Overpressure Effects from Propane Detonation: Comparison of Simulation Results with Experimental Data

Vyazmina E.[1,*], Lecocq G.[2], Commanay J.[3], Grégoire Y.[2], Jallais S.[1], Krumenacker L.[4], Mahon A.[3], Trélat S.[5], Tripathi A.[4]

[1] *Air Liquide Research and Development, Jouy en Josas, France*
[2] *INERIS, Verneuil en Halatte, France*
[3] *APSYS, Blagnac, France*
[4] *Fluidyn, Saint-Denis, France*
[5] *IRSN, Fontenay-aux-Roses, France*
**Corresponding author's email: elena.vyazmina@airliquide.com*

ABSTRACT

Accidental gas explosion is a standard scenario considered in risk assessment for process industries. Blast walls or barriers are an efficient way to reduce the effects of pressure waves originated from an explosion. However, the proper design of a blast wall requires heavy investigation considering real accidental scenarios. CFD-based method can be used for a parametric investigation and for design optimization instead of experimental investigations. Nevertheless, the first CFD codes must be validated versus corresponding experimental data. The purpose of this paper is to present comparison of CFD simulations of propane/oxygen detonation and experimental measurements for small scale explosions.

KEYWORDS: CFD, detonation, blast wave, protective walls, validation.

INTRODUCTION

Accidental gas explosion is a standard hazard usually considered in risk assessment for process industries. Pressure waves originating from an explosion can result in unacceptable risk for infrastructures and people present on and outside the site. Blast walls are an efficient way to significantly decrease the effects of the overpressure, and hence to protect people and infrastructures. However, the proper design of a blast wall requires heavy investigation, considering real accidental scenarios. The prediction of blast effects behind the blast walls requires a detailed understanding of the phenomenon, taking into account the interaction of blast waves with the barrier and with the ground. This interaction strongly depends on the wall dimensions (height, width and thickness), the angle of the inclination of the front and the back side, the distance to the blast wall, etc.

Due to the complexity of the phenomenon associated with blast wave interactions with the wall, a computational fluid dynamics (CFD)-based method may be used for a parametric investigation or for design optimization.

In France, CFD is not commonly used for the modeling of on-shore explosions at industrial sites. In most cases engineering models [1] are used for the definition of safety distances. These methods are developed for hemispherical or spherical symmetries, with explosions of constant flame speeds. They do not take into account different flow effects, obstacles, or the time history of the flame velocity. CFD can bring more accurate results, involving 3-D Navier-Stokes and combustion

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equations. However, first CFD the codes must be validated in terms of their correspondence with experimental data.

A French Workgroup led by INERIS including industrial companies, design offices, and national institutions was created to obtain a practical state-of-the-art on strengths and weaknesses of CFD tools. 10 explosion test cases were selected, each based on published experimental data.

Five partners (Air Liquide, INERIS, IRSN, Apsys, Fluidyn) joined together to perform comparison of CFD results and experimental data. The computations are compared to the experimental results for a laboratory-scale detonation of a hemispherical gaseous charge with (see Eveillard [2]) and without (see Trélat [3]) the blast walls.

SMALL-SCALE EXPERIMENT

An explosion in a hemispherical soap bubble of 6cm radius is investigated. The bubble initially contained a propane oxygen mixture in stoichiometric proportions. This mixture was at rest initially.

Ignition was initiated by an exploded wire. The nominal electrical energy associated with the discharge according to Trélat [3] was 200 J. However, it is difficult to estimate exactly how much energy was transmitted to the flammable mixture.

A trapezoidal barrier made of a wood was used in the experiments of Eveillard [2]. The barrier was 60 cm wide and 80 cm long, see Fig. 1. Pressure sensors (P1-9) were located on the centerline upstream and downstream of the barrier.

