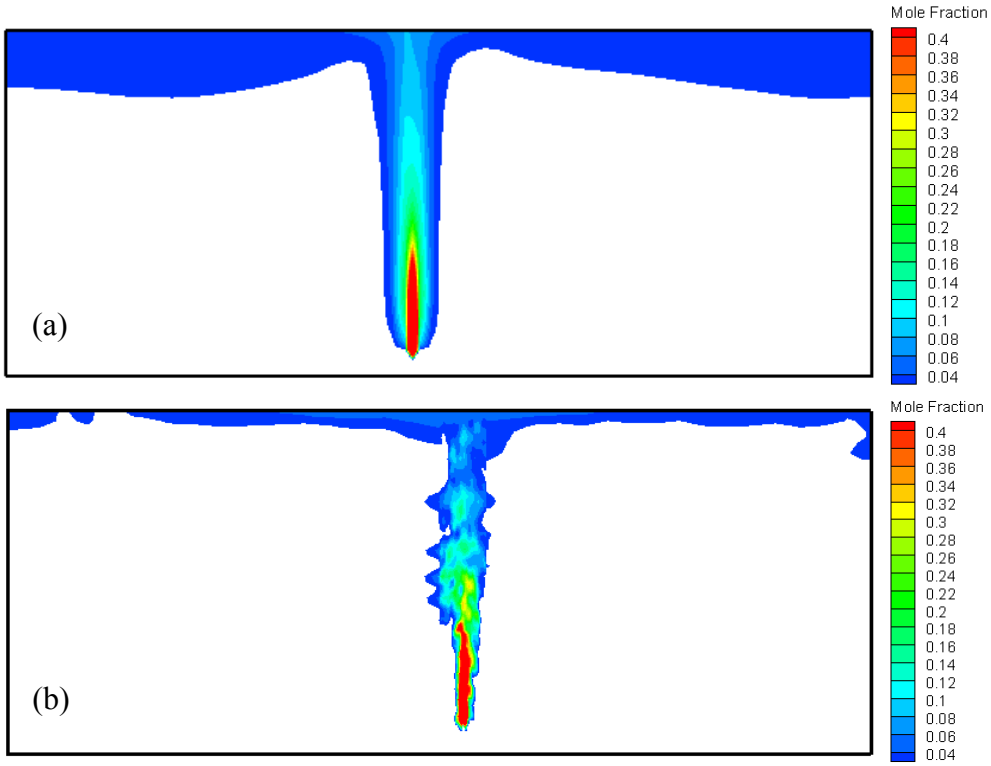

Figure 2. (a) RANS contour of hydrogen volume fraction at 60 seconds (jet impingement) and (b) LES contour of hydrogen volume fraction at 60 seconds (jet impingement)

Prior to 240 s there is a central region with high hydrogen concentration at the centreline. After the hydrogen supply was ceased at 240 s, this central region gradually disappears as a result of mixing and diffusion. Buoyancy effects maintain the higher concentration of hydrogen in the top of the vessel. Some time after injection only diffusion is the important phenomenon, which was turbulent in the first stage but becomes laminar in the last ones. After 300 s computation was carried out using laminar approach (for RANS approach) with time step of 1 s. A general observation for the calculations is that predicted mean concentrations were generally in good agreement with respect to experiment in the jet centreline region.

