

# MODELLING OF LEAN UNIFORM AND NON-UNIFORM HYDROGEN-AIR MIXTURE EXPLOSIONS IN A CLOSED VESSEL

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## ABSTRACT

Simulation of hydrogen-air mixture explosions in a closed large-scale vessel with uniform and non-uniform mixture compositions was performed by the group of partners within the EC funded project “Hydrogen Safety as an Energy Carrier” (HySafe). Several experiments were conducted previously by Whitehouse et al. in a 10.7 m<sup>3</sup> vertically oriented (5.7-m high) cylindrical facility with different hydrogen-air mixture compositions. Two particular experiments were selected for simulation and comparison as a Standard Benchmark Exercise (SBEP) problem: combustion of uniform 12.8% (vol.) hydrogen-air mixture and combustion of non-uniform hydrogen-air mixture with average 12.6% (vol.) hydrogen concentration across the vessel (vertical stratification, 27% vol. hydrogen at the top of the vessel, 2.5% vol. hydrogen at the bottom of the vessel); both mixtures were ignited at the top of the vessel. The paper presents modelling approaches used by the partners, comparison of simulation results against the experiment data and conclusions regarding the non-uniform mixture combustion modelling in real-life applications.

## 1.0 INTRODUCTION

There is a potential for hydrogen to serve an important role as an energy vector in future efficient energy management. To be publicly acceptable hydrogen should be at least the same safe as present day hydrocarbon fuels [1]. Workpackage “Standard Benchmark Exercise Problem” (SBEP) was established within EC funded Network of Excellence “Hydrogen Safety as an Energy Carrier” (HySafe) to investigate adequacy of models used in Computational Fluid Dynamics (CFD) in view of their practical application to hydrogen safety engineering problems. The workpackage partners identify experimental data and perform SBEP simulations in order to draw conclusions about the suitability of models and numerical tools. Performed previously SBEP simulations and simulation results may be found in open literature: on hydrogen release and distribution in a closed vessel – in [2], on hydrogen release and distribution in a garage environment – in [3], on deflagration dynamics in a simulated hydrogen fuel station environment – in [4].

## 2.0 EXPERIMENT DETAILS

Deflagration experiments in quiescent dry hydrogen-air mixtures with concentration gradient (stratified mixtures) and hydrogen-air mixtures without concentration gradient (uniform mixtures) are described in the paper by Whitehouse and co-authors [5]. The combustion experiments were conducted in the closed facility having diameter 1.5 m, height 5.7 m high and 3 manholes installed to provide access to the instrumentation and equipment. The vessel had internal volume 10.7-m<sup>3</sup>. Fans were installed in the vessel to create a uniform mixture. The hydrogen concentration was measured in 11 sample points located along the vertical line. Pressure histories were recorded using the piezoelectric type pressure transducers. The flame movement was deduced from the flame arrival

times, detected by array of thermocouples, located on either side of the vessel axis midway between the axis and the vessel wall. Outline of the vessel geometry is shown in Figure 1.

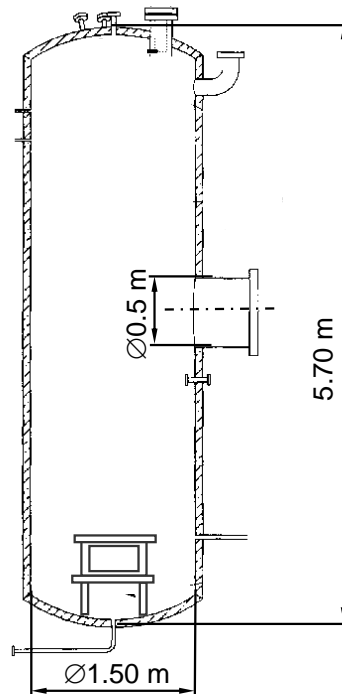


Figure 1. Combustion Test Facility geometry.

