AN INTERCOMPARISON EXERCISE ON THE CAPABILITIES OF CFD MODELS TO PREDICT DEFLAGRATION OF A LARGE-SCALE H_2-AIR MIXTURE IN OPEN ATMOSPHERE

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ABSTRACT

This paper presents a compilation of the results supplied by HySafe partners participating in the Standard Benchmark Exercise Problem (SBEP) V2, which is based on an experiment on hydrogen combustion that is first described. A list of the results requested from participants is also included. The main characteristics of the models used for the calculations are compared in a very succinct way by using tables. The comparison between results, together with the experimental data, when available, is made through a series of graphs. The results show quite good agreement with the experimental data. The calculations have demonstrated to be sensitive to computational domain size and far field boundary condition.

1. INTRODUCTION

As part of the activities within the HySafe Network of Excellence ("Safety of Hydrogen as an Energy Carrier"), experimental tests collected and proposed by the partners of the consortium have been selected for code and model benchmarking in areas relevant to hydrogen safety. Such selected exercises have been identified with the acronym SBEPs –standing for "Standard Benchmark Exercise Problems" – and follow the main objectives of establishing a framework for the validation of codes and models for simulation of problems relevant to hydrogen safety, and identifying the main priority areas for the further development of the codes/models.

Comparative assessments of code performance are being made and directions towards further development have been identified. Different codes and models are being assessed by the partners involved. These tools cover the different approaches used in each phenomenon, i.e. integral, CFD (1D to 3D), in-house, commercial both specific and multi-purpose. Benchmarking exercises should therefore benefit from the complementarities arising from the variety of codes, models, approaches, user experience and points of view from industry and research agents participating in this network. Quality and suitability of codes, models and user practices are being identified by comparative assessments of code results, which constitute the essentials of the SBEPs. Directives towards further development and recommendation for optimal tools and user best practices for phenomena and approaches are to be provided.

It was proposed to use existing data to start this activity. Therefore, relevant cases for SBEPs have been selected, based on the relevance to hydrogen safety of the phenomena explored in the tests, the availability and feasibility of the data and their possibility to be used for validating mainly CFD codes.

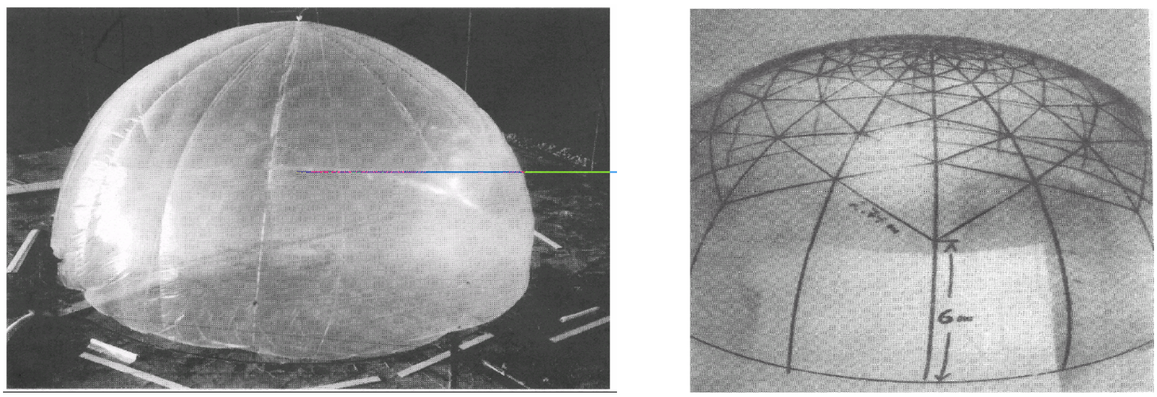
A first experiment on hydrogen combustion was selected and identified as SBEP-V2. In the paper, first, this experiment is described. Next, the main characteristics of the models used for the calculations are briefly compared. Afterwards, the comparison between results and experimental data, when available, is presented. Finally, a discussion about the results and conclusions obtained is made.

2. EXPERIMENT DESCRIPTION

The experiment was performed by one of the partners of the HySafe network, the Fraunhofer Institut Chemische Technologie (Fh-ICT), Germany, in 1983 [1, 2]. For the experiment, a 20 m diameter polyethylene hemispheric balloon (total volume 2094 m^3) was placed on the ground and filled in with a homogeneous stoichiometric hydrogen-air mixture (see Fig. 1a). The balloon was fixed to the ground by weights placed inside, where the balloon wall met the floor. These weights alone did not compensate the upward buoyancy, thus an additional rhombus-shaped wire net was laid over the balloon and fastened to the ground at 16 points, as shown in Fig. 1b.

The filling process of the gases was closely observed in order to produce a homogeneous mixture to avoid an enrichment of the hydrogen in the upper areas of the balloon. The required air was provided from the atmosphere using a fan and introduced into the balloon via a tube fitted with a flutter valve. The hydrogen was supplied from several bottles connected in parallel, where the required quantity was determined based on the known bottles volume and pressure. The air fans created an effective mixing of the gas in the balloon. Gas samples were taken at different heights inside the balloon and analysed using gas chromatography in order to check the hydrogen-air mixture homogeneity.

The initial pressure was equal 98.9 kPa and the initial temperature 283 K. The combustion was initiated by ignition pills of 150 J at the centre of the hemisphere basement. After ignition, the turbulent wrinkled flame was propagating in almost hemispherical form. At the same time, the balloon stretched slightly outwards until it burst at the seams bordering the ground and along longitudinal welds. This occurred at the moment when the flame had reached about half of the radius of the balloon, i.e. about 5 m. In the further course of the flame propagation, the balloon segments expanded. Flow must be disturbed when the remaining unburned gas flowed between the segments of the balloon shell and was burned after that.



(a) (b)

Figure 1. 10 m radius hemispherical balloon (a) and wire net (b).

Pressure dynamics was recorded using 11 transducers, installed on the ground level in a radial direction of the hemisphere basement at the following distances from the centre: 2.0, 3.5, 5.0, 6.5, 8.0, 18.0, 25.0, 35.0, 60.0 and 80.0 m. In addition, one “a-head” pressure transducer was installed along an axis running at right angle and mounted on a vertical timber wall of 1×1 m² placed on the ground at 25 meters far away from the ignition point.