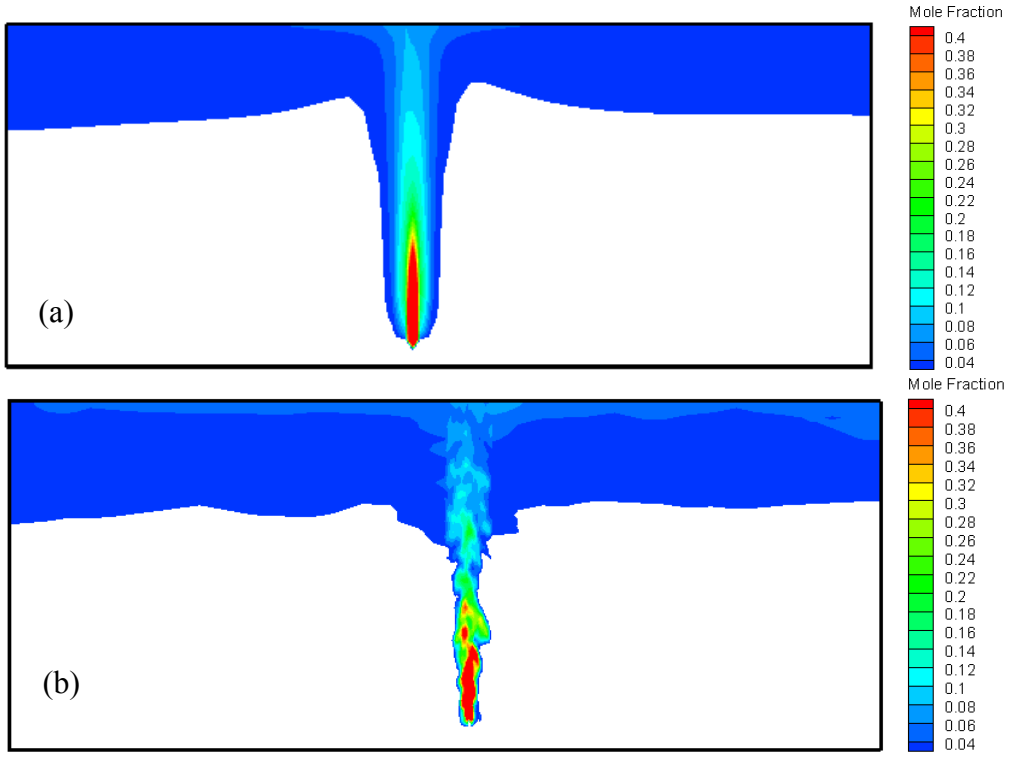

Figure 3. (a) RANS contour of hydrogen volume fraction at 120 seconds (spread along the ceiling) and (b) LES contour of hydrogen volume fraction at 120 seconds (spread along the ceiling)

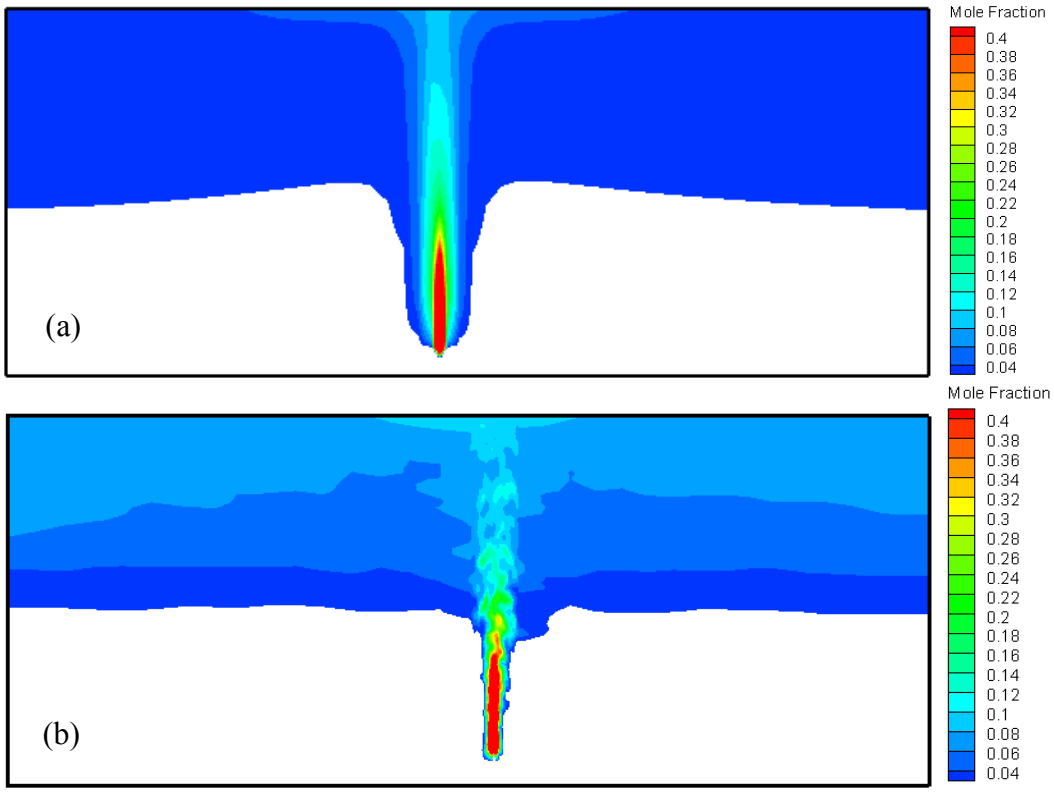

Figure 4. (a) RANS contour of hydrogen volume fraction at 240 seconds (downward movement) and (b) LES contour of hydrogen volume fraction at 240 seconds (downward movement)