The NoE HySafe partners decided to choose for simulations two particular experiments with approximately the same amount of hydrogen from the range of the experiments described in [5]: deflagration of the uniform 12.8% vol. hydrogen mixture and deflagration of the non-uniform hydrogen mixture, corresponding to the average 12.6% vol. hydrogen concentration. In the latter case hydrogen concentration at the top of the vessel was 27% and at the bottom of the vessel - 2.5%. Hydrogen distribution for the stratified mixture composition was reported in the experimental paper [5]. The mixture was ignited at the top of the vessel (15 cm below vessel's dome) for both experiments.

### 3.0. PARTICIPATING ORGANISATIONS AND CFD MODELS

List of organizations, which performed simulations and submitted results for the comparison, is as follows:

1. Forschungszentrum Karlsruhe GmbH, Germany (FZK)
2. Joint Research Centre, Institute for Energy, The Netherlands (JRC)
3. Research Centre "Kurchatov Institute", Russian Federation (KI)
4. University of Ulster, United Kingdom (UU)

The acronyms of the organizations, shown in the brackets, will be used through the paper, tables and figures. Table 1 gives the list of numerical codes and the corresponding reference for its description and/or validation, the major characteristics of the codes (discretisation method, numerical schemes,

time step). The partners FZK, JRC and KI used their in-house codes, while the partner UU used for implementation of its own combustion model the commercial CFD code FLUENT.

Table 2 gives numerical grid type, mesh resolution, the computer resources (CPU type and required RAM), and the CPU time. Typical CV size used in simulations ranged from as little as 0.02 m in simulations by the partner KI to 0.2 m in simulations by the partner JRC. Generally, total CVs number used by the partners in this SBEP exercise was relatively low: the total number of CVs remained under 1,000,000 CVs even in simulations by the partner KI, where the grid resolution was finest. The partner JRC used adaptive meshing (based on specified pressure and temperature range), but even with the adaptive mesh the minimum CV size was 0.1 m and the maximum number of CVs in simulations was up to 22,000 CVs.

Table 3 gives list of turbulent models, combustion models and expressions for the mass burning rate and/or burning velocity. The models to describe viscous terms ranged from the inviscid fluid model (used by KI) to the Large Eddy Simulation approach to modeling turbulence (used by UU). FZK and JRC used the standard k- $\epsilon$  turbulence model [6] to describe the flow turbulence. The partner UU used LES subgrid scale model based on the renormalisation group analysis [7].

Table 1. Characteristics of the codes/models

Participant & Code	Type of solver and pressure-velocity coupling	Discretisation scheme C = convection terms D = diffusion terms T = temporal terms	Time step requirements
FZK, COM3D-3.4 (similar to CREBCOM [8])	Finite difference	C = Ami Haarten , TVD 2nd order non-oscillative, D = 2nd order central difference, T = 1 <sup>st</sup> order explicit	CFL = 0.96
JRC, REACFLOW v0.8.6 [9, 10]	Finite volume solver, Roe's approximate Riemann solver – Flux- vector splitting type solver	C = 2nd order Roe solver, D = 2nd order central difference, T = 1st order Euler explicit method	CFL <1
KI, B0B [8]	3D Eulerian explicit solver	C = 1st order upwind, D = 2nd order central difference, T = 1st order, Pressure gradients — 2nd order central difference	CFL = 0.3
UU, FLUENT v6.3.26 [11]	Finite volume, explicit coupled solver, density- based pressure-velocity coupling	C = 2nd order upwind, D = 2nd order central -difference, T = 1st order explicit linearisation	CFL = 0.8