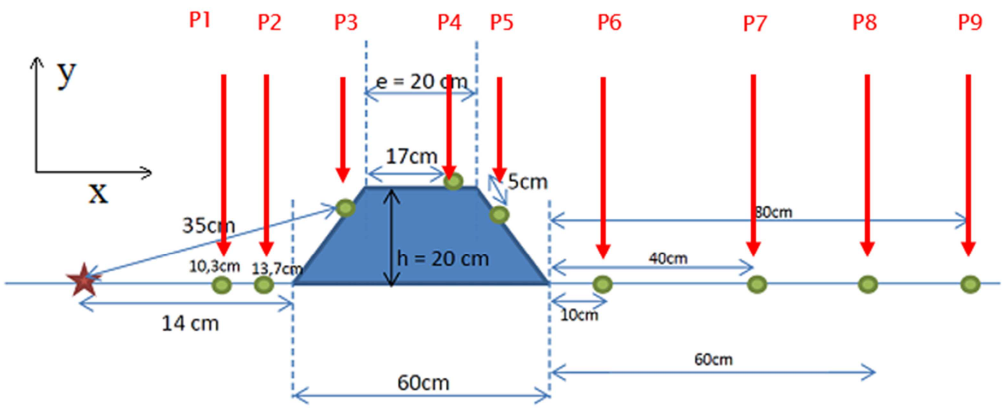

Fig. 1. Experimental set-up of Eveillard [2]. The green dots are the pressure sensors positions; the red star is the explosive charge location.

According to Eveillard [2], the experimental uncertainty was estimated to be +/- 14% in pressure. The temporal uncertainty was 5-8%. Trélat [3] performed the same experiments as Eveillard [2] but in a free field. The difference between the two experiments for the pressure at 10 cm (P1) was ~ 10%, which is in agreement with the values previously mentioned. Hence, 15% error on the experimental results is considered in the current investigation for the overpressure.

For comparison with simulations, only reliable sensors are considered: P1, P2, P4, P7 and P9.

Modeling approaches for the small scale experiments of a Rupture of a High Pressure, High Temperature Reservoir containing equivalent energies. All Participants used this modelling approach, and the 5 Bench Particpants used 5 different Codes.

MODELING APPROACHES FOR THE SMALL SCALE EXPERIMENT

Pressure waves from an explosive charge could be modelled by the ones originating from a rupture of a high pressure- high temperature reservoir containing the equivalent energy. All participants of the bench used this modeling approach.

For modeling, 5 bench participants used 5 different CFD codes.

Description of CFD codes and corresponding mesh

Air Liquide (AL) used a commercial CFD code FLACS V10.6 [5]. FLACS solves the compressible Navier-Stokes equations on a Cartesian grid. Simulations are fully 3D, with the k-ϵ model used for turbulence representation. FLACS [5] recommendations for a time step are applied in this investigation for the CFL number: CFLC = 0.1, CFLV = 0.1 and the option “keep low” is also applied. This option prevents the initial step from growing in a far-away distance to reduce diffusivity in the far field. AL models a computational domain of 1.2 m in downstream and cross-stream directions [-0.6m; 0.6m] and 0.6 m in the vertical direction. Two meshes made of 1cm and 0.5cm wide cells are used, which corresponds to ~0.5M and ~1.5M cells. For simulations with a protective wall AL uses a longer domain of 2.3 m downstream [-0.6m; 1.6m], 2.4m in the cross-stream [-1.2m, 1.2m] and 0.6 m in the vertical directions. For this case AL used 3 meshes with cells width of 1cm, 0.5cm and 0.25cm, which corresponds to ~2.5M, ~15.2M and 18.2M cells correspondingly. In this case all meshes are kept uniform in the region of interest (the region covering the explosive charge, barrier and pressure detectors), and they are stretched in the less sensitive regions (in particularly in the cross direction far from the barrier). Results only for the finest meshes are discussed in the paper.

APSYS used OpenFOAM (Open source Field Operation And Manipulation) [6], which is a C++ toolbox of customized numerical solvers and pre/post processing utilities for the solution of continuum mechanics problem, including CFD. It includes a varied range of solvers that are available for computation, either within structured / unstructured mesh, of simulation cases using the finite volume method. In the current simulations, “RhoCentralFoam” solver (solves the Euler equations with the central Kurganov and Tadmor scheme [9] for the convection operator. A 3D domain (size 1.95 m x 0.6 m x 0.6 m) that contains around 1.8 billion elements is used. Mesh is refined along obstacles and in the near field of the explosion center, with cell size between 7.5 mm and 3.75 mm. Explosion was modelled by the pressure release of a compressed hot air hemisphere. Hemisphere radius has been chosen to be close to the one used in experiment (6cm) and hemisphere Chapman-Jouguet Temperature was estimated to be T_{CJ} = 3815 K. Knowing the energy contained in the hemisphere (around 4100 J), the Brode equation was used to determine initial hemisphere pressure.