The observed variation between the predicted and experimental (for RANS) values can in general be attributed to different empirical constant especially C_3 and modelling of G_B. Various

values have been suggested for C_3 for modelling buoyant turbulent flow. Modelling of G_B by SGDH is simplified approach as it does not take into account the horizontal component of density gradient and can not accurately predict the spread rate. Figure 6 to 13 shows the comparisons of the hydrogen mole fraction between the CFD prediction and experimental data at different locations. Figures 6, 7 and 8 are for locations 16, 13, 14 along the jet centreline figures 9, 10, 11 and 12 are for locations 1, 4, 6 and 7 located along the ceiling, and figure 13 for location 11 along the side wall. The LES based computations are in very good agreement with the experimental predictions in general.

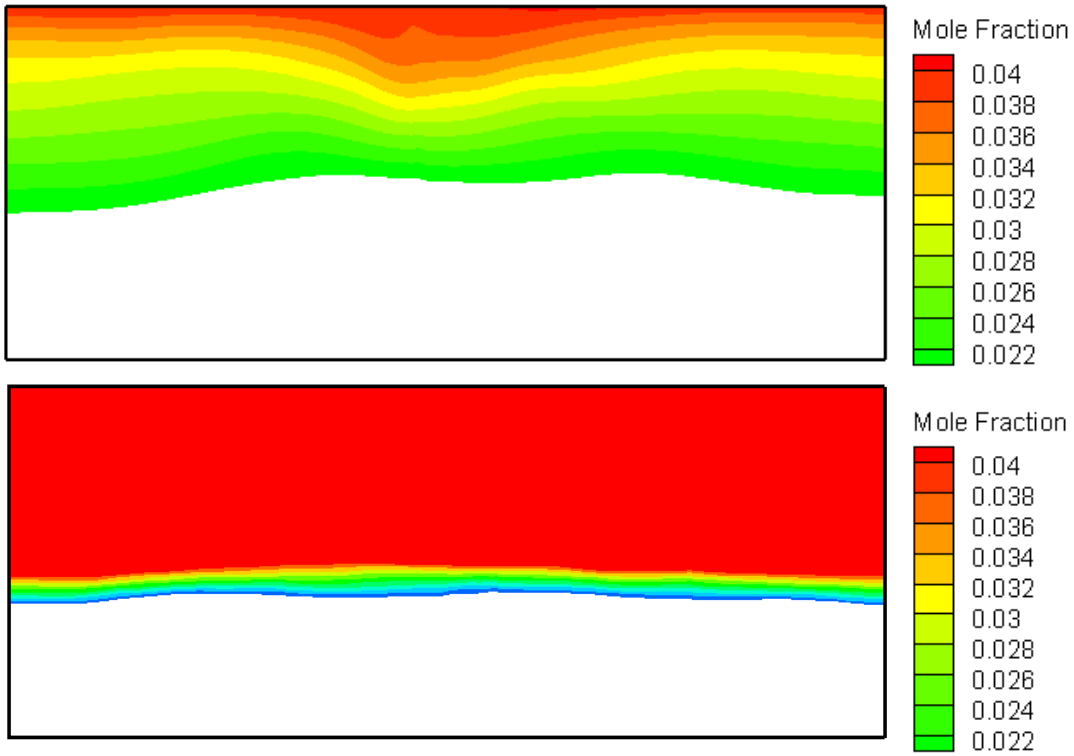

Figure 5. (a) RANS contour of hydrogen volume fraction at 360 seconds (stratification) and (b) LES contour of hydrogen volume fraction at 360 seconds (stratification)