Table 2. Calculation domain, numerical grid, CPU type and used RAM

Participant & Code	Type of grid	Characteristic CV size, resolution and total CV number	CPU type, RAM used and CPU time
FZK	Cubic structured	$\Delta x = 0.04$ m in whole calculation domain. 67x53x142, 504,242 CVs	16 processors Opteron-AMD CPU type, 1 GB RAM CPU. CPU time: ~2 h gradient mixture, ~10 h uniform mixture
JRC	Unstructured tetrahedral grid, adaptive meshing	$0.1 \text{ m} < \Delta x < 0.2 \text{ m}$ Adaptive meshing $\Delta x \sim 0.1$ m. Initial No. CV 19,000, maximum No. CV 22,000 CV	1 AMD CPU, 1.8 GHz, RAM: 2 GB x CPU, CPU time: ~2 h gradient mixture, ~16 h uniform mixture
KI	Cubic structured	$\Delta x = 0.02$ m, 40x69x319, 880,440 CVs	Intel Core2Duo 2.66 GHz, RAM: 40MB, CPU time: ~ 40 h for both mixtures
UU	Unstructured tetrahedral	$\Delta x \approx 0.08$ m, 157,352 CVs	Intel DualCore 3.0GHz, RAM: 200MB, CPU time: ~15 h gradient mixture, ~50 h uniform mixture

The combustion and flame propagation models also belonged to different classes. The code B0B by partners KI realizes CREBCOM combustion model [8], which algorithm assumed that combustion in a particular CV takes place when the neighbouring CV has burned out to some explicitly defined extent. In this model the burning rate is defined as  $\partial Y_f / \partial t = K_0 / \Delta x$ , where  $Y_f$  is the fuel mass fraction,  $K_0$  is the burning rate constant,  $t$  is time and  $\Delta x$  is the CV size. Then the combustion rate constant can be estimated as a function of the turbulent burning velocity  $S_t$ :  $K_0 = S_t(\sigma + 1)/4$ , where  $\sigma$  is the expansion ratio of combustion products. The partner KI used the constant burning velocity for both uniform and gradient mixtures, though the mixture properties were dependent on the mixture composition assumed to vary linearly along the vertical centreline of the vessel. CREBCOM model [8] suggests correlations for the maximum turbulent burning velocities of various uniform mixture compositions. For the uniform mixture the partner KI chose burning velocity value as  $S_u = 0.739$  m/s, and  $S_u = 1.000$  m/s for the stratified mixture. Burning velocity dependence on pressure was modelled in the following form:  $K_0 = S_u \cdot \left\{ a \exp[b(p - c)^2] + d \arctan(e(p - f)) \right\}$ , where  $S_u$  - burning velocity at initial condition,  $a, b, c, d, e, f$  - empirical constants.

The code of the partner FZK is also based on the CREBCOM model [8], but uses variable burning velocity: for first 50 ms the burning velocity maintained equal to the laminar value, then - the expression for the turbulent burning velocity value obtained from Kawanabe correlation as described in [12]. The burning velocity dependence on the mixture composition was chosen according to [13]. The model also accounts dependence of burning velocity on temperature, which makes it function of pressure as well (through adiabatic heating):  $S_u(T) = S_{u,298} \sqrt{\lambda_{air}(T) / \lambda_{air}(298 K)} (T/298)^n$ , where  $S_{u,298}$  - burning velocity at  $T=298$  K,  $\lambda_{air}$  - thermal conductivity of air,  $n$  - model parameter dependant on hydrogen concentration.

The JRC combustion model used classical Eddy Dissipation Concept [14] (see Table 3), where the burning rate is controlled mainly by the turbulent motion. The modification by Hjertager [15] was introduced to account flame extinction. A more detailed description of the code REACFLOW and its validation are given in [9, 10]. The model doesn't allow explicit simulation of the burning rate dependence on pressure and mixture composition, though accounts them through the pressure effect on density and mass fraction of the limiting component (see Table 3).

UU used its own LES combustion model to describe burning velocity, which accounts for initially laminar flame propagation regime and major mechanisms for flame acceleration: 1) flow turbulence using the turbulent combustion model by Yakhot, 2) turbulence generated by the flame front itself according to the theory by Karlovitz, 3) fractal-like flame wrinkling mechanism in a fully developed turbulent combustion regime according to the experimental data by Gostintsev. The model description and validation of the model for uniform mixtures were published elsewhere, e.g. [16].

