A COMPARISON EXERCISE ON THE CFD DETONATION SIMULATION IN LARGE SCALE CONFINED VOLUMES

Yáñez Escanciano, J.[1], Kotchourko A. [1], Lelyakin, A. [1], Gavrikov, A. [2], Efimenko, A. [2], Zbikowski, M. [3], Makarov, D. [3], Molkov, V. [3],

[1] Institute for Energy and Nuclear Energy, Karlsruhe Institute of Technology, Germany
[2] Kurchatov Institute, RU, Russian Federation
[3] University of Ulster, UK, United Kingdom

ABSTRACT

The use of hydrogen as an energy carrier is going to widen exponentially in the next years. In order to ensure the public acceptance of the new fuel, not only the environmental impact has to be excellent, but also the risk management of its handling and storage must be improved. As a part of modern risk assessment procedure, CFD modeling of the accident scenario development must provide reliable data on the possible pressure loads resulted from explosion processes. The expected combustion regimes can be ranged from slow flames to deflagration-to-detonation transition and even to detonation. In the last case, the importance of the reliability of simulation results is particularly high since detonation is usually considered as a worst case state of affairs. A set of large-scale detonation experiments performed in Kurchatov Institute at RUT facility was selected as benchmark. RUT has typical industry-relevant characteristic dimensions. The CFD codes possibilities to correctly describe detonation in mixtures with different initial and boundary conditions were surveyed. For the modeling, two detonation tests, HYD05 and HYD09, were chosen; both tests were carried out in uniform hydrogen/air mixtures; first one with concentration of 20.0% vol. and the second one with 25.5% vol. In the present exercise three CFD codes using a number of different models were used to simulate these experiments. A thorough inter-comparison between the CFD results, including codes, models and obtained pressure predictions was carried out and reported. The results of this inter comparison should provide a solid basis for the further code development and detonation models' validation thus improving CFD predictive capabilities.

INTRODUCTION

The use of hydrogen is going to grow increasingly in the near future in parallel to its industrial and economic importance, representing a large amount of activity around it, such as large industrial plants, large storage facilities, refueling stations, etc. meaning an increasing iteration, and handling not only with experts, but also with the population. In order to address the safety issues of hydrogen storage, transport and infrastructure in a coordinated way all along Europe, the European co-funded HySafe Network of Excellence "Hydrogen Safety as an Energy Carrier" (HySafe) [1] was founded by European Commission, focusing on a safe transition to a sustainable development in Europe by facilitating the safe introduction of hydrogen technologies and its applications. As a work methodology, every partner member of the Network, identify a set of Standard Benchmark Exercise Problems (SBEPs) representative of the problems to be found on the praxis such as, experiments on hydrogen releases and distribution, jet fires, deflagrations and detonations. The partners acknowledge, as a fundamental tool to analyze the mentioned problems, the Computational Fluid Dynamics (CFD) codes. Inside the project, a specific target is to evaluate and improve, if possible, the accuracy of them, assessing their range of applicability. This is achieved by the comparison of the code performance against available experimental data and of the results obtained by different partners. An indication of the quality and suitability of the models, numerical codes and user practices is finally obtained for application to practical real size industrial hydrogen safety problems.

Following the state of the art, it is publicly accepted that a joint CFD simulation exercise is a useful method for achieving the enunciated goals, as may be confirmed in [2, 3]. Similar exercises for the validation of CFD simulations against hydrogen combustion experiments in nuclear reactor environment has been described in [4] as well as the validation of simulations against large-scale industrial explosions has been performed in [5]. For the benchmark problem we deal with, the large scale test RUT facility was chosen. It consists of a 60 m. long channel with variable cross-section, which can also be separated into several interconnected rooms and is being operated by the Kurchatov Institute with the aim of being able to perform realistic accident scenarios analysis in complex, multi-compartment geometries with variables hydrogen concentrations, pressures and temperatures. The HYD05 and HYD09 tests chosen for this problem were carried out in uniform hydrogen/air mixtures, the first with 20 % vol. and the second 25.5% vol. [6]. The tests were identified for benchmarking purposes and relevant data have been made available to interested users inside the project. The predictive capabilities on the calculation of a big scale detonation of the codes could be assessed with different mixtures, ignition location, and geometries. Thanks to the special shape and size of the RUT facility, and to the fact that the magnitudes of industrial facilities and RUT are comparable, results could be extrapolated to real industrial safety assessment scenarios. On the scope of this particular exercise, the main target and task of the organizations participating on it, is correctly simulate the pressure, impulse and velocity of the detonation.