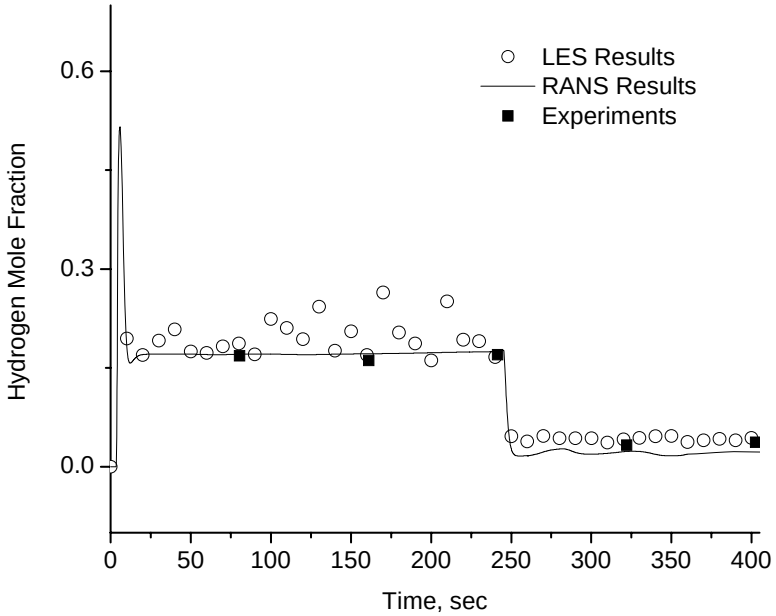

Figure 6. Hydrogen volume fraction at location 16

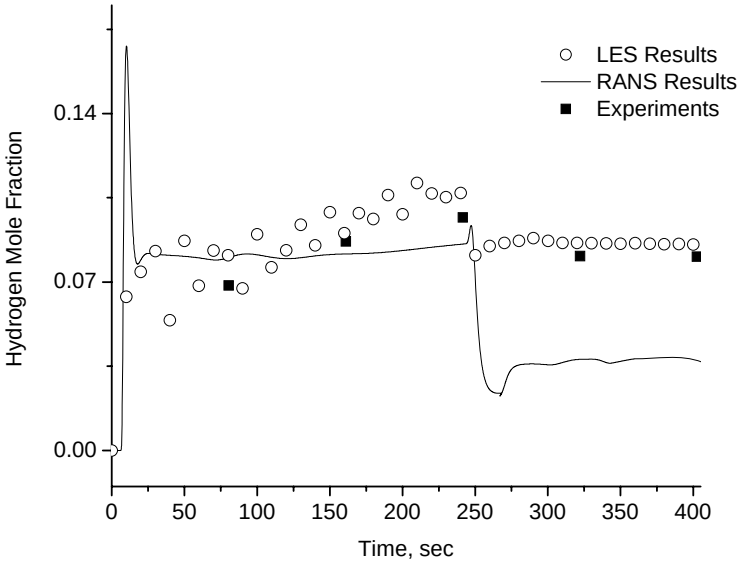

Figure 7. Hydrogen volume fraction at location 13

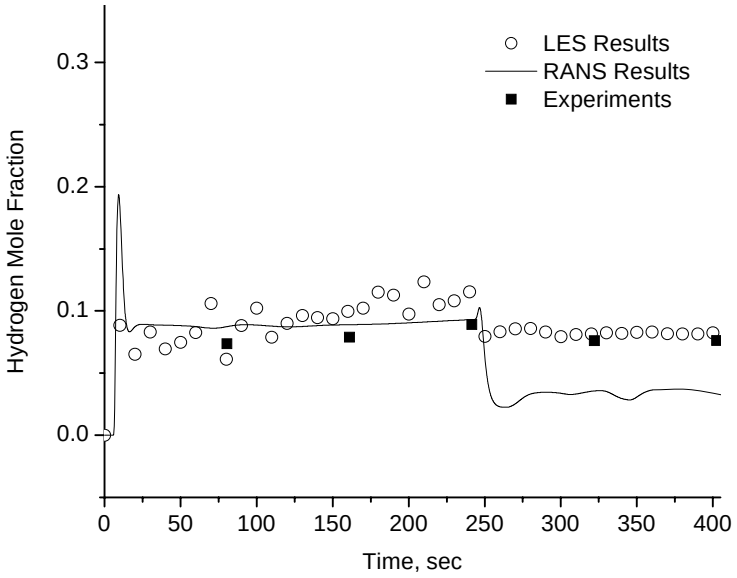

Figure 8. Hydrogen volume fraction at location 14

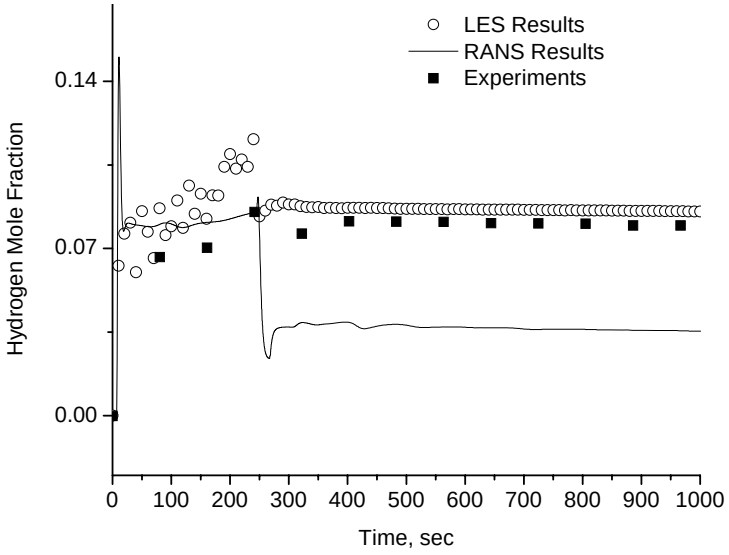

Figure 9. Hydrogen volume fraction at location 1

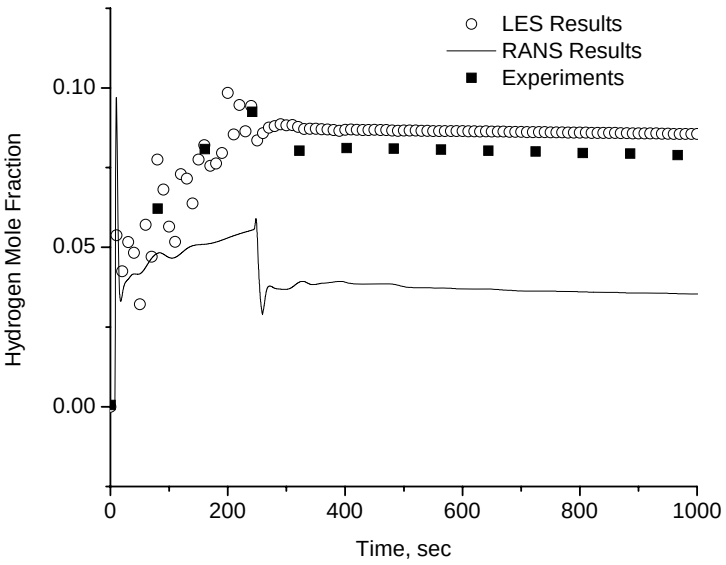

Figure 10. Hydrogen volume fraction at location 4

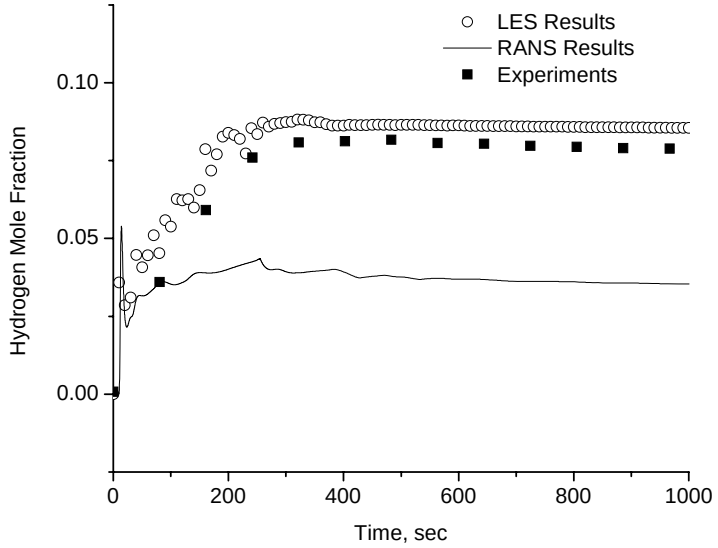

Figure 11. Hydrogen volume fraction at location 6

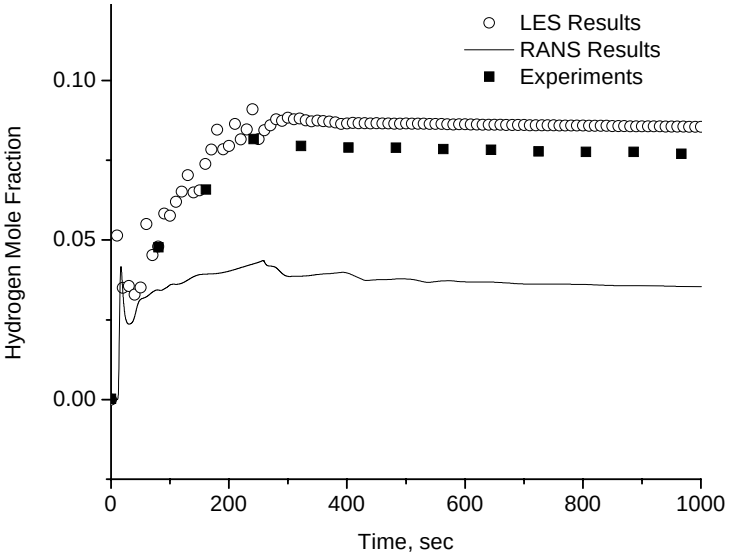

Figure 12. Hydrogen volume fraction at location 7

The RANS CFD predictions generally agree (less than LES) with the experimental data along the centreline. At the ceiling, the hydrogen mole fraction increases with time and reaches its peak at 240 s when hydrogen supply is stopped, after 240 s hydrogen mixes through diffusion and the hydrogen mole fraction eventually becomes constant, about 0.05, slightly lower than the experimental value, about 0.08. The centreline data in Figure 6 shows that at location 16 CFD code predicts a nearly constant value of 0.17, which