The deflagration front propagation was filmed using high-speed cameras. The dynamics of the flame shape profiles with time, filmed by cameras, positioned along to the pressure measurements axis and normal to it, is available for comparison and shown in Figure 2. The flame propagation was evaluated along the radial paths between 45° and 135° from the ignition point and the average values of the flame front radius and the flame front velocity were derived. The error, arising from indistinctness of the flame contour and fluctuations in picture frequency, was estimated by the authors [1] as ±5% without taking into account certain asymmetries in flame propagation.

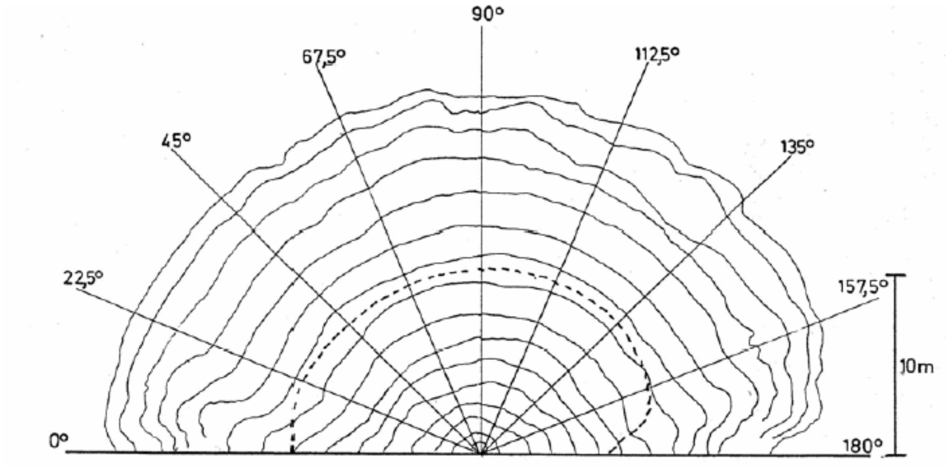


Figure 2.Variation of flame front contours with time.

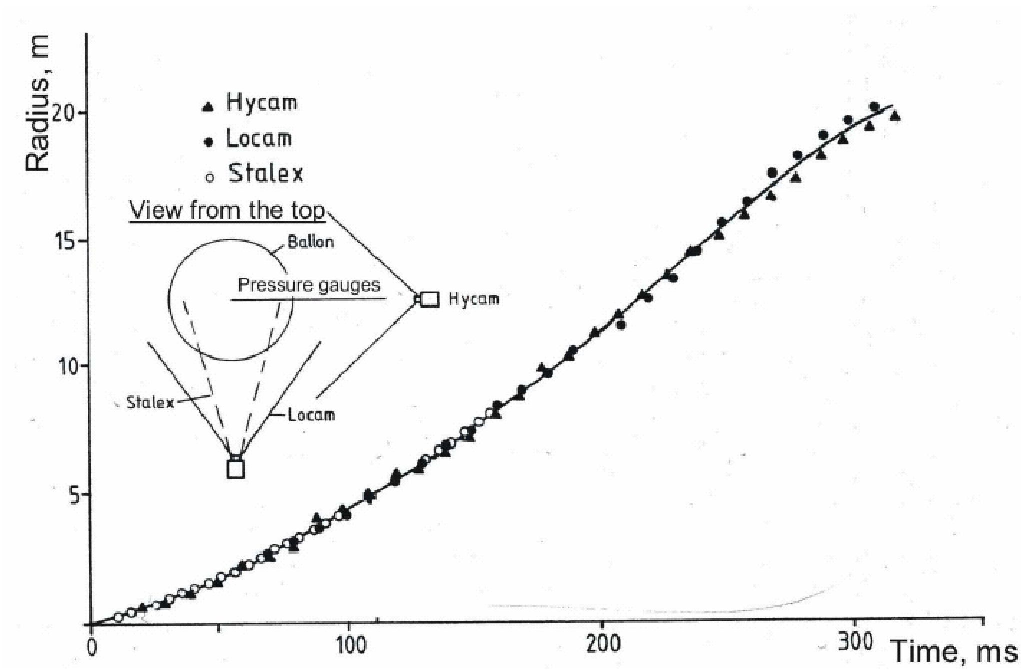


Figure 3. The flame front radius vs. time, obtained from post-processing of films from different cameras, and the averaged flame front radius.

3. MODELS

Different codes and models have been used by the HySafe partners involved in this exercise. These tools make use of different approaches and assumptions, which are summarized in Table 1.

Table 1. Summary of codes and models used by the participants.

Participant & Code	Turbu-lence model	Chemical model	Discretisation scheme & resolution method	Grid	Computer & CPU time
CEA (Commissariat à l'Energie Atomique) **CAST3M** [3]	-	One chemical global reaction, (CREBCOM combustion model)	Operator splitting technique. First Euler equations without source term, second, in each mesh cell, the ODE system involving the source terms. Euler explicit algorithm in time.	1D spherical domain cell size 0.1 m	Not available
GexCon **FLACS** v8.1 [4]	k-ε standard	Beta flame model solves a linear differential equation to control the flame thickness (3-5 grid cells). Reaction rate based on one step model with burning velocity from flame-library	SIMPLE, second order schemes.	3D-Cartesian cell size:0.5 m A: with 2 planes of symmetry B: full domain	1 CPU PCs (2-3GHz) 0.5-4 Gb RAM Linux 4h CPU
FZK (Forschungs-zentrum Karslruhe) **COM3D** [5]	k-ε standard	Combustion model CREBCOM. Adjustable parameter C_f, governing the rate of chemical interaction and therefore a visible flame speed. Multicomponent (e.g. H_2, O_2, N_2, H_2O) with enthalpies and heat capacities as polynomial fits of JANF tables.	Hydrodynamic solver coupled with the turbulence and chemical kinetics models. Euler equations used to model the process.	Arbitrary-shaped 3D equidistant orthogonal grid. 80x80x80 cells (0.3 m) to simulate in detail the combustion process. 50x50x160 cells (0.59 m) to study the pressure wave	Cluster of 7 Athlon PC - 2 CPU each. Linux 2.4.20. ≈ 14 days /with 14 processors
JRC (EC Joint Research Centre) **Reacflow** [6]	k-ε standard	Modified Eddy Dissipation combustion model	Explicit scheme - Second order Variants of Roe`s (Roe, 1980) Riemann Solver	3D unstructured adaptive grid	Multi CPU system. 26.5 to142 h CPU
NH (Norsk Hydro) **FLACS** v8 [4]	k-ε standard	beta flame model (flame front defined to the location where 10% (vol) of the present H_2 has reacted with O_2)	SIMPLE, second order schemes	3D-Cartesian	6 days CPU (1 s experiment)
TNO **AutoReaGas** v3.0 [7]	k-ε standard	combustion is mixing controlled; flame thickness 3-5 cells; flame speed correlates via empirical relations with the calculated turbulence parameters; calibrated for hydrocarbons	SIMPLE, first order scheme	3D Cartesian space 8000 cells (1 m^3) **TNO-1**: 27000 cells (1m^3)	
UU (University of Ulster) **FLUENT** v6.1.18 [8]	LES (RNG)	Gradient method	Explicit method for solution of linear equation set. 2[nd] order upwind for convective terms. 2[nd] order central difference for diffusive terms	3D unstructured tetrahedral grid **Case a**: 258671 cells **Case b**: 677729 cells	2/6 CPU IBM Pwer 4 4/12 Gb RAM 142/197h CPU (0.32/0.63 s experiment)