An Euler solver with the properties to handle shocks properly (Shock-Capturing-schemes) should handle detonation calculations if the correct value for the heat release rate due to chemical interaction is provided. On a well resolved grid, fine but not necessarily so fine as to resolve the inner structure of the detonation wave, results should be correct. The authors experience show that good practice implies reproducing the 3D structure of detonation cell, but not the thickness of the shock itself [26]. Therefore around 50 mesh nodes are required inside of every detonation cell at least e.g. [25]. For stoichiometric air-H2 mixtures, this constrain will leave the demanded resolution on a maximum of 3 mm. For engineering applications with domains of the order of 1 hm^3 this resolution is absolutely unreachable. This article is dedicated to proof the ability of models and codes taking part on the exercise to properly resolve big industrial problems performing completely three dimensional calculations in which constrains relative to the resolution are unavoidable.

EXPERIMENTAL DETAILS

The two tests already presented above were carried out to measure the effect of initiator location, hydrogen concentration and 3D geometry on the loads suffered by the walls of the facility. Hydrogen concentrations were 20% vol. and 25.5% vol. The scheme of the experimental facility is presented in the Figure 1. It must be underlined that the length of the volume was almost 30 m (263 m^3), including the curvilinear part of the channel.

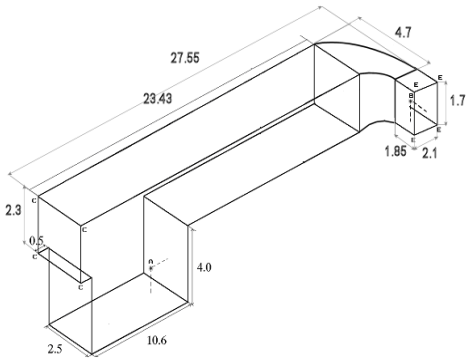

Figure 1. Schematic of the RUT-2200 facility segments used in detonation experiments HYD05 and HYD09.

The measurements preformed during the test were carried out using a high-frequency measurement system, including piezoelectric pressure transducers "Kistler", models 701 and 7031, tenso-resistive pressure transducers "ENDEVCO", models 8511A-5K and 8530B-1000. Signals from pressure transducers were recorded with the DL-2800 register with a sample rate of 5 μs.

Two lines of pressure transducers were arranged inside the experimental volume. The first one was placed in the *canyon* (lower part of the facility) and included transducers 1-6 (line 1); the second one in the channel and includes transducers 7-11(line 2). The scheme of transducers location in the experimental volume is shown in Fig 2. The pressure transducers number 2 to 5 were located on a longitudinal wall as represented in Fig. 1 & 2 on the *canyon,* and the transducers 7 to 11 on the opposite wall Fig. 1 & 2 of the channel. Transducers 1, 6, 11 were placed in the middle of the transversal walls.

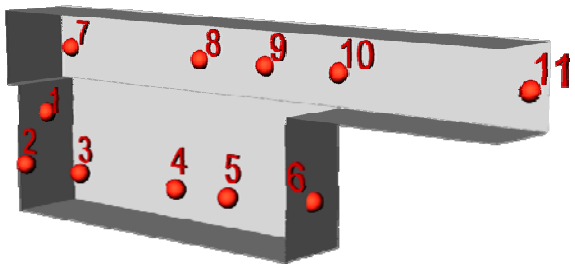

Figure 2. Position of the transducers.

In the tests, two different initiator locations were used (Figure 1, A and B points). High explosive charges (200 g) were used as initiators. The ignition points were located at distances 80 cm from the floor and 50 cm from the wall.

Table 1. Main characteristics of the experiments

File name	Volume of H_2-air mixture (cubic m)	H_2 concentration (vol. %)	Initiator location	Initiator mass (g of HE)
HYD05	263	20.0	A	200
HYD09	263	25.5	B	200

The mixture temperature and pressure were 20^{o}C and 1atm in both tests. Mixing was assured by fans. Hydrogen concentration and mixture uniformity were checked taking samples from two different points of the experimental volume. It was found that the non uniformity was less than 0.5% vol. on hydrogen concentration.

PARTICIPANTS AND MODELS

Three organizations have participated into this validation exercise, using three different CFD codes. The organizations were: the “Karlsruhe Research Centre” (FZK); the “Russian Research Centre Kurchatov Institute” (KI) and the “University of Ulster“(UU). The Table 2 shows the CFD codes used: COM3D [21, 22], developed and used by FZK, b02 [7] developed and used by KI, and FLUENT [8] a commercial CFD package used by UU as a platform for implementation of its detonation model [9], [10].

The partners do not perform any kind of simplification on the geometry of the calculation, such as, reduction to two dimensions with simplified geometry from a three dimensions problem with complex geometry [30], or consider one dimension of restricted size [31]. A review of detonation main calculation approaches could be found in [34] [35]. In agreement with the statement made in [25], that detonation must be a three dimensional procedure, the partners choose the aforementioned approach. This gives the additional advantage compared with the calculation presented in [30] of being able to compute focusing and reflections of the waves. Due to the conditions of the problem, it is not necessary take into account auto ignition phenomena [32].