FLUIDYN used a commercial code that they developed, fluidyn-VENTEX. VENTEX solves the compressible Navier-Stokes equations on structured or unstructured mesh. Several turbulence models are available; the k-ϵ model was used in the simulations presented here for turbulence representation. Among the possible numerical schemes, the Euler scheme was used for time resolution and the UDS scheme was used for convection resolution. The domain of simulation is a 2D-axisymetrical domain, with the vertical axis through the center of the explosive volume as symmetry axis. The domain size is 2 x 0.5m and the mesh was comprised of 363000 elements, with a cell size between 1 and 2 mm. A preliminary simulation was done for a similar experience, without the presence of the wall. The Chapman-Jouguet pressures and temperature were estimated to be T_{CJ} = 3815 K and P_{CJ} = 34.1 bar g. The explosion was modelled by the pressure release of a hemisphere containing compressed air, with a radius of 6 cm and with internal pressure and temperature those of Chapman-Jouguet. Hence, the energy inside the hemisphere is equal to 3900 J. The equation of state is that for a perfect gas. The choice had been made to take the volume of the equivalent hemisphere equal to the volume of the bubble to represent the case the same way Fluidyn should have done it with a more geometrically complex scenario.

INERIS used the OpenFoam 3.0.0 code [6] for this calculation. It has been decided to use the rhoCentralFoam solver i.e. to solve the Euler equations with the central Kurganov and Tadmor scheme [9] for the convection operator. A 2D axisymmetric domain (centered on the explosive charge) of 2m by 1 was used, decomposed with a 4 million cell mesh (Δx = 0.7 mm). At such a scale both the wall and the charge can be explicitly resolved on the mesh with a satisfying accuracy. was chosen to rely on the Stanyukovich model [10] of an instantaneous detonation in the soap bubble. The detonation wave in propane travels at about 2360 m/s [11], which implies a delay of 0.02 ms in the considered bubble. It corresponds to about one-tenth of the duration of the wave recorded on the first sensor, so we say it is still acceptable for our calculation. A theoretical approach based on a Riemann problem of a 1D detonation wave propagating in a tube, leads to relatively simple pressure temperature and velocity profiles in the bubble that can be found in almost any detonation course. Averaging those profiles over the distance on Cartesian coordinates, between the center of the detonated bubble and its shell leads to $P = P_{CJ}/2$, $T \approx 0.9T_{CJ}$ and $u \approx u_{CJ}/4$ (the CJ subscript standing for the Chapman Jouguet state). For our calculations, we chose to keep in the bubble $P = P_{CJ}/2$ (P_{CJ} = 35 bar according to [11]. For the temperature, it is considered that thermal equilibrium does not have the time to be attained, and the maximum temperature $T = T_{CJ}$ is kept. Representing the speed is more difficult in terms of programming the initial conditions, because of the variable direction of the velocity vector, so we left it at 0. At last, due to the small size of the load, compared to the calculation volume, it was decided not to model the gases differently in the bubble, with respect to the atmosphere outside the bubble. Several approximations are made, but the calculations only rely on limited data for the firing configuration, (bubble size, position and dimensions of the merlon), These remain the same in the model, and the information published in the scientific literature (in the present case the measurements of pressure and detonation temperature CJ of the propane oxygen mixture, that are completely independent of the test modelled). Thus, this method is not based on any adjustment to the analyzed test, and aims to provide a generalizable and predictive result, rather than the best possible agreement with the experimental data.

IRSN used a commercial software LS-DYNA that solves the compressible Euler equations. A very short time step of 0.2 μs is used. For the free field geometry IRSN uses for the size of the computational domain 1.5 m horizontal direction [0 m; 1.5 m] and 0.8 m in the vertical direction [0m, 0.8 m]. The grid is stretched from 1 up to 5 mm corresponding to ~120 000 cells. For the geometry with a protection barrier IRSN uses the same size of the computation domain and the same mesh, corresponding to ~450 000 cells. Finer cells are used close to the barrier to properly model the reflection of pressure waves in this area.

All the participants model the generation of the shock wave from the gaseous detonation by an equivalent burst. In AL and IRSN calculations, the radius R of this high-pressure and high-temperature equivalent hemispherical vessel is calculated as follows:

$$\frac{2}{3}\pi R^3 \frac{\Delta P}{\gamma - 1} = E,$$

where ΔP is the overpressure inside the vessel, E is the energy released by the burst. Burst parameters used by bench participants are given in Table 1.