It is important to note that for this exercise all details of experimental results were known to the modellers several months before the submission. Further, some modellers submitted their results after the initial deadline, with full access to the results predicted in time by other modellers. Since most of the model predictions will strongly depend on user choices (grid, choice of sub-model, etc.) little can be said about prediction capabilities from the simulation performed. Being a first exercise, we were more interested in learning about the strength and limitations of the available models to simulate the phenomena than in the predictive power of each team. Optimally, predictive power should be tested against blind simulations, with no knowledge about experiment results or the predictions of the other modellers when submitting.

Some participants submitted two sets of results (UU and TNO) varying the grid and the calculation domain sizes. The boundary definition was observed critical as it is discussed below.

According to the CEA interpretation of the phenomenon, the experimental results show that, before the flame reaches the interface between the stoichiometric hydrogen-air mixture and the air, we are dealing with a one-dimensional point-symmetrical flow generated by a constant speed flame. If the medium would be homogeneous and the flame width would be negligible, the solution would be self-similar, as pointed out in the works of Sedov and Kuhl [9, 10]. In this case, the solution would consist in a shock wave, followed by an isentropic compression region, followed by the (infinitely-thin) flame, and then the flow at rest behind the flame. Because of the hyperbolicity of the phenomenon, the solution remains self-similar until the pressure wave reaches the interface, and afterwards, is "almost self-similar" until the flame reaches the interface. Thus, the CEA model is a one-dimensional spherical model, opposite to the 3-D models used by the other participants. Nevertheless, the use of 3-D models would allow taking into account buoyancy effects that are far from axial symmetric. This may not be an essential effect with such a reactive gas mixture, but the effect of buoyancy will definitely influence the flame shape after the gas has been burnt.

4. RESULTS

Before going to the comparisons between experimental and numerical results, a few considerations related to the experimental conditions and the data recorded should be taken into account:

- First, gauges at 2, 8 and 18 m have to be influenced by combustion products; their signal did not recover ambient pressure as the other gauges did.
- The influence of the polyethylene film is unclear; however it could be supposed small or negligible.
- Additional pressure due to film weight is excluded due to the presence of the supporting constructions.
- Turbulence generation by the supporting constructions should be small since no noticeable flame acceleration at R = 10 m appears. However, in the upper part, where the wire net was denser, there seemed to be an effect, visible on the video from the tests but not measured, creating turbulence and flame acceleration that could influence in particular the far field pressures.
- Errors in the flame velocity measurements are difficult to evaluate.

At the initial moment the hemispherical balloon is filled with quiescent mixture, so the initial conditions employed for the calculations, in all cases, were for the temperature $Ti=283\ K$ and for the pressure p_i=98.9 kPa. The dynamics of the averaged flame front radius with time, including both experimental and numerical results, is presented in Fig. 4. From this figure it can be inferred an absolute front flame velocity between ~40 m/s at the beginning to ~80 m/s at the end, these values correspond to turbulent combustion regime. In Figs. 5 to 10 the pressure dynamics at different radii are shown, including the experimental and the numerical results obtained by the different modellers.

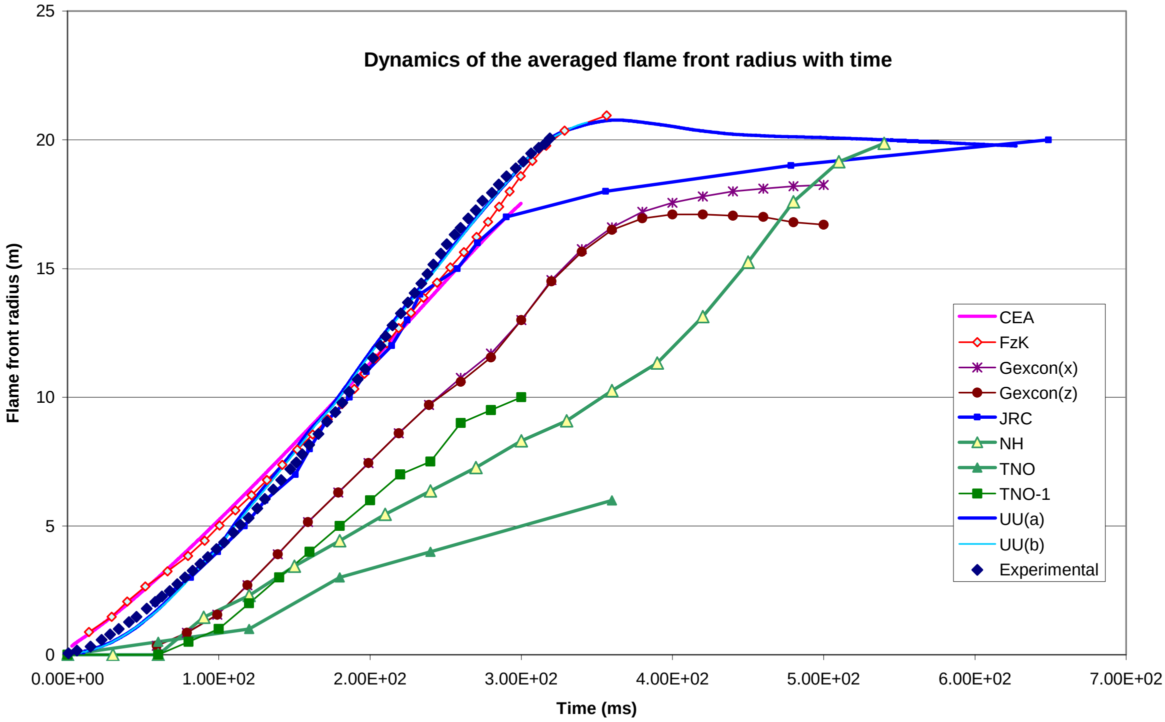


Figure 4. Dynamics of the averaged flame front radius with time.