Some relevant information about the numerical schemes used in the codes is provided in Table 3. FZK has used the Van Leer-Hänel scheme [11, 12], while KI employed pressure gradient central differences scheme [7], and UU used the AUSM+ [13] scheme. For this simulation, the three codes employed structured Cartesian grid as described in Table 4. FZK and KI have chosen a computational domain with the same cell size, number of cells and cell resolution (for both 3.832.192 cells) while UU have performed their calculations in the same domain but with a coarser mesh resolution of 0.1 m. which accounts for 237005 cells. The execution time of the codes was found to be between six and sixty hours.

In its calculation FZK used the code COM3D-v.3.5. The Heaviside Detonation Model [15] was used, which is based on the fact that the Chapman-Jouguet parameters are independent on the chemical kinetics. It is a simplified model, specially created for the problems in which constrains make the cell very coarse. It is intended to be used just to study how a detonation will propagate in a system, and is specially indicated for worst scenario studies. The consumption formula stated in Table 5 has limited physical meaning, being a mechanism to provide enough species consumption to maintain the detonation. The turbulence and the heat losses for the calculation of the detonation were neglected as stated in [14], based on the fact that, the time scale of the detonation and heat transmission are much longer than the detonation's.

In the calculation performed by the KI the in-house code B02 was used. B02 is used to describe the detonation regime of the combustion process. It is assumed that the ignition mechanism of the mixture is adiabatic, and is being calculated with a one-step Arrhenius reaction. The wave thickness is quite thin and it cannot be resolved on a grid that covers the entire domain. Therefore, even if it is possible to use a more complex scheme, such as, for instance, the one presented in [28] with several reactions including chain branching [29], the partner consider this would be pointless for the aforementioned reasons. Therefore:

$$\partial C/\partial t = \rho \cdot K_0 \cdot \exp(-E_a/T), \tag{1}$$

where C — mass fraction of n component, ρ — gas density in computational cell, K_0 — pre-exponential factor of reaction rate of reaction m, E_a — activation energy of reaction m, T — temperature in computational cell.

To take into account the energy release rate the following equation is used in each computational cell:

$$\frac{\partial E}{\partial t} = Q \cdot \rho \frac{\partial Ci, j, k}{\partial t} \tag{2}$$

where Q — chemical energy release of reaction, C — mass fraction of reagent, ρ — gas density. The turbulence and the heat transfer was neglected too.

Table 2. List of organizations and codes

Participant Organisations	Codes
FZK, Research Center Karlsruhe, Germany	COM3D-v.3.4 [21,22]
KI, Russian Research Centre Kurchatov Institute, Russia	B02 [7,23]
UU, University of Ulster, UK	FLUENT v6.3.26 [8]

Table 3. Main features of the codes

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-v.3.5	Finite differences Van Leer	C = Van Leer, 2nd order non-oscillative, T=2nd order explicit	CFL=0.96
KI, B02	3D Eulerian explicit solver	C=1st order upwind, T=1st order, Pressure gradients - central difference	CFL=0.9
UU, FLUENTv6 .3.26	Finite volume coupled solver, density-based coupled pressure-velocity coupling, AUSM+	C=2nd order upwind, D=2nd order central -difference, T=1st order explicit linearization	CFL=0.05

Table 4. Computational domain, mesh, CPU time and RAM

Participant	Domain size LxWxH, m	Type of grid	Resolution and total Control Volume number	CPU type, RAM used and CPU time
FZK, COM3D-v.3.5	6.53x6.27x27.73	Cubic structured	98X94x416 0.0666 m. 3,832,192 cells	3 processors Opteron-AMD CPU type, 1 GB RAM per processor. CPU time: ~6 h
KI – B02	6.53x6.27x27.73	Cubic structured	0.066666666cm 3,832,192 cells	Pentium 4, 3.2GHz RAM ~ 150MB Simulation Time ~20 hours
UU - FLUENT	27.75x6.55x6.3	Cubic structured	CV=0.1m 237005 cells	CORE 2 QUAD 775 Q9400 2.66GHz, RAM : 8GB CPU time : ~60 h.

Table 5. Turbulence, combustion and heat losses model

Participant	Turbulence model	Combustion/flame tracking model	Expression for burning tracking model	Heat losses
FZK, COM3D-v.3.5	None	Heaviside Detonation Model	$\Delta y_{H_2} = 100 \cdot Cf \frac{\Delta t}{\Delta x} y_{H_2} \cdot Rr$ Cf- const eq. 6, Δt time step, Δx cell size, y mass fraction	Neglected

			$Rr = \begin{cases} 0 & T < T_0 \\ \dfrac{T - T_1}{T_1 - T_0} & T_0 < T < T_1 \\ 1 & T > T_1 \end{cases}$	
KI – b02	None	Adiabatic, one-step Arrhenius reaction	$\partial C/\partial t = \rho \cdot K_0 \cdot \exp(-E_a/T)$ C - mass fraction of n component, K_0 - pre-exponential factor, E_a - activation energy, T - temperature	Neglected
UU	RNG-LES	Customised RNG premixed combustion model. Gradient method	$\overline{S}_E = H_c \cdot \overline{S}_c$ $\overline{S}_c = \rho \cdot D \cdot \lvert \nabla \widetilde{c} \rvert$ S_c - the source term in the progress variable equation, ρ_u - unburnt mixture density, D - detonation velocity, ∇c - gradient of the progress variable H_c - heat of combustion	Neglected