compares very well with the experimental result. At location 13, hydrogen mole fraction increases gradually to 0.08 and at Location 14 to 0.09. For the sensors along the ceiling CFD code under predict the concentration as k-ε model does not accurately predict the spread rate with SGDH assumption. Parametric study is required with different modelling approaches used for GB i.e. Generalised Gradient Diffusion Hypothesis, Algebraic stress modelling and vorticity based formulation.

As previously discussed, after the hydrogen supply is stopped, hydrogen at the upper layer will diffuse to the lower layer, which causes the hydrogen mole fraction at the upper layer to decrease and the hydrogen mole fraction at the lower layer to increase. Figure 13, which shows the comparisons of CFD calculations and experimental data at locations 11, confirms experimentally and numerically this phenomenon. At location 11 the hydrogen mole fraction increases with time before 240 s, after which it slowly decrease with time. Very poor predictions at locations 4, 6 and 7 as mentioned in figure 10, 11, 12 are because of the use of k-ε model. k-ε model under predicts the jet concentration near the edge as it under predicts the spread rate because of lack of momentum and/or species diffusion obtained using the k- ε model. Figure 6 to 12 show a characteristic spike in the hydrogen concentration around 20 seconds, this peak was observed because of numerical modelling approaches and has been observed by various investigators [1],[2]. Because of unwinding nature the main flow i.e. in vertical direction is predicted first rather than in horizontal direction during initial transients.

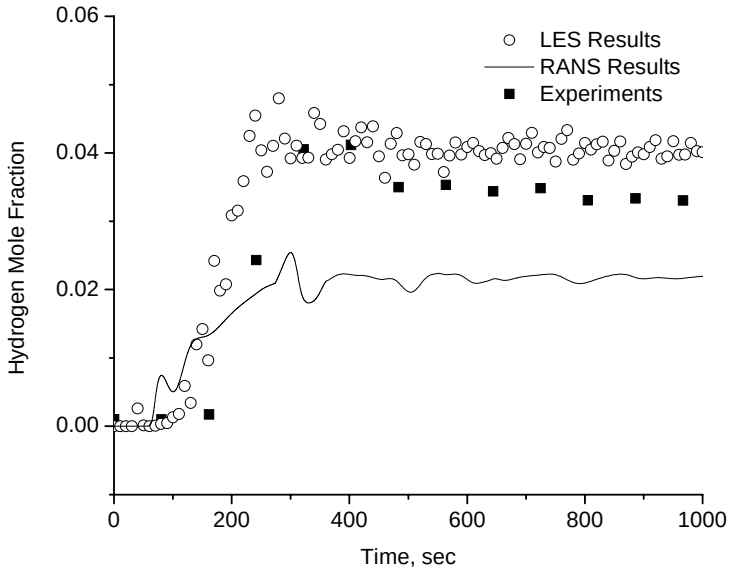

Figure 13. Hydrogen volume fraction at location 11

6. Conclusion

Hydrogen dispersion within an enclosure was numerically studied using RANS based in-house CFD code and also with LES based FDS code. CFD model requiring significant computation time enabled a more detailed analysis. During the release phase use of k-ε model with buoyancy modification, with turbulent Schmidt number=0.7, small time step and second order convective scheme is recommended in literature. Same approach was utilized during the release phase and for the centreline hydrogen mole fraction there was a good agreement between the experimental data