In order to compare the results obtained with the different codes and approaches, perhaps the main parameter is the flame velocity. For the flame position versus time one should expect some deviation, as it is unclear how the video camera predicted flame corresponds to the numerically estimated flame. It can also be mentioned that some models show a delay in the initial phase of the simulation. Taking this into account, we can say that, despite of use of different models and approaches, all codes demonstrated ability to correctly estimate mean flame velocity. All simulations (except the old version of FLACS used by NH and the imperfectly calibrated calculation of TNO) reproduced quite well the mean flame velocity. In particular the results obtained using “Large Eddy Simulation” (UU) showed an excellent agreement with the experimental flame acceleration.

For NH, using an old version of FLACS code, it seemed unclear whether the fans were running upon ignition, and they used a “characteristic velocity” of 0.5 m/s inside the tent upon explosion. A turbulence intensity of 0.05 was chosen along with a turbulent length scale of 0.5 m. This showed out to produce too slow flame propagation and late arrival of explosion pressures. The FLACSv8 was issued 2003. In the period since that release a significant upgrade and validation effort for hydrogen explosions have been carried out. The performance for FLACSv8 for hydrogen has been questionable. Significant improvements are seen with FLACSv8.1, issued March 2005.

In the TNO case, the problem seemed to be caused by a gas leaking as a result of an inappropriate boundary definition, probably combined with the lack of calibration of the model for H_2. A better definition of boundary conditions in a second calculation (TNO-1) clearly improved the results.

The pressure-time curves corresponding to transducers installed outside the balloon, at radii 18, 35 and 80 m, (Fig. 8 to 10) show an almost linear increase corresponding to the compression waves travelling ahead of the flame front. When the flame is extinguished the gases are no longer pushed by the flame and an expansion wave follows. Because of the spherical character of the phenomenon the intensity of the waves decreases with the distance to the centre of the hemisphere.

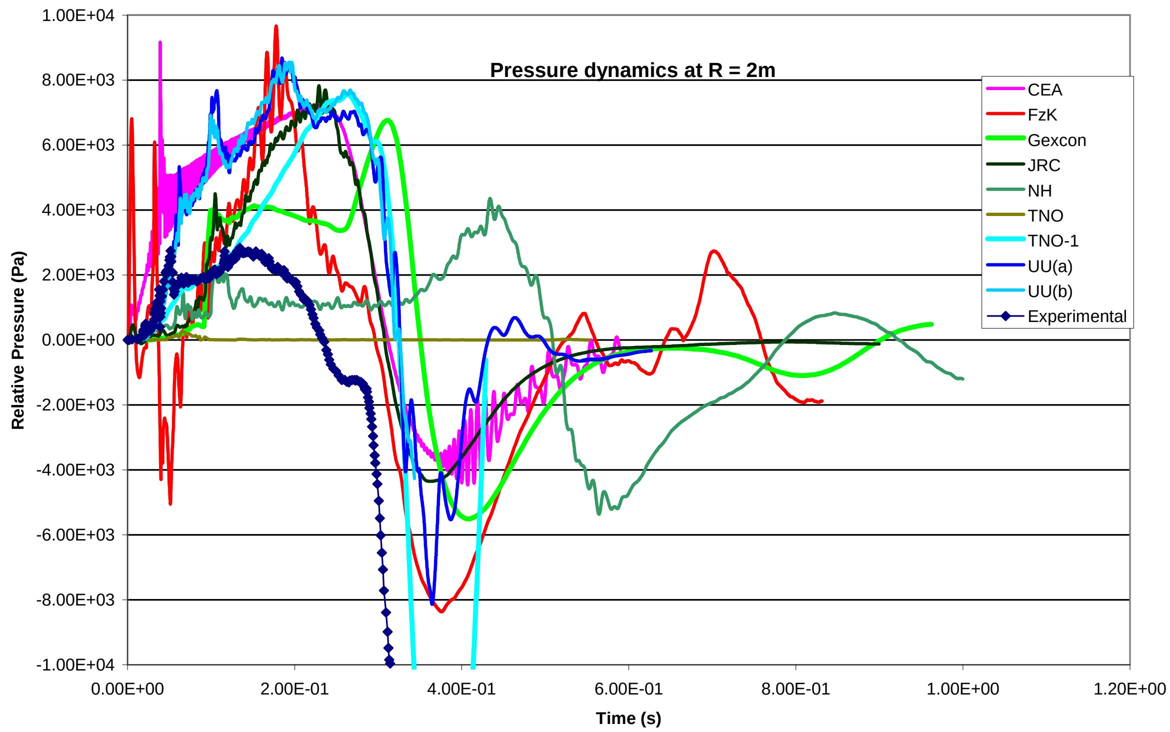


Figure 5. Pressure dynamics at R=2 m.