In the calculation done by the UU the FLUENT commercial code was used. Its ability to handle strong shocks as well as its validation against experimental data was studied by the co-authors in [24]. The comprehensive model description can be found in [16]. The turbulence was modeled with Large Eddy Simulation (LES). The effective viscosity was calculated according to renormalization group (RNG) LES model [17]. The gradient method was used to prescribe the reaction rate during the detonation stage of explosion [18]. $\overline{S}_c = \rho \cdot D \cdot \lvert \nabla \widetilde{c} \rvert$, where S_c -the source term in the progress variable equation, ρ_u - unburnt mixture density, D - the detonation velocity, ∇c - the gradient of the progress variable. The source term for energy equation is associated with combustion reaction rate $\overline{S}_E = H_c \cdot \overline{S}_c$, where S_E is the source term in energy conservation equation and H_c the heat of combustion. UU co-authors consider detonation as a part of the broader physical phenomena (deflagration-to-detonation transition), where the effects of viscosity and turbulence may not be neglected, and therefore consider modeling of turbulence.

RESULTS AND DISCUSSION

Hyd5

"Hyd5", (20% H2) is the first test case to be calculated in the field of this Standard Benchmark Exercise Problem. Sensors 2, 3, 4, 5 have been selected for the comparison between the experimental data and the simulation results (see Figure 3). The sensors are located along the side wall of the tunnel and have 1.2, 3.6 and 5.08 m interval between them. The first sensor reached by the explosion (number 2) is taken as a reference. The evolution of the over-pressure signal, the propagation speed and or the delay of the signals could be compared with the experimental one in different gauges. Joining the first signal peaks as well as later ones (reflections) the propagation of the detonation on the facility could be studied. The slope of this line represents the speed of the detonation, further reflections, etc.