and CFD results. The CFD model correctly predicted the diffusion process after the hydrogen supply was ceased as observed in the experiment. During diffusion phase constant stratification was observed in the enclosure. A layer of hydrogen exists close to the ceiling which is horizontally homogeneous and vertically stratified. The important points for such calculation are time step, vertical grid spacing and order of convective scheme. In general the result obtained by CFD code has a good agreement with experiments. But LES based simulations were better as compared to RANS based predictions. The performed simulation provides useful insight regarding performance of CFD code to simulate hydrogen transport problem and this capability can be further utilized to simulate the hydrogen transport in the real containment geometries.

Nomenclature

ρ	Density of mixture, (kg/m^3)
p_{ref}	Reference pressure, (101325 N/m^2)
T	Absolute temperature of the mixture, (K)
R_u	Universal gas constant, (8314 J/Kmol K)
Y_i	Mass fraction of i^{th} species
MW_i	Molecular Weight of i^{th} species
ϕ	General Transport Variable
t	Time
$\vec{U}$	Velocity Vector
Γ_Φ	Diffusion Coefficient for variable ϕ
S_Φ	Source term for variable ϕ
u	X- component of velocity
v	Y- component of velocity
w	Z- component of velocity
μ	Dynamic viscosity, (Ns/m^2)
μ_t	Turbulent viscosity
μ_{eff}	Effective viscosity
g	Acceleration due to gravity, (9.81 m/s^2)
D	Diffusion Coefficient, (m^2/s)
Sc_t	Turbulent Schmit Number
k	Turbulent Kinetic Energy, (m^2/s^2)
ε	Turbulent Dissipation Rate, (m^2/s^3)
Pr_k	Turbulent Prandtl Number for kinetic energy
Pr_ε	Turbulent Prandtl Number for Dissipation
G_k	Generation term for turbulent kinetic energy because of mean shear
G_B	Generation term for turbulent kinetic energy because of buoyancy
C_1, C_2, C_3, C_μ	Empirical constants used in k- ε model

References

[1] Zhang, J., Hereid, J., Hagen, M., Bakirtzis, D., Delichatsios, M. A., Venetsanos, A. G. Numerical Studies of Dispersion and Flammable Volume of Hydrogen in Enclosures. in 2007 Proceedings of the HYSAFE International Conference on Hydrogen Safety.

[2] Venetsanos, A. G., Papanikolaou, E., Delichatsios, M., Garciac, J., Hansen, O. R., Heitsch, M., Huser, A., Jahn, W., Jordan, T., Lacome, J. M., Ledin, H. S., Makarov, D., Middha, P., Studer, E., Tchouvelev, A.V., Teodorczyk, A., Verbecke, F. and Voorto, M. M. V. An Inter-Comparison Exercise on the Capabilities of CFD Models to Predict the Short and Long

Term Distribution and Mixing of Hydrogen in a Garage. International Journal of Hydrogen Energy, 2009. 34: p. 5912-5923.

[3] Patankar, S. V. Numerical Heat Transfer and Fluid Flow. 1980. Hemisphere Pub. Co. Washington, DC.

[4] Launder, B. E. and Spalding, D. B. The Numerical Computation of Turbulent Flows. Comput Methods Appl Mech Eng, 1974. 3: p. 269–289.

[5] Viollet, P. L. The Modeling of Turbulent Recirculating Flows for the Purpose of Reactor Thermal-Hydraulic Analysis. Nuclear Engineering and Design, 1987. 99: p. 365–377.

[6] Rodi, W. Turbulence Models, their Application in Hydraulics—a State of Art Review. University of Karlsruhe, SFB/80/T/127, 1978.

[7] Ferziger, J.H. Subgrid-Scale Modeling, In: Large Eddy Simulation of Complex Engineering and Geophysical Flows. Editors: B. Galperin and S.A. Orszag, Cambridge University Press, Cambridge, 1993 pp 37-54.

[8] Smagorinsky, J. General Circulation Experiments with the Primitive Equations. Monthly Weather Review, 91 pp 99-165.

[9] Baum, H. R. and Rehm, R. G. Numerical Computation of Large-Scale Fire Induced Flows, In: Eighth International Conference on Numerical Methods in Fluid Dynamics. Editors: E. Krause, Lecture Notes in Physics, Springer-Verlag, Berlin, 1982. 170: p. 124-130.