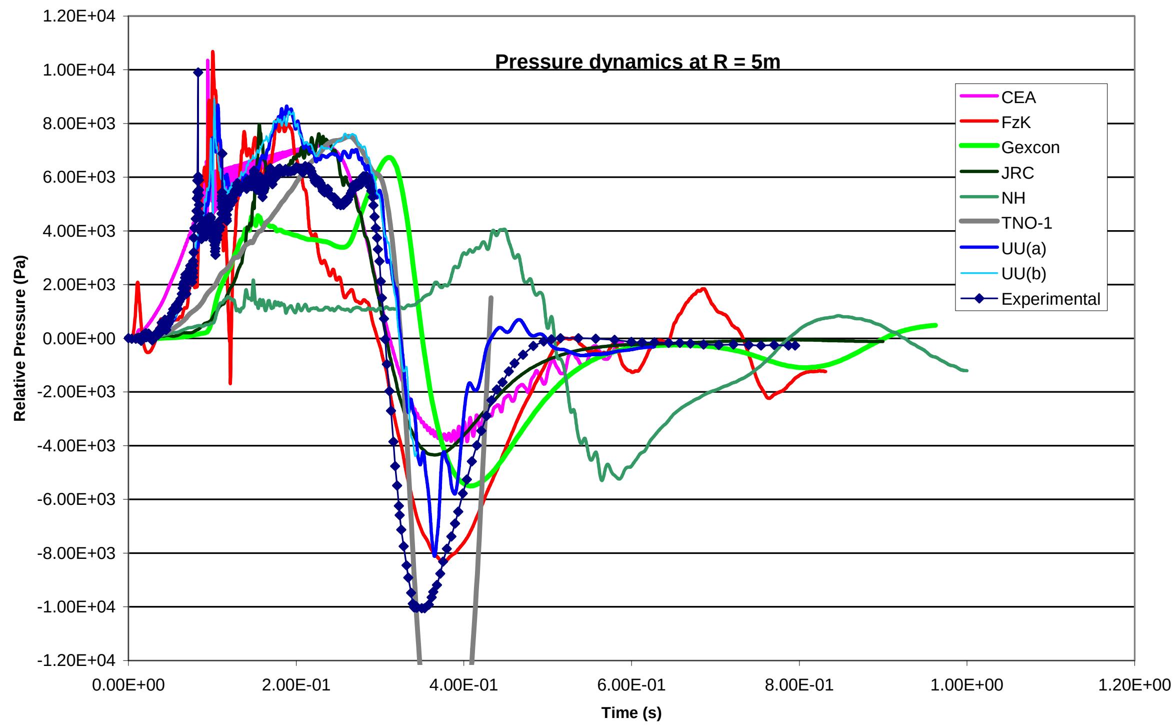


Figure 6. Pressure dynamics at R=5 m.

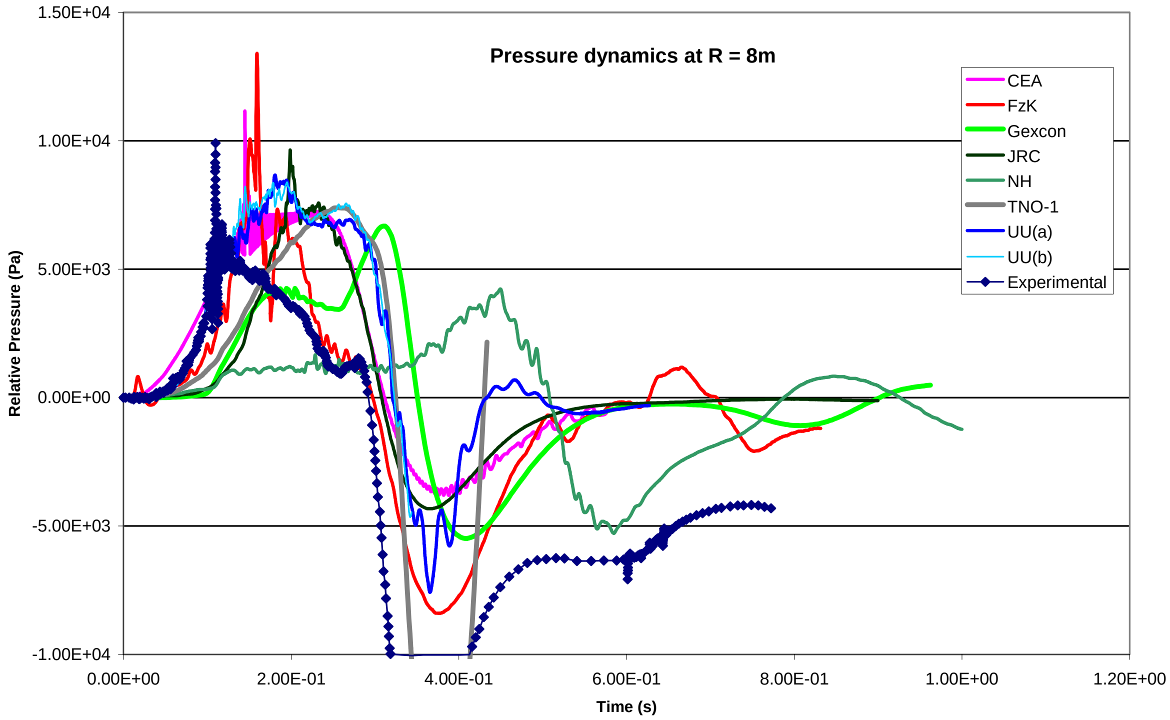


Figure 7. Pressure dynamics at R=8 m.

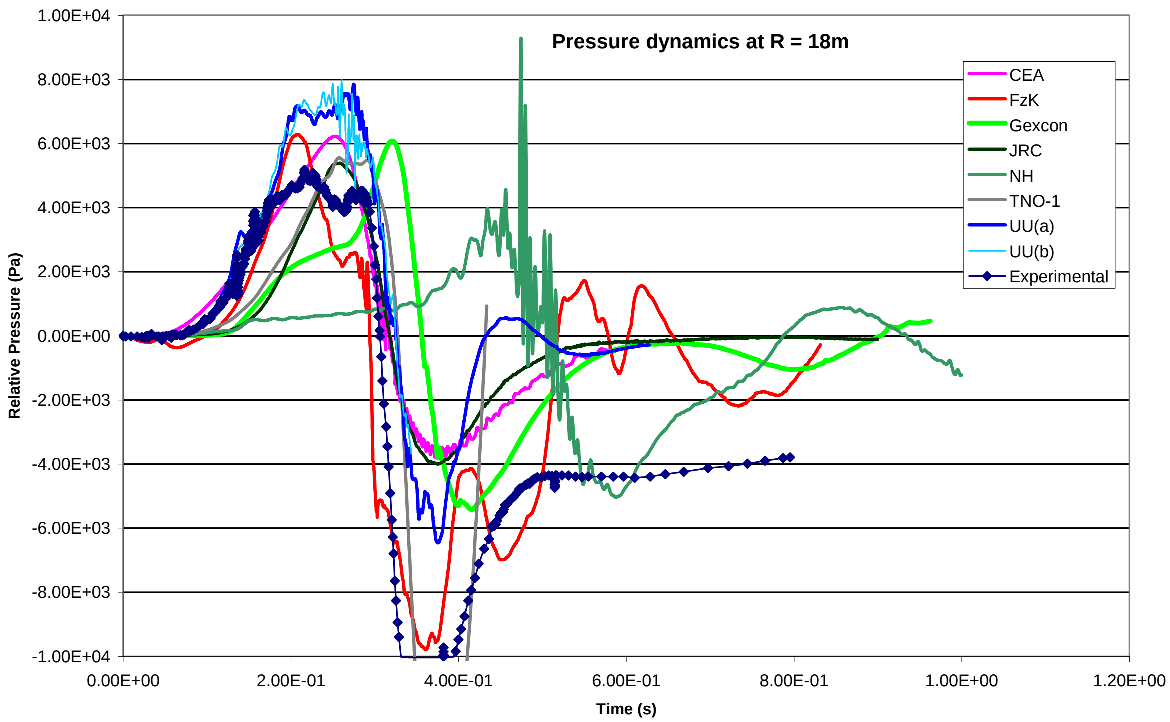


Figure 8. Pressure dynamics at R=18 m.