Table 3. Turbulence and combustion models used by the exercise participants

Participant	Turbulence model	Combustion/flame tracking model	Expression for burning velocity $S_t$ or mass burning rate $\dot{m}$
FZK	Standard k-ε model	CREBCOM model for flame tracking [8]	$S_t = S_u (1 + 1.25(u'/S_u)^{0.7}),$ $S_u(T) = S_{u,298} \sqrt{\lambda_{air}(T)/\lambda_{air}(298 K)} (T/298)^n$ $S_{u,298}$ - burning velocity at $T=298$ K, $\lambda_{air}$ - thermal conductivity of air, $n$ - model parameter dependant on hydrogen concentration
JRC	Standard k-ε model	Eddy Dissipation Concept [14, 15]	Mass burning rate $\begin{cases} \dot{m} = -c_f \frac{\varepsilon}{k} \rho Y_{lim} & \text{if } \tau_{ch}/\tau_{tu} < D_{ie} \\ \dot{m} = 0 & \text{if } \tau_{ch}/\tau_{tu} \geq D_{ie} \end{cases}$
KI	Inviscid fluid	CREBCOM model for flame tracking [8]	$\partial Y_f / \partial t = K_0 / \Delta x;$ $K_0 = S_u \cdot \{a \exp[b(p-c)^2] + d \arctan(e(p-f))\}$ $S_u=0.739$ m/s for uniform mixture, $S_u=1.000$ m/s for gradient mixture, $a, b, c, d, e, f$ - empirical constants
UU	RNG-LES	Customised RNG premixed combustion model, [19]	$R < R_0$ $S_t = \left[ S_u(Y_{H_2}, T, p) \cdot \chi_{ip} \cdot \left\{ 1 + (\chi_{Karl_{max}} - 1) \left[ 1 - \exp\left(-\frac{R}{R_0}\right) \right] \right\} \right] \cdot \exp\left(\frac{u'}{S_t}\right)^2$ $R \geq R_0$ $S_t = \left[ S_u(Y_{H_2}, T, p) \cdot \chi_{ip} \cdot \left\{ 1 + (\chi_{Karl_{max}} - 1) \left[ 1 - \exp\left(-\frac{R}{R_0}\right) \right] \right\} \cdot \left(\frac{\varepsilon_{R_0}}{\varepsilon} \cdot \frac{R}{R_0}\right)^{D-2} \right] \cdot \exp\left(\frac{u'}{S_t}\right)^2,$ $S_t$ - turbulent burning velocity, $\chi_{ip}$ - flame wrinkling due to preferential diffusion, $\chi_{Karl}$ - flame wrinkling due to turbulence generated by flame front itself.

UU model also accounted the preferential diffusion mechanism of flame acceleration based on the leading point concept by Kuznetsov and Sabel'nikov [17] and implemented according to the Zimont-Lipatnikov model [18]. Details of the leading point concept implementation in UU LES combustion model and its validation are available in [19]. The UU combustion model uses burning velocity as a function of the hydrogen concentration according to experimental data [20]. Burning velocity dependence on pressure is accounted as  $S_u = S_{u0}(Y_{H_2})(p/p_0)^\varepsilon$ , where  $S_{u0}(Y_{H_2})$  is the laminar burning velocity at initial pressure,  $\varepsilon$  is overall thermokinetic index as a function of the hydrogen concentration.

The KI model accounted heat losses, which reflected on the lower maximum overpressure and lower pressure in the pressure dynamics tail achieved in simulations. The heat losses in explosion experiments are known to decrease the deflagration overpressure - the longer time, the larger decrease of pressure. This may be seen in closed vessel deflagration experiments, where maximum experimental overpressure is smaller than predicted by analytical models without heat losses. As a result the simulated pressure dynamics, obtained assuming zero heat losses, should give larger overpressures and steeper pressure dynamics than the experimental one affected by heat transfer.