[10] Baum, H. R., Rehm, R. G. and Mulholland, G. W. Computation of Fire Induced Flow and Smoke Coagulation. Nineteenth Symposium (International) on Combustion/The Combustion Institute, 1982 pp 921-931.

[11] Rehm, R. G., Tang, H. C., Baum, H. R., Sims, J. S. and Corley D. M. A Boussinesq Algorithm for Enclosed Buoyant Convection in Two Dimensions, NISTIR 4540, U.S. Department of Commerce, National Institute of Standards and Technology, Computing and Applied Mathematics Laboratory, Gaithersburg, MD 20899, U.S.A., 1991.

[12] Baum, H. R., McGrattan, K. B. and Rehm, R. G. Mathematical Modeling and Computer Simulation of Fire Phenomena. in 1994 Fire Safety Science Proceedings of the Fourth International Symposium, Ottawa, Ontario, Canada, pp 185-193.

[13] Rehm, R. G., McGrattan, K. B., Baum, H. R. and Cassel, K.W. Transport by Gravity Currents in Building Fires, in 1997 Fire Safety Science Proceedings of the Fifth International Symposium, pp 391-402.

[14] Baum, H. R., McGrattan, K. B., and Rehm, R. G. Large Eddy Simulations of Smoke Movement in Three Dimensions. in 1996 Proceedings of the Seventh International Interflame Conference, Interscience Communications, London, pp 189-198.

[15] Baum, H. R., McGrattan, K. B. and Rehm, R. G. Three Dimensional Simulations of Fire Plume Dynamics. in 1997 Fire Safety Science Proceedings of the Fifth International Symposium pp 511-522.

[16] Baum, H. R. Large Eddy Simulations of Fires – from Concepts to Computations. Fire Protection Engineering, 1999. 6: p. 36-42.

[17] McGrattan, K. B., Baum, H. R. and Rehm, R. G. Large Eddy Simulations of Smoke Movement. Fire Safety Journal, 1998. 30: p. 161-178.

[18] Sharma, P. K., Markandeya, S. G., Ghosh, A. K., Kushwaha, H. S. and Venkat Raj, V. A Computational Fluid Dynamics Study of a Buoyant Plume in a Cross Flow Condition. in 2001 Proceedings of the 28th National Conference on Fluid Mechanics and Fluid Power, Punjab University, Chandigarh.

[19] Spearpoint, M., Mowrer, F. W. and McGrattan, K. Simulation of a Compartment Flashover Fire Using Hand Calculations, Zone Models and a Field Model. in 1999 Proceedings of the International Conference on Fire Research and Engineering (ICFRE3), Society of Fire Protection Engineers (SFPE), National Institute of Standard and Technology (NIST) and

International Association of Fire Safety Science (IAFSS), Chicago, IL, Society of Fire Protection Engineers, Boston, MA.

[20] McGrattan, K., McDermott, R., Hostikka, S., and Floyd, J. Fire Dynamics Simulator (Version 5) , User's Guide NIST Special Publication 1019-5, In cooperation with: VTT Technical Research Centre of Finland National Institute of Standards and Technology, Gaithersburg, Maryland, June 23, 2010.

[21] McGrattan, K., Hostikka S., Floyd, J., Baum, H., Rehm, R. Fire Dynamics Simulator (Version 5), Volume -1 Mathematical Model, Technical Reference Guide NIST Special Publication 1018-5, In cooperation with: VTT Technical Research Centre of Finland National Institute of Standards and Technology, Gaithersburg, Maryland, 2007.

[22] Clement, J. M. Experimental Verification of the Fire Dynamics Simulator (FDS) Hydrodynamic Model, Ph D. Thesis, University of Canterbury, Christchurch, New Zealand, 2000.

[23] McGrattan, K., Hostikka, S., Floyd, J., Baum, H., and Rehm, R. Fire Dynamics Simulator (Version 5) Volume -2, Validation, Technical Reference Guide NIST Special Publication 1018-5, In cooperation with: VTT Technical Research Centre of Finland National Institute of Standards and Technology, Gaithersburg, Maryland, 2007.

[24] McGrattan, K., Hostikka, S., Floyd, J., Baum, H., and Rehm, R. Fire Dynamics Simulator (Version 5) Volume -3, Verification, Technical Reference Guide NIST Special Publication 1018-5, In cooperation with: VTT Technical Research Centre of Finland National Institute of Standards and Technology, Gaithersburg, Maryland, 2007.