All bench participants use the same gas (air) at the same temperature. All modelers have chosen, except INERIS, a pressure about 35 barg (Chapman-Jouguet pressure) in the burst bubble. The choice of the radius value varies according to the modelers between 5.05 cm and 6 cm. Note, however, that the energy theoretically deposited varies by a factor of two between INERIS/IRSN modeling choices and AL/APSYS/Fluidyn ones.

Table 2 gives description of physical and numerical approaches used by bench participants.

Table 1. Description of the equivalent source used by bench participants

	AL	APSYS	Fluidyn	INERIS	IRSN
Eq. source	Hemisphere, R=5.05cm	Hemisphere, R=6cm	Hemisphere, R=6cm	Hemisphere, R=6cm	Hemisphere, R=5.05cm
T	3843 K	3815 K	3815 K	3830 K	3843 K
P	35.1 barg	36.3 barg	34.1 barg	17.5 barg	35.1 barg
Gas	air	air	air	air	air
γ	1.213	1.4	1.4	1.4	1.4
ρ	3.26kg/m^3	3.3 kg/m^3	3.18 kg/m^3	1.65 kg/m^3	3.18 kg/m^3
E	4.4kJ	4.1 kJ	3.9 kJ	1.9 kJ	2.4 kJ

Table 2. Modeling approaches used by bench participants

	AL	APSYS	Fluidyn	INERIS	IRSN
Transport equations	Navier-Stokes	Euler	Navier-Stokes	Euler	Euler
Domain topology	3D	3D	2D-axi	2D-axi	2D-axi
Grid size in zone of inter.	2.5 mm	3.75 – 7.5 mm	1 – 2 mm	0.7 mm	1 - 5 mm
Numerical schemes	Time: Euler Conv.: weighted centered 2nd order/Upwind	Time: Euler Conv.: Tadmor /Kurganov	Time: Euler Conv.: UDS	Time: Euler Conv.: Tadmor/ Kurganov	Time: Euler Conv.: CE-SE

AL and APSYS chosen 3D approach, which could allow them to model lateral overturning waves, which is not possible to obtain by a 2D approach.

SIMULATION RESULTS FOR SMALL SCALE EXPERIMENT

For the detailed comparison of simulation results with experimental data, the following parameters can be used: maximum accidental overpressure; travel time of the pressure wave between sensors (more objective than the arrival time of the shock wave, since current approaches do not model the explosion combustion); pressure rise:

$$\frac{dP}{dt} = \frac{P_{max} - P_0}{t_{pmax} - t_{p0}}.$$

The thickness of a shock wave in air is of the order of the mean free path, i.e. about 100 nm. With a pressure wave ranging from 5 bar to a few tens of mbar, impact velocities of 800 to 350 m/s are considered, i.e. a pressure rise time of 100 to 300 picoseconds. The reason for focusing on the pressure rise rate of the experimental, or simulated signal, is purely qualitative. As we are in the presence of a detonation in the soap bubble, a shock wave steep profile is expected outside. However, the time resolution of real sensors as well as simulated ones is being insufficient to capture the rate of rise in pressure. Consequently, we compare the *dP/dt* of the digital signals to know if we are approaching the shape of a shock or not. It is a qualitative estimate, to assess to which extent, the physical phenomenon is reproduced or not.

Free field geometry [3]

Free field geometry (Trélat [3]) was modeled only by 3 participants of the bench: AL, IRSN and Fluidyn. The corresponding source terms described in Table 1 are used.

Figure 2 shows the pressure signals at various distances from the center of the charge: 10 cm, 20 cm and 30 cm. Results of AL with FLACS and IRSN with LS-DYNA/CESE match well with experimental data for the maximum overpressure and for the corresponding impulse. AL pressure signal in slightly more diffusive compare to IRSN results due to two main differences. AL uses Navier-Stokes, whereas IRSN uses non-viscous equations (Euler equations), which are less diffusive. AL used mesh of 5 mm wide cells, whereas IRSN cells width is 1 mm. AL simulations with a finer mesh comparable to the one from IRSN should show less diffusion. However, in both simulations (from AL and from IRSN) the error on the maximum overpressure for each monitoring point is less than the experimental error (15%). Fluidyn overestimates the overpressure at 10 cm and 20 cm by 26% and 14% correspondingly and predicted a pressure at 30 cm lower than the experimental error.