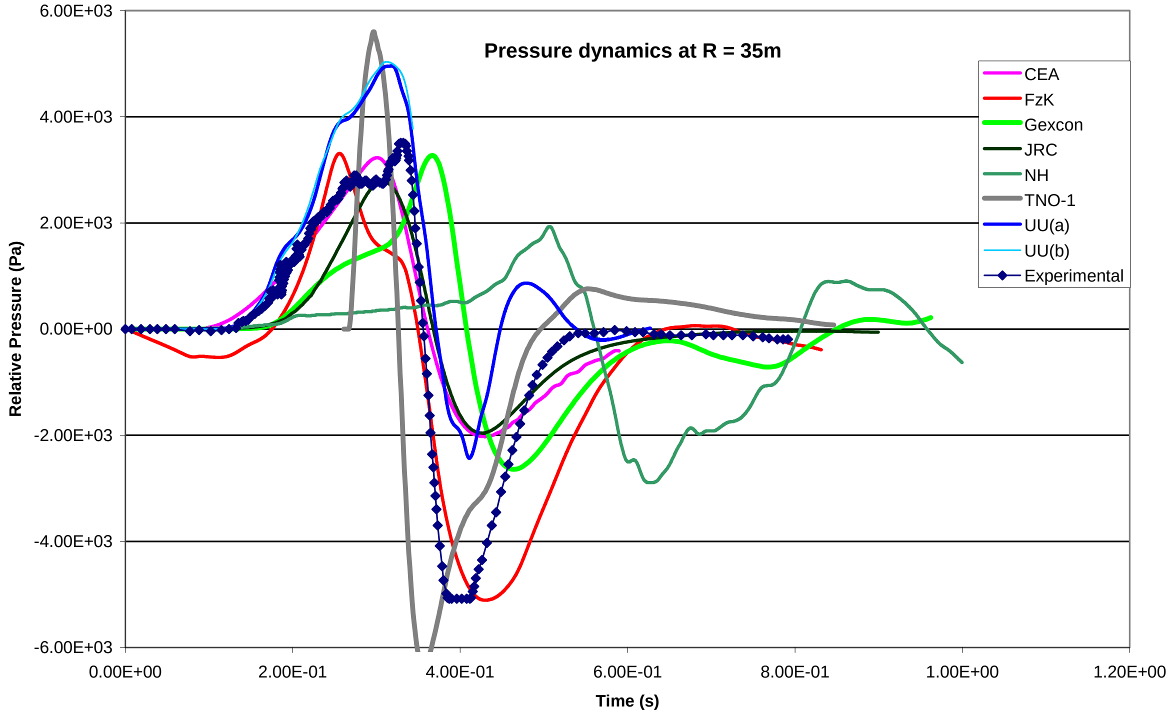


Figure 9. Pressure dynamics at R=35 m.

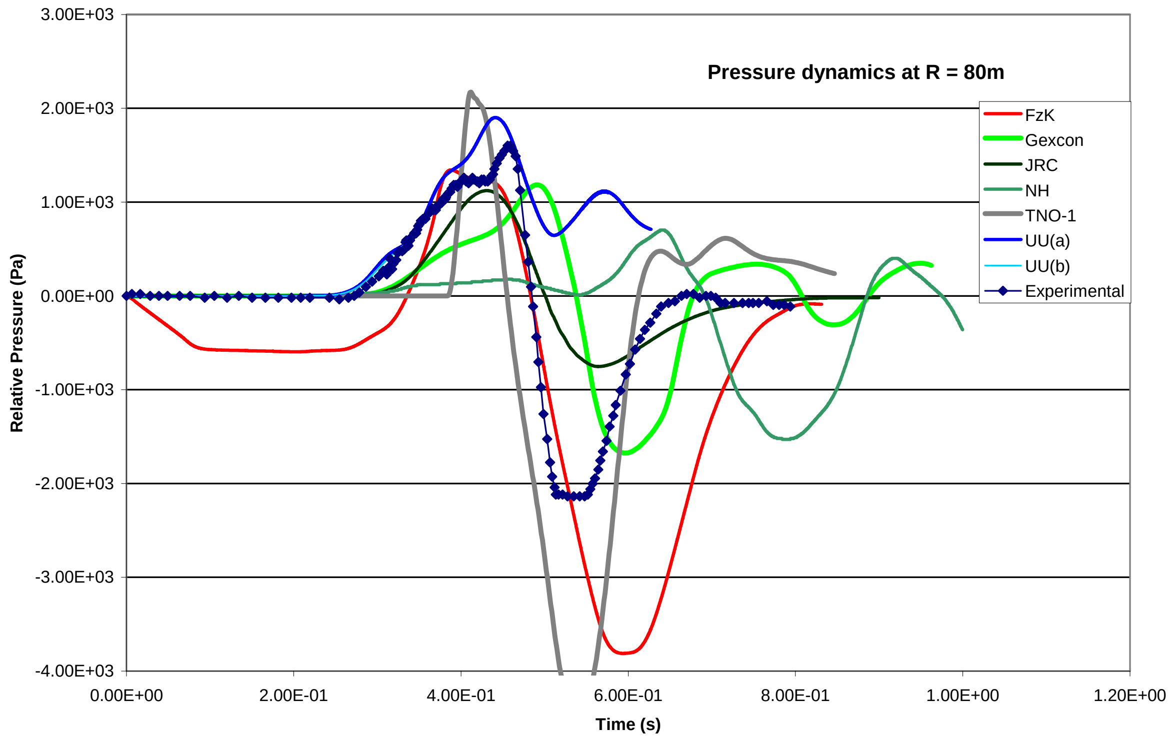


Figure 10. Pressure dynamics at R=80 m.