The authors would like to stress that they are not targeting to make conclusions about superiority of any model or simulation approach, but investigate what level of performance one may expect in CFD simulation of the non-uniform mixture deflagration for realistic safety assessment and/or safety design.

#### 4.0 RESULTS AND DISCUSSION

The simulation results, requested in this SBEP for comparison against experimental data, included pressure and flame dynamics for both uniform and gradient mixtures. The pressure distribution inside of the vessel may be assumed uniform and a single pressure dynamics for the whole vessel was compared against the experimental data. The experimental data was digitised manually as it was reported in [5] and follows experimentally recorded pressure oscillations only in general. However the pressure dynamics tendency is preserved: pressure dynamics of the uniform mixture deflagration was much smoother than the highly oscillating pressure dynamics of the gradient mixture deflagration.

Figure 1 shows comparison of the experimental and simulated pressure dynamics inside of the vessel for the uniform 12.8% vol. hydrogen-air mixture. The experimental record indicates that there may be mass burning rate acceleration at the very final stage of combustion, leading to the increasing pressure rise rate. KI simulations with empirical constants for burning velocity demonstrates an impressive agreement with the observed pressure dynamics. UU model accounts fractal character of the flame front acceleration in the fully turbulent flame propagation regime and burning velocity dependence on pressure, both contributing to the rising mass burning rate. As a result, the increase in the pressure rise rate is qualitatively similar to the experimental one, though faster. Simulated pressure dynamics by FZK and JRC have a more linear pressure dependence with time.

Comparison of the experimental and simulated flame arrival times for the uniform mixture is given in Figure 3. The analysis is conducted based on assumption that the flame propagation along the centreline reflects its propagation in the vessel generally. The models provided close agreement with the experiment pressure dynamics are expected to have close to the experimental flame dynamics too. KI model, which fitted ideally the experimental pressure curve, has a very close agreement with the experimental flame dynamics. Generally, simulation results by JRC are very close to the experimental data too. However, KI and JRC flame dynamics have different tendencies: when KI flame dynamics accelerates at about  $t=0.50-0.55$  s, JRC flame decelerates at about the same time. Results by FZK and UU model are further from the experimental data and they have different tendencies: FZK flame decelerates along the vessel, when the flame propagation speed in UU simulation is accelerating.

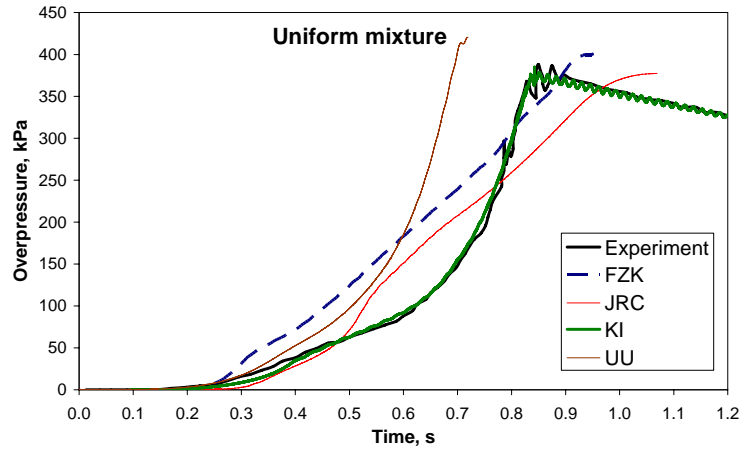


Figure 2. Experimental and simulated pressure dynamics for the uniform 12.8% vol. hydrogen-air mixture.