Geometry with a protection barrier [2]

Figure 3 shows comparisons of predicted and measured of pressure signals at monitoring points P1 and P2 upstream to the barrier.

This comparison demonstrates that APSYS and Fluidyn overestimate the overpressure at both positions by 17.6, 26.6, 18.9, and 19.3 % respectively. AL slightly underestimates the overpressure at P1 by 15.2% and slightly underestimates at P2 by 17.7%. In the case of the monitor position P2 (located on the ground, 13.7 cm from the center of the explosive charge), the pressure signal has a two peak-shape. The first peak corresponds to the incident peak (from detonation), whereas the second one is the pressure reflection from the barrier. AL uses the coarsest grid compare to other bench participants, which does not allow for a correct separation of these peaks. The finest AL grid is of 0.25 cm, where the distance from monitor point to the barrier is only 0.3 cm. APSYS uses a coarse grid too, which also interferes a correct separation of two pressure peaks. For the correct resolution of this double-peak structure, the simulation grid should be at least twice smaller than the distance between the monitor point and the barrier.

INERIS computation underestimates the overpressure at P1 and P2 by ~25% and 20%, simulations show that the reflected pressure peak at P2 is higher than the accidental one.

IRSN results are in the best agreement with experimental data at both positions P1 and P2.

Figure 4 shows pressure signals at monitoring points P4 and P5 located on the barrier. INERIS computation underestimates the overpressure at P4 and P5 by ~19% and 14% (experimental error is 15%). APSYS overestimates the overpressure at P5 by 17%, all other results are within the experimental error.

Figure 5 demonstrates pressure signals at monitoring points P7 and P9 located behind the barrier. INERIS computation underestimates the overpressure at P7 and P9 by ~28% and 13% (experimental error is 15%). Results from all other bench participants are within the experimental error.