Inside the balloon (r = 2, 5 and 8 m) the behaviour is different; the flame front pushes out the unburned gases increasing the pressure of the air confined between the flame front and the balloon; this pressure reduces suddenly when the balloon bursts, at t=0.1 s approximately, and then, the pressure is almost constant until the expansion wave, originated by the flame extinction, reaches the transducer producing the minimum pressure that finally adapts to ambient pressure. At radii equals to 2, 8 and 18 m this pressure recovery is not properly detected by the sensors, probably due to a problem with these sensors, which resulted affected by heat radiation, while all the calculations show the pressure recovery up to around the ambient pressure.

Regarding pressure dynamics, and excluding the sensor at r=2 m, all codes reproduce qualitatively well the maximum pressure (except the TNO code), as a consequence of the good prediction of the flame velocity. We think that this sensor did not provide a correct measurement (the maximum pressure load is 20 mbar while in the others in the flame region is 60 mbar, i.e. this sensor does not respect the initial self-similarity of the flow). In general, as already said, all gauges inside the flame (r <= 10 m) should have to be strongly influenced by heat radiation and their measurements have to be carefully considered.

The models show more difficulties to capture the minimum pressure due to the expansion wave, originated when the combustion extinguishes. Amplitudes of negative pressures demonstrate considerable dispersion. Reason could be connected with ‘open’ boundary conditions in the simulations. This can be avoided by using larger computational domains. Besides, at larger distances from the centre of explosion, the grid cells are greater than near the origin, and this could explain the decay of the simulated negative pressure. In general, a finer grid produces better numerical results and less oscillation. For instance, JRC calculation with the REACFLOW code used a resolution of 0.27 m in the reaction zone by means of the adaptive meshing, achieving an average accuracy of about 8.5% over 3 sensor probes. However, in the far field region, the average mesh size was about 2 m, with an average accuracy of about 25% over two sensor probes. Increasing the mesh resolution in the outer region will contribute to obtain a similar accuracy.

CEA has performed the computations with a first order accurate scheme, since the second-order reconstruction method tends to amplify the oscillations due to the combustion model CREBCOM [11]. This explains why their results are damped in the low pressure region.

FzK did not consider the initial stage of the flame development in the simulation; this resulted in almost ‘steady state’ regime of deflagration with average velocity of 60 m/s

In figures 11 and 12 the flame front surface profiles at t= 120 and 240 ms, obtained with different 3D models are represented. Experimental data are not available, except for the average radius given in Fig. 4. The results from FzK and UU are very similar, with a more corrugated surface for FzK as a consequence of the combustion model. GexCon results (not represented) also showed a quasi-symmetrical profile, close to that of UU but with slower development. However NH and TNO results differ from previous ones, as expected, because the flame velocity is not correctly predicted in these models (see Fig. 4).

5. CONCLUSIONS

We can conclude that most of the calculations reproduced quite well the flame velocity, an important parameter for safety purposes. The pressure dynamics obtained numerically are in good agreement with the experiments, for the positive values. The negative pressures are more sensitive to far field boundary condition and, as a consequence, to the size of the computational domain. Therefore, the numerical values obtained present more dispersion. This can be avoided using larger domains and finer grids. Nevertheless, taking into account the possible errors in some measured pressures, the agreement cannot be considered bad for the negative pressures.

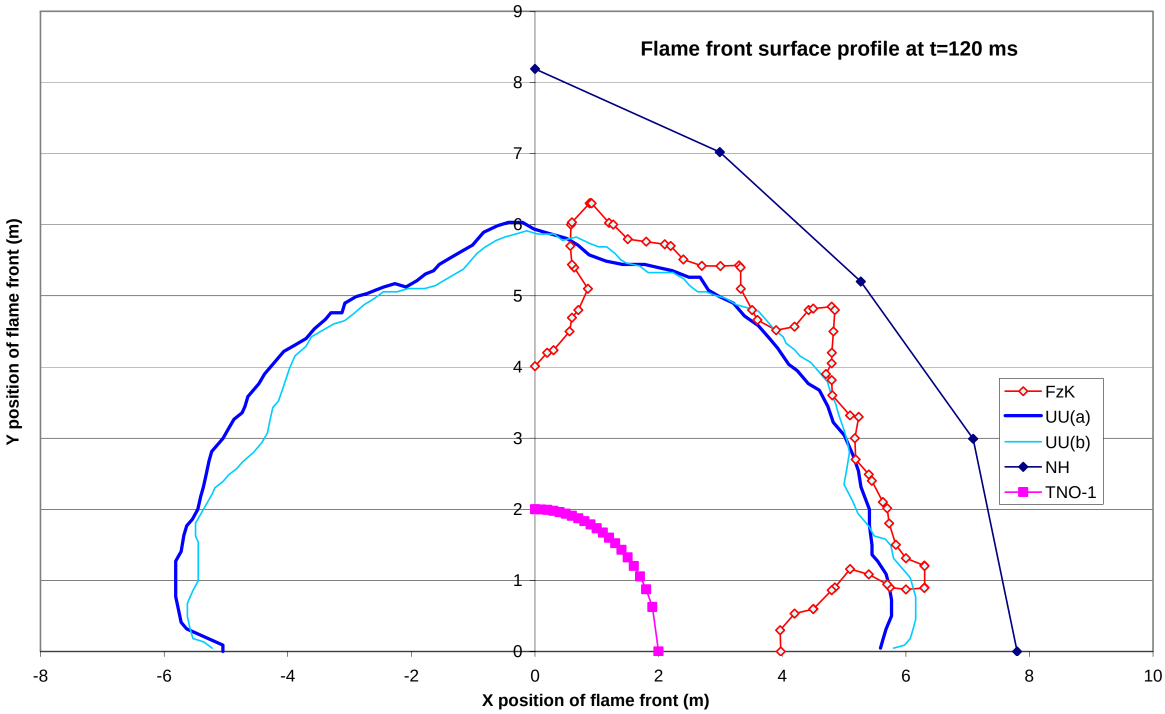


Figure 11. Flame front profiles at t=120 ms.