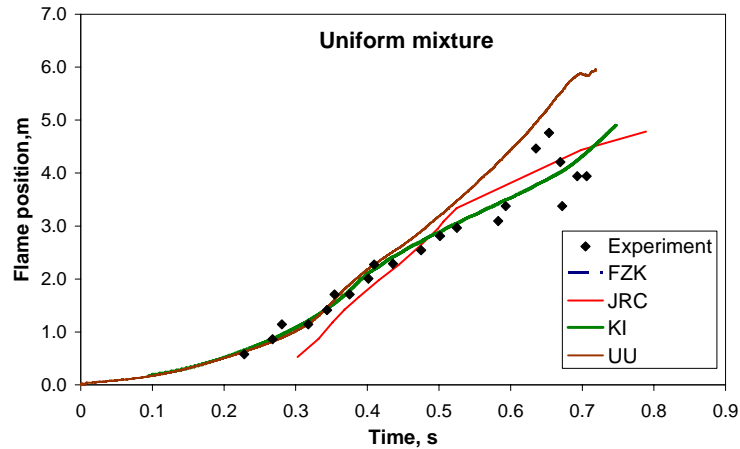


Figure 3. Experimental and simulated flame dynamics for the uniform 12.8% vol. hydrogen-air mixture.

Figure 4 gives comparison for experimental and simulated pressure dynamics in the gradient mixture. The gradient mixture deflagration is faster than the deflagration of the uniform one. One may see that 1) for the gradient mixture deflagration the simulated pressure records are much closer to the experimental data, and 2) all simulated pressure dynamics reproduced pressure oscillations similar to the experimental ones, when there was no comparable pressure oscillations in simulation results for the uniform mixture. Again, the KI simulation which uses empirical combustion model achieved impressive agreement between the experimental and simulated pressure rise rate and values of the first two pressure peaks. In simulations by JRC the timing of the first pressure peak is later and the peak itself is lower than the experimental values. UU simulations provided good correspondence of the 1<sup>st</sup> pressure peak value and time compare to the experiment. FZK simulations have larger pressure oscillations and earlier time of the first pressure peak than in the experiment.

Figure 5 gives comparison of the experimental and simulated flame arrival times for the deflagration in the mixture with concentration gradient. General agreement between the simulation results and the experimental data is good: the simulation results are concentrated around the experimental

measurements. Characteristic behaviour of the flame dynamics agrees well between the partners' simulations and the experimental observations: at about  $t=0.025 - 0.040$  s the flame front accelerates and then decelerates at about  $t=0.045 - 0.050$  s.

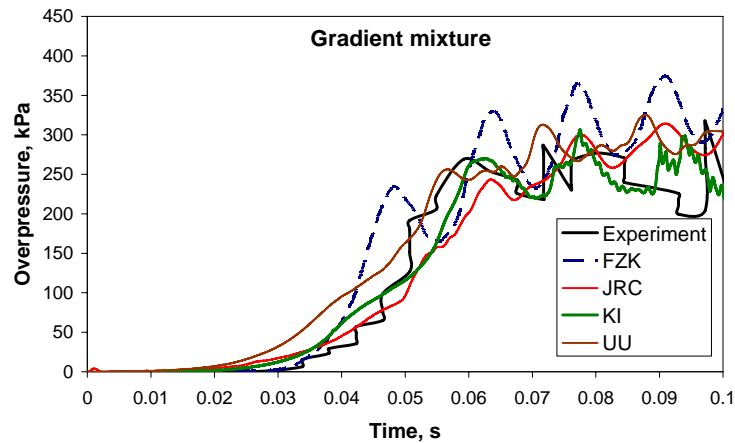


Figure 4. Experimental and simulated pressure dynamics for the gradient (average 12.6% vol.) hydrogen-air mixture.

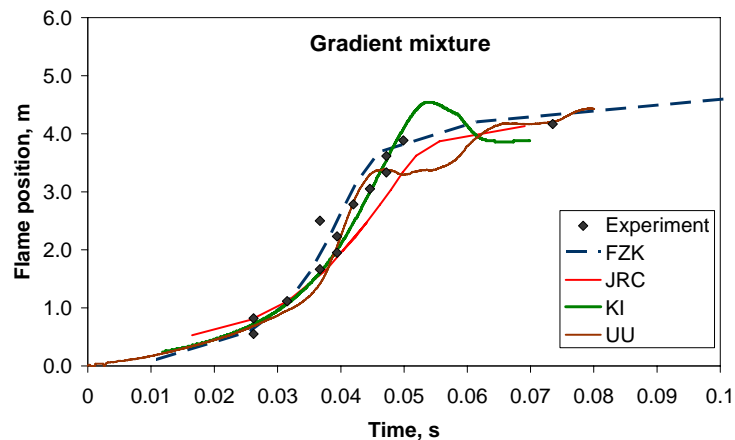


Figure 5. Experimental and simulated flame dynamics for the gradient (average 12.6% vol.) hydrogen-air mixture.

Overlooking the results, one may conclude that discrepancy between simulation results and experimental observations are larger for the deflagration in the uniform hydrogen-air mixture than in the mixture with concentration gradient, which was expected to be more difficult to model. In author's opinion the reason for such a result is in the fact that the uniform hydrogen-air mixture was lean and experience in modelling of such mixtures is not so extensive as for near stoichiometric mixtures. The combustion in the mixture with concentration gradient starts in the hydrogen-air mixture with the concentration close to the stoichiometric (27% vol. hydrogen), and this is probably why all partner's simulations provided here much better results, especially for the flame front dynamics.

Pressure rise rate was close to linear in FZK and JRC simulations of the uniform mixture deflagration, which suggests that the burning rate at initial moment of combustion is overestimated and the burning



rate doesn't change much during combustion. Deeper analysis is required to conclude on the reasons for such behaviour. Potentially, this may be down to the fact that purely turbulent combustion models were used by the partners FZK and JRC under low level of turbulence. Simulation results from the gradient mixture composition are inconclusive to judge if it is the case or not. Since in KI simulation the burning velocity depends only on pressure, one could draw the conclusion that describing the correct dependence of the burning rate on pressure is an essential step in order to capture the correct flame speed and subsequently the correct pressure history in explosion computations in closed vessels without obstacles. Simulations by UU are slightly aside from the tendency of results by FZK and JRC as the increase of the burning velocity with distance from the ignition point is incorporated in the burning velocity expression. Besides, the UU combustion model incorporates the leading point concept, which potentially should improve results for turbulent combustion of lean hydrogen mixtures. On the other hand, UU simulations were conducted on the relatively coarse grid ( $\Delta x \approx 0.08$  m), which was comparable to JRC mesh (about  $\Delta x \approx 0.1$  m), which should be also taken into account. Yet, simulation results achieved in this exercise must be treated as relatively good – all pressure rise rates are within 50% error margin from the experimental value. One must keep in mind that in a similar SBEP exercise on simulation of deflagration dynamics in a hydrogen fuel station environment [4] the majority of the simulated pressure rise rates (compared against experimental measurements in different locations for the same experiment) had errors much higher than 50% for all participating models.

It is interesting to note that in spite of the relatively simple combustion model (burning velocity depending on pressure only), simulation results by the partner KI are in a very good agreement with the experimental data for uniform mixture and still close to the experimental data for the gradient mixture. In the same time the partner KI used the best grid resolution between the partners. One practical conclusion, which may be drawn from this, is that the sophisticated model is not the only solution and in many cases cannot substitute for the simple model and better grid resolution.

## 5.0 CONCLUSIONS

CFD simulations of lean uniform and non-uniform hydrogen-air mixture deflagrations with similar amount of hydrogen, performed by four NoE HySafe partners were presented and discussed. The comparison of simulation results provided information on the level of quantitative precision one may expect with present days CFD codes and combustion models for prediction of hazards in hydrogen safety engineering.

Simulations demonstrated that available CFD codes and models are capable to simulate a hydrogen deflagration dynamics in realistic non-uniform hydrogen-air mixtures. In the same time, simulations highlighted that there is a potential for the models' improvement for lean hydrogen-air deflagrations.

This benchmark exercise demonstrated availability of CFD technique as a practical engineering tool for hydrogen explosion safety even with relatively moderate computer hardware.

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