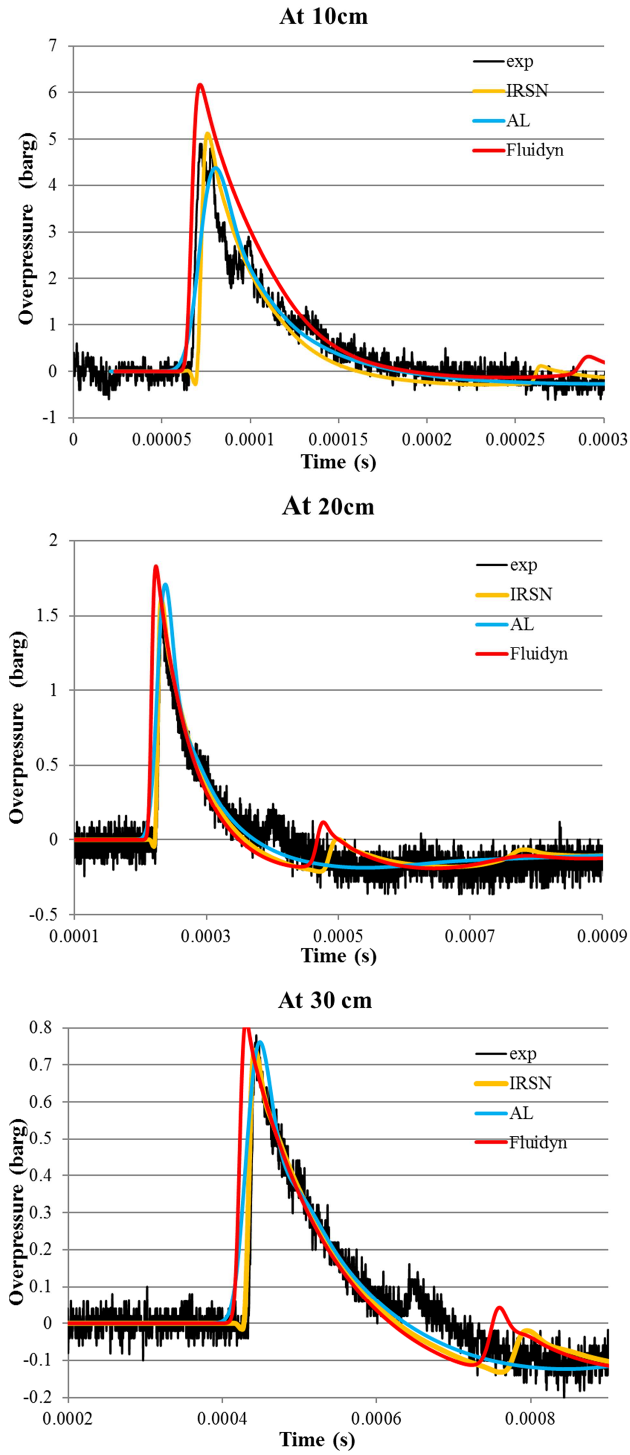

Fig. 2. Simulation results for pressure wave propagation in a free field geometry, exp – data from Trélat [3].

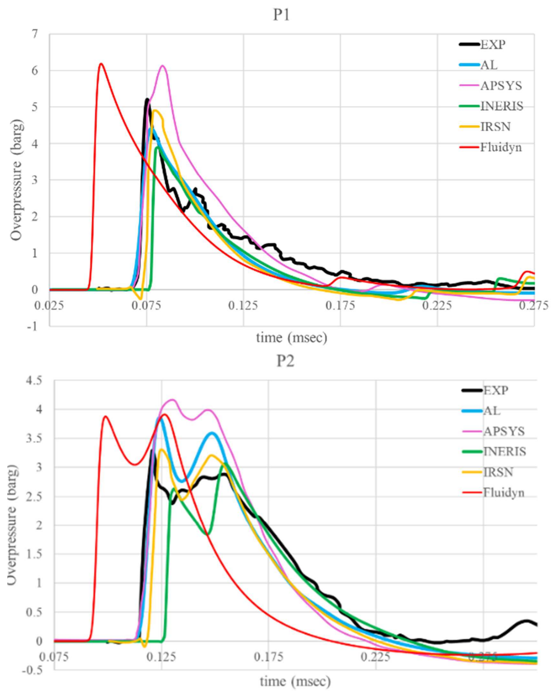

Fig. 3. Simulation results for pressure wave propagation in the presence of the barrier (exp – data from Eveillard [2]): pressure sensors located upstream of the barrier.

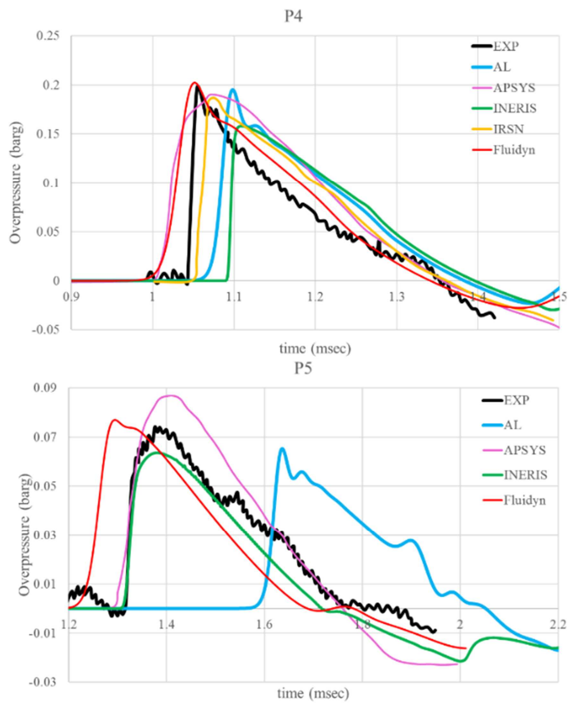

Fig. 4. Simulation results for pressure wave propagation in the presence of the barrier (exp – data from Eveillard [2]): pressure sensors located on the barrier.