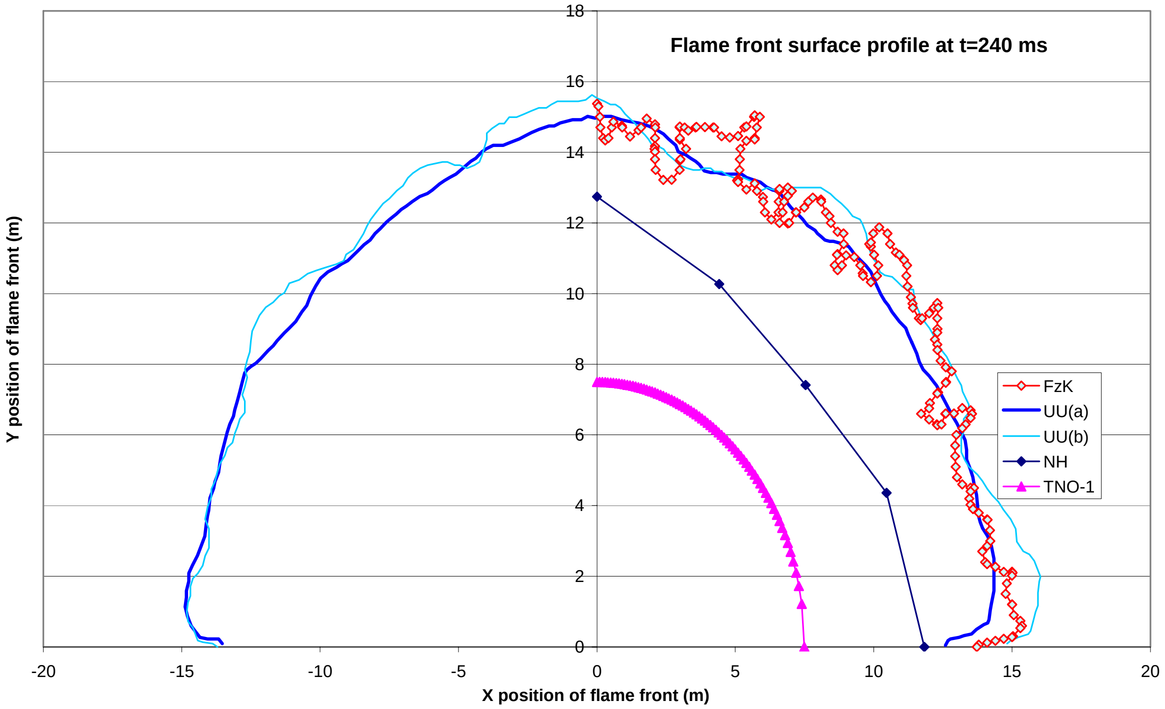


Figure 12. Flame front profiles at t=240 ms.

Lessons learnt from this exercise will be useful for improving our models and codes that will be tested soon against new SBEPs. This is only the first of a series of exercises to be developed along the HySafe duration through which validation of the models against further experiments will be reached. Depending on the numerical implementation of the same combustion model CREBCOM [11], numerical oscillations appeared in CAST3M [3] and not in the COM3D code [5]. A future modification of the combustion criterion is expected to eliminate these oscillations and to allow using a second-order reconstruction and then to provide more accurate results. The AutoReaGas [7] model will be properly calibrated for H_2 and will make use of larger domain to avoid underprediction of the flame velocity. The code used by NH was and old version of FLACS [4] that, together with the assumption of non stationary initial velocities inside the balloon, lead to an inaccurate flame front propagation. However, with the newest version of FLACS, previously validated against several experiments [4], GexCon obtained results considerably improved. The adaptive meshing used by the REACFLOW [6] code is a peculiar characteristic that seems to contribute to improve the accuracy of the pressure wave propagation both in the reaction zone and beyond it into the far field region. The LES combustion model used by UU is based on the use of the progress variable equation and the gradient method to reproduce flame front propagation with proper mass burning rate. This approach helps to decouple physics and numerics of the simulated process and make simulations less grid dependent.

ACKNOWLEDGMENTS

The help of Dr. Schneider (Fh-ICT) in supplying the experimental information and its interpretation is warmly acknowledged.

The authors also like to acknowledge the collaboration of H. Wilkening (JRC) and D. Makarov (UU), in their organisation's contribution to this paper.

This work was supported by the HySafe Network of Excellence *("Safety of Hydrogen as an Energy Carrier")* of the VI Framework Research Programme of the European Commission (contract no. SES6-CT-2004-502630).

REFERENCES

1. Schneider H., Pförtner H. PNP-Sichcrheitssofortprogramm, Prozebgasfreisetzung-Explosion in der gasfabrik und auswirkungen von Druckwellen auf das Containment. Dezember 1983.
2. Becker T., Ebert F., Vergleich zwischen experiment und theorie der explosion grober, freier gaswolken. *Chem.-Ing.-Tech.,* V.57, N.1, pp.42-45, 1985.
3. CAST3M: http://www-cast3m.cea.fr/cast3m/index.jsp
4. Hansen, O.R., Renoult, J., Tieszen, S.R. and Sherman, M., Validation of FLACS-HYDROGEN CFD Consequence Model Against Large-Scale H_2 Explosion Experiments in the FLAME Facility. Paper to be presented at the *International Conference on Hydrogen Safety*, Pisa 8-10 September, 2005.
5. Kotchourko, A., Breitung, W., Numerische Simulation der turbulenten Verbrennung von vorgemischten Gasen in komplexen 3D-Geometrien. FZK-Nachrichten, Forschungszentrum Karlsruhe, 2000.
6. Wilkening H. and Huld T. An adaptive 3-D solver for modelling explosions on large industrial environment scales. *Combustion Science and Technology*, 149, pp361-387. 1999
7. Berg A.C. van den, Robertson, N.J., and Maslin, C.M. AutoReaGas, for gas explosion and blast analyses. In *Course on Explosion Prediction and Mitigation*, University of Leeds, 7-10 November, 2000.
8. FLUENT v6.1.18: http://fluent.com/software/fluent/ .
9. Sedov, L. I. Similarity and Dimensional Methods in Mechanics, Academic Press 1959.
10. Kuhl, A. L., Kamel M. M. and Oppenheim A. K. Pressure Waves Generated by Steady Flames, *Fourteenth Symposium on Combustion*, The Combustion Institute, 1973.
11. Efimenko, A.A. and Dorofeev, S.B. CREBCOM code system for description of gaseous combustion. Technical report, Russian Research Kurchatov Institute, Moscow, 1998.