HYDROGEN COMBUSTION BENCHMARK USING EXPERIMENT IN DOUBLE-COMPARTMENT EXPERIMENTAL VESSEL

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ABSTRACT

The accident at the Fukushima Daiichi nuclear power plant (NPP) in Japan has put again the spotlight on the issue of hydrogen explosion and its consequences.
About that, so called lumped-parameter (LP) codes remain, for the time being, the customary tool for simulating hydrogen combustion in actual NPPs. Namely, the volumes of actual containments are much too large for performing calculations with CFD codes. Thus, estimations of hydrogen combustion consequences still rely on LP codes, which use relatively simple models of combustion.
Although hydrogen combustion in single compartments has already been simulated quite often, there were not many opportunities so far to simulate flame propagation between compartments. With this purpose, a benchmark exercise was organized, based on a laboratory-scale hydrogen combustion experiment, performed in a parallelepiped shape double-compartment vessel of 1.48 m^3 total volume at the University of Pisa (Italy). In the experiment, many hydrogen combustion tests were performed by varying the initial hydrogen concentration and the area of the orifice in the wall separating the two compartments.
Three different tests were simulated and the main results, which consist of time dependent pressure and temperature, are presented, compared between them and to experimental results (for the pressure increase). This work is focused on the assessment of flame propagation models of the codes, with the aim of identifying their limitations