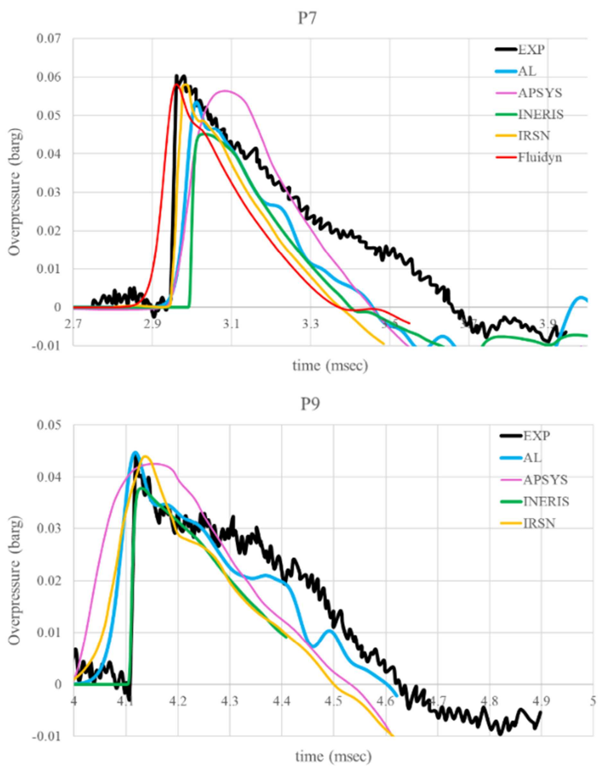

Fig. 5. Simulation results for pressure wave propagation in the presence of the barrier (experimental data by Eveillard [2]): pressure sensors behind the barrier.

Table 3. Simulation results for the maximum overpressures

		P1	P2	P4	P5	P7	P9
Exp. P (barg)		5.21	3.28	0.2	0.074	0.055	0.044
AL	Sim P(barg)	4.42	3.86	0.2	0.065	0.056	0.045
	Error, %	-15.2	17.7	within exp. error	within exp. error	within exp. error	within exp. error
APSYS	Sim P(barg)	6.13	4.15	0.19	0.087	0.056	0.042
	Error, %	17.6	26.7	within exp. error	17.2	within exp. error	within exp. error
INERIS	Sim P(barg)	3.9	2.6	0.16	0.063	0.045	0.038
	Error, %	-25.2	-20	-19.2	within exp. error	-18	within exp. error
IRSN	Sim P(barg)	4.9	3.3	0.19	Not calculated	0.058	0.044
	Error, %	within exp. error	within exp. error	within exp. error		within exp. error	within exp. error
Fluidyn	Sim P(barg)	6.2	3.9	0.2	0.077	0.058	Not calculated
	Error, %	18.9	19.3	within exp. error	within exp. error	within exp. error	

Table 3 shows the comparison of simulations results with experimental measurements in terms of maximum overpressure at each pressure sensor. According to this table, results of IRSN are in the best agreement with experimental data: the error between simulations and measurements is within the experimental error for all pressure detectors. Fluydin & APSYS overestimate the overpressure at the closest pressure sensors P1 & P2 (upstream of the barrier). AL underestimates the overpressure at P1 and overestimates at P2, whereas pressure at other pressure sensors is within the experimental error. INERIS underestimates the overpressure at sensors P1, P2, P4 and P7 by 20-25%. This underestimation is due to the difference in the burst energy: energy used by INERIS is ~20% less than the energy used by IRSN. All bench participants demonstrate a better match with the experimental data behind the barrier.

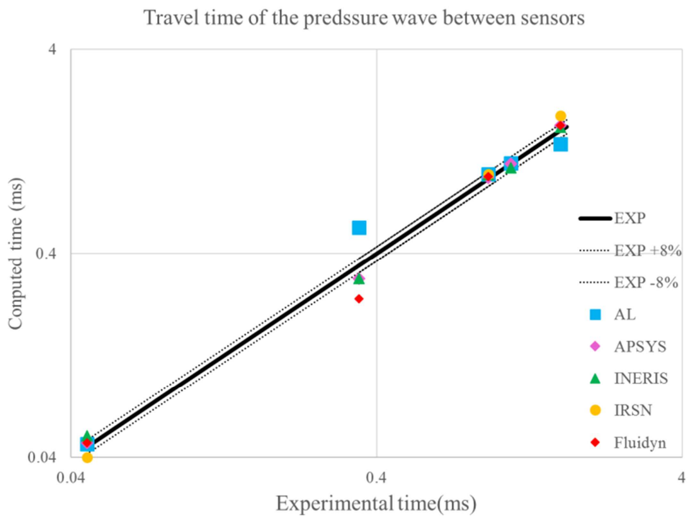

Fig. 6. Scatter plot of comparison simulates with experimental data by Eveillard [2]: travel time.