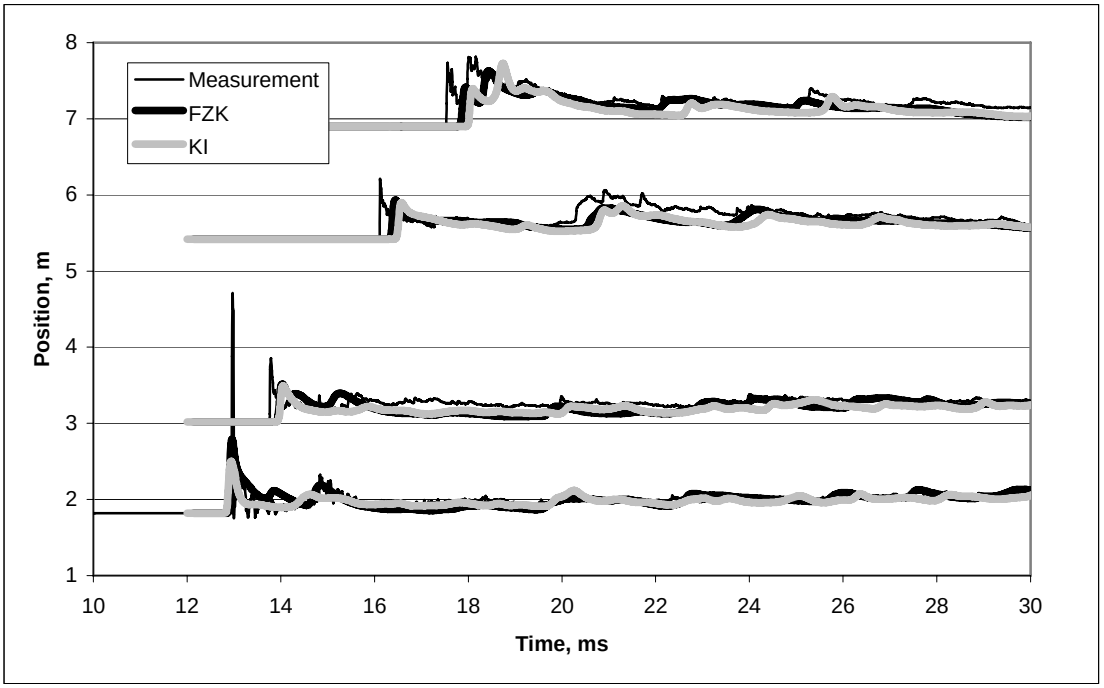

Figure 3. R-t diagram

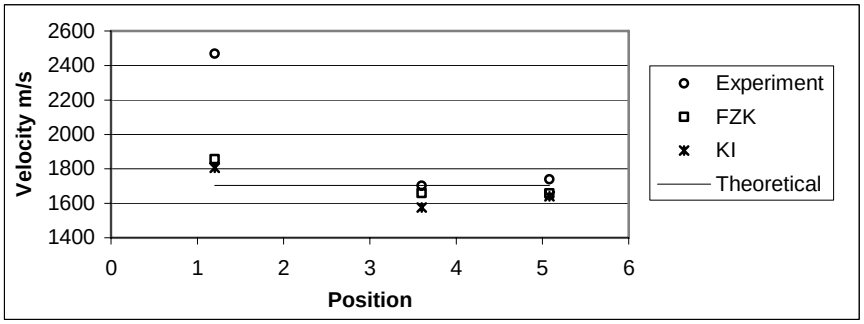

Figure 4. Detonation speed

This is represented in the Figure 4 as well as the speed of a flat detonation front which resulted to be 1703 m/s following [20]. In the interval between the first and the second gauge, the experimental results show an overdriven detonation plus the effect of a curved detonation front (effect of the oblique wall and spherical initial detonation blast). In the calculations of the partners the effect of the curved front is present. It is represented as the deviation (increase) from the predicted theoretical detonation speed of the planar flame. The rest of gauges, are further away from the initial detonation position. Thus the effect of the initial explosive charge no longer is present. Also the curvature of the detonation front is negligible. Therefore in the two last measurement points all codes show a good agreement with the calculated, theoretical and registered values under the expected normal deviation of around 5% (85 m/s). For the last two positions, the differences between the theoretical value and the test on one side and the theoretical value and the calculations on the other are of the same magnitude.

In the Figures 5 and 6 the pressure and impulse signal have been shown. The gauge number 2 has been chosen as most representative. In the pressure signal diagram, KI and FZK calculation show a good agreement with the registered values, both for the peak and for the shape of the curves.

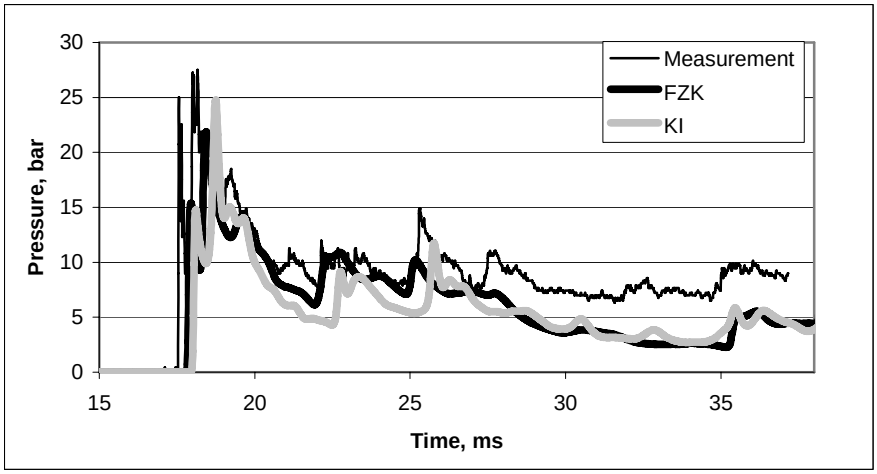

Figure 5. Pressure gauge number 2. Pressure readings.

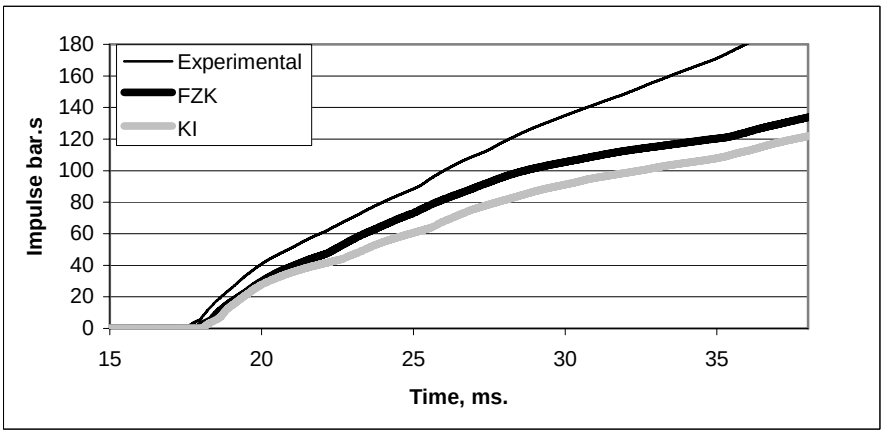

Figure 6. Impulse of the gauge 2.

The partners under predict significantly the values of the impulse. It should be noted that high heat sensitivity of piezo-electric transducers results in the "thermal" signal drift at large times. Thus impulse calculations from experimental data are not very precise. The results of those two last diagrams may indicate the presence of an over driven detonation in the experiment [32]. This supposition is further hinted by the presence of a huge charge of explosive used for initiation. That may result in measurements in which the speed, pressure and impulse are significantly higher than theoretically predicted ones.

The statistical analysis in Figure 6 has been performed following the method that was proposed by the MEGGE group [19]. It may also confirm the previous hypotesis. The geometric mean bias (GB) and the geometric mean variance (GV) are given by the formulas:

$$GB = \exp\left(\overline{\ln\left(PP/PO\right)}\right);\ GV = exp\left(\overline{ln\left(PP/PO\right)^2}\right) \tag{3}$$

where the overbar symbol means averaging, PP stands for the calculated value and PO stands for the measured value. The statistical analysis is a very useful method to evaluate the performance of different models and approaches against a common data set. A model with 100% accuracy should have a value of GB and GV equal to 1, that is located in the vertex of the parabola with coordinates (1;1) in Figure 7. The closer to that point that are the values of GB and GV, the more accurate is the

code. The vertical line passing through the vertex divides the graphs into two areas: the area on the right hand side of the line identifies the over-predictions while the area on the left hand side the under-predictions. The data close to the parabola means systematic mistake whilst the one closer to the central axis means dispersion. In the Figure 7, the KI calculation shows slightly more systematic mistake than FZK one which is coherent with the fact that the predicted speed is slightly further away than the registered one. On the other hand, the data of the FZK is more disperse, which may indicate a slightly bigger difference on the tails of the signals. The fundamental conclusion to be obtained from the figure is a general under prediction of both partners which confirm the conclusion what was already supposed about the initiation.

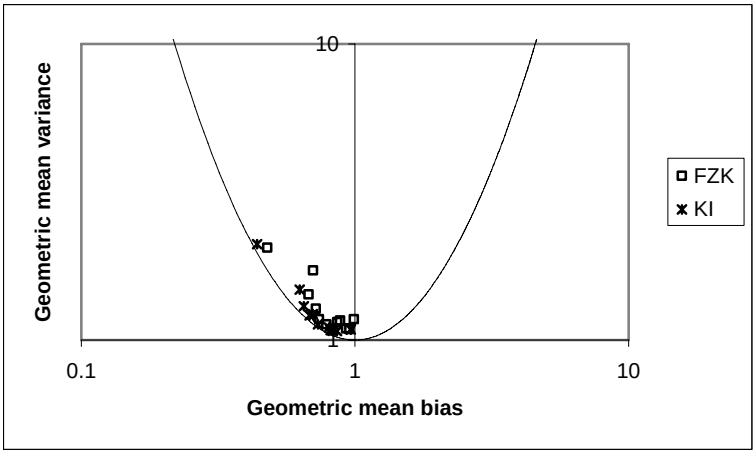

Figure 7. Geometric mean variance and bias

HYD09

The "Hyd9" is the second experiment performed in the field of this SBEP in which the concentration of H2 was 25.5% vol. The sensors selected to perform the principal comparisons are placed in the channel of the facility (sensors 7-11) Figure 2. The distances between the different transducers are 6.2, 8.93, 11.53, 17.2 m. measured from transducer number 11 which was taken as a reference.

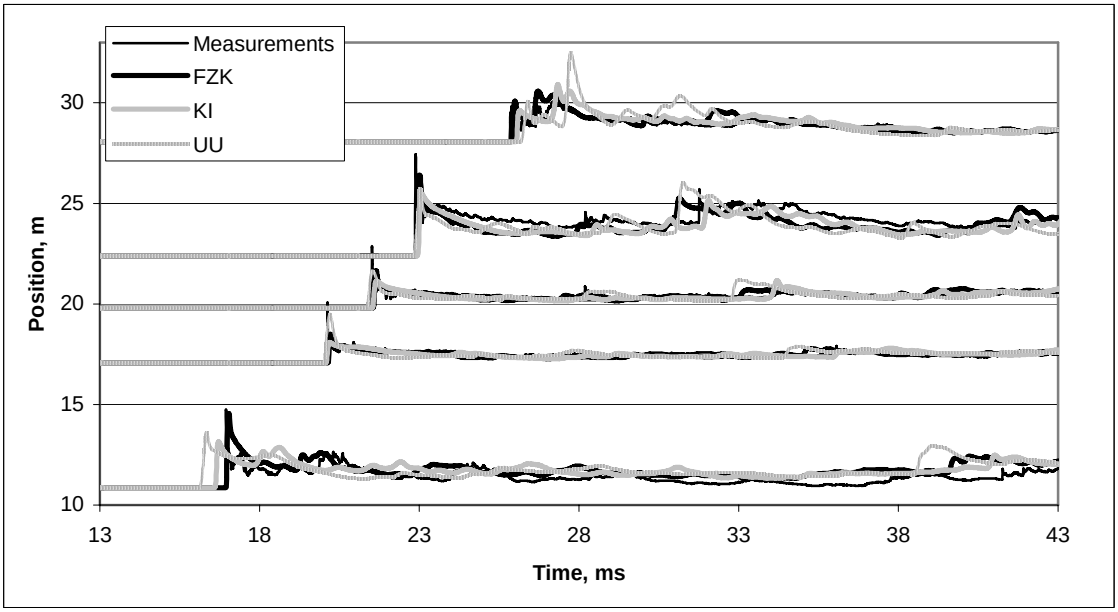

Figure 8. R-t diagram

From the Figures 8 and 9 it could be seen that the main shape of the detonations signals is well represented in the results provided by all partners. The R-t diagram shows the delay or early arrival of the signals. All partners represent qualitatively good the initial detonation front and the reflection. The slope of a hypothetical line joining the arrival of the detonation signal represents the speed of the detonation, which is plotted in the Figure 9.

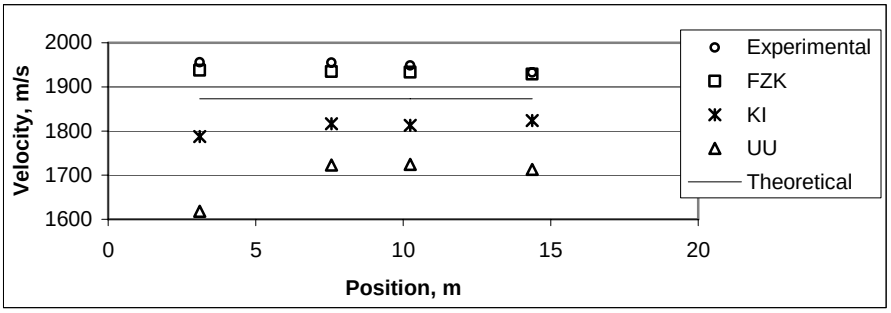

Figure 9. Detonation speed diagram

For this concentration, the speed of a flat detonation front was found to be 1873 m/s [20]. The FZK prediction of the detonation speed agrees with the sampled experimental values but differs form the theoretical planar one in a maximum of 60 m/s. The KI calculation presents an underprediction regarding the theoretical planar speed of 80 m/s and of the sampled data of 150 m/s. For these two partners the difference between the calculated and the theoretical planar detonation speed is of the order of magnitude of the accuracy of the calculation (5% or 80 m/s). The UU calculation presents an under prediction of around 200 m/s of the theoretical value and of around 250 of the sampled one. Though the value of the theoretical detonation velocity is defined in the model as a constant, the simulation results give under predicted propagation of the detonation front. This under prediction in detonation velocity is due to the relatively coarse mesh and numerical diffusivity, which becomes pronounced in simulation of 3D propagating detonation wave.

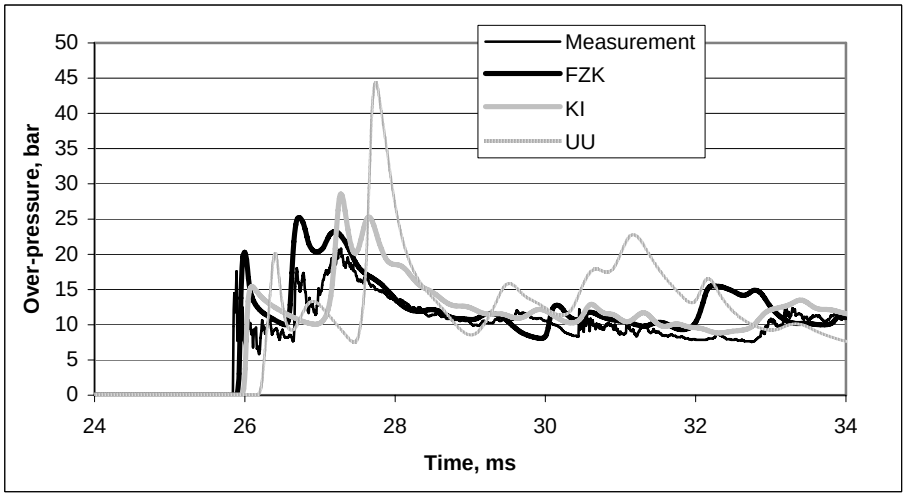

Figure 10. Pressure diagram for gauge 7

In figure 10 the pressure signal is shown. As could be seen, the results obtained with all codes present good qualitative agreement in the shape of the signal, predicting the peaks and reflections. The gauge number 7 was chosen as more significant as is located further away of the ignition source and closer to the wall than the others. The peaks of the pressure, both detonation and reflection, are overpredicted in

the calculation done by FZK. The overprediction of the reflected peak, Figure 10 (26.8 ms), is due to the fact that the heat transfer is neglected, which can have a significant effect both on the curved part of the channel and on the wall in which the reflection takes place. In data provided by KI the first detonation front is calculated quite accurately but the reflection is overpredicted. In the data supplied by UU both the first peak and the reflection are overpredicted. This is believed to be caused by the numerical instability of strong shock waves due to CV size and time step (CV size 0.1 m used in this SBEP simulation). UU partner expects that the use of finer CV size and smaller time step will improve modeling of the propagating and reflected shock waves. As it is patent in the impulse diagram, Figure 11, all codes predict in a similar way the impulse. The overprediction, may be considered of the order of the accuracy of the calculation, due to the fact that the tails of the pressure signals are quite well predicted by all partners. The thickness of the detonation wave depends on the size of the control volume. UU partner believes that the increase of impulse is due to the fact that an increase in the control volume will widen the detonation front, a mechanism that will cause the increase of impulse.

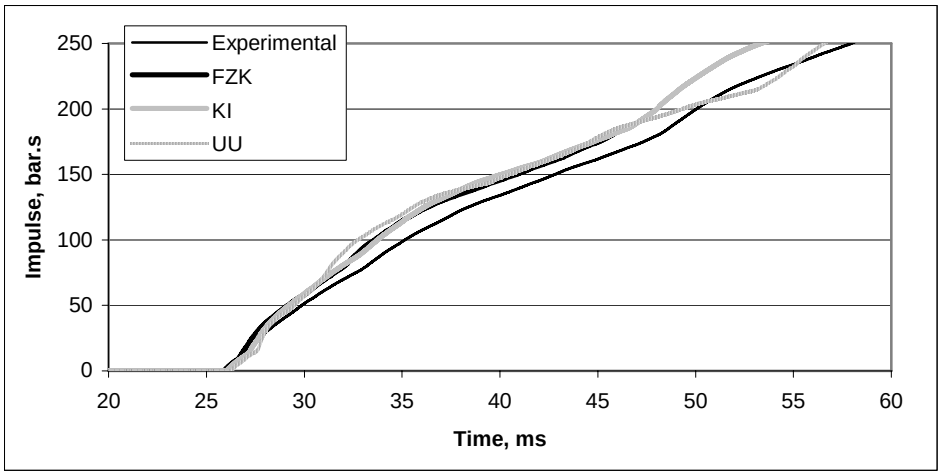

Figure 11. Impulse gauge diagram for gauge 7

The figure 12 shows the geometric mean bias (GB) vs. the geometric mean variance. The figure presents symmetry to the Y axes and confirms that that the over and under prediction of the pressure depend of the gauges and has no defined tendency, excluding a defined systematic mistake on the models. The detected systematic mistake in experiment "Hyd5" was, with all probability, the product of the explosive charge used to start the detonation on the experiment. All partners achieve in this experiment good agreement. The improvement compared with "Hyd5" is very significant.

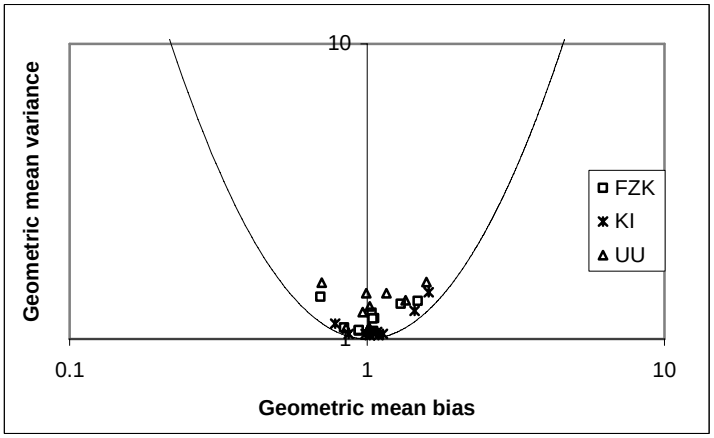

Figure 12. Geometric mean & variance bias.

CONCLUSIONS

This paper discusses the results of the CFD simulation of two uniform hydrogen-air mixture detonations with concentrations of 20% vol. and 25.5% vol. of H_2 and different ignition locations, which was experimentally studied by the Kurchatov Institute (RU).

A total of three partners submitted five simulation results obtained using various CFD tools. The detailed analysis, comparison of the simulations and of the divergences between them was the object of this paper. The exercise was carried out simulating industrial scales, with the goal of the evaluation of the capabilities and limitations of CFD simulations in the hydrogen safety engineering praxis.

The comparisons presented include the results of the pressure, impulse, detonation speed and the representation of the R-t diagram for both the 20% and 25.5% vol. H_2 cases. A quantitative comparative analysis of the quality of the result of every partner was carried out. Its results are depicted on the geometric mean vs. bias diagram.

Note that the results of all codes are in better agreement with the experimental measurements for the 25.5% case than for the 20% one. The divergences between them and the theoretical values calculated following the 1D detonation theory are due to the strength of the ignition source and position of the walls, creating possibly an overdriven detonation.

In the areas of steady state detonation, it is remarkable, that even on the coarse grids, with a typical calculation cell size of ~ 6-10 cm, considerably larger than the detonation cell size ~ 1.2 to 1.4 cm, the quantitative results are very good for the propagation speeds, overpressures and impulses.

The fundamental outcome of this exercise is that the simulation of detonations in large scale in CFD based safety analysis can be considered as reliable and trustworthy.

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