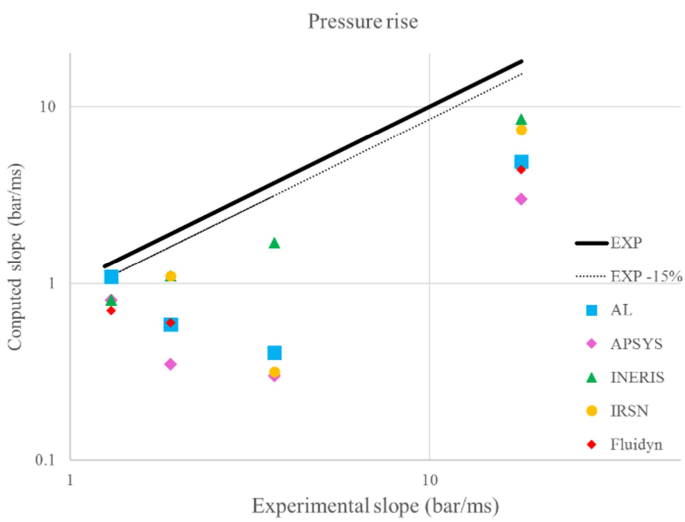

Fig. 7. Scatter plot of comparison simulations with experimental data by Eveillard [2]: pressure rise.

The speed of the shock is directly related to the amplitude of the pressure peak through the following law

$$V_{onde} = c\sqrt{\frac{\gamma+1}{2\gamma}\frac{P_1}{P_0}+\frac{\gamma-1}{2\gamma}}.$$

Hence, the travel time of the pressure wave between sensors is also a very important parameter. In general all bench participants correctly estimate travel time, see Fig. 6.

Figure 7 illustrates the comparison of simulation results with experimental data for pressure rise behind the barrier. Underestimation of the preesure rise can be attributed to numerical (mesh) and physical (Navier-Stokes equations) diffusion. The best results for the pressure rise are obtained by INERIS who uses Euler equation and the finest grid compare to other bench participants. IRSN results are slightly more diffusive due to a coarser grid. APSYS uses the coarsest grid, which increases the numerical diffusion and leads to the lowest pressure rise compare to other bench participants. Actually, this numerical diffusion is more important than the physical diffusion specified by the approach of Navier-Stokes equations used by AL and Fluidyn. Behind the barrier AL and Fluidyn use similar meshes (2.5 mm for AL and 2 mm for Fluidyn), that is why the pressure rise is almost the same.

CONCLUSION

Based on the current investigation several conclusions can be made:

- The methods based on 2D-axisymmetric approaches demonstrates a better conservation of the shock compared to the meshes 3D due to a finer mesh.
- The accuracy obtained by the 2D and 3D approaches for the overpressure magnitude, and wave arrival times are very similar. Nevertheless, the best results are obtained by a 2D mesh (IRSN simulations).
- Accurate modeling of the burst is essential for correct prediction of the far-field overpressure effects related to a charge explosion. INERIS suggested a universal model, which was previously tested for other configurations and gases. Additional bench participant will test this approche in the future.
- The underestimation of the overpressure peaks is related either to the source term or to the numerical diffusion. Hence, for the risk assessment it is better to use validated term source
- The results obtained for the peak of overpressure are quite satisfactory (max error and 26%) compared to the experimental measurement error (15%).
- The good agreement in terms of the travel time is found for AL, APSYS and IRSN calculations (the relative difference of simulation and lower than the measurement error).
- A fine mesh for pressure should be preferred to simulate the wave propagation: the effect of numerical diffusion due a coarse mesh can exceed the effect of physical diffusion. However, the numerical diffusion can also be due to the precision of the numerical scheme, corrective flux, artificial viscosity (for example, used in the k-epsilon model), Gibbs error etc.
- Euler equations (APSYS, INERIS and IRSN) give better conservation of the shock even for a coarse mesh. The Navier-Stokes approach requires a much finer mesh to keep the shock. In this case, it is also possible to assume the turbulent viscosity to be 0 with an ad

hoc initiation of the characteristic sizes of the turbulence. Results will be less diffusive and this approach will help to conserve the shock.

- A qualitatively correct shape of the overpressure signal at the sensor close to the barrier (including the maximum overpressure, the impulse and the nature of the peak, incident or reflected) can be predicted if at least 1 cell is set between the sensor and the barrier. 3 cells is an ideal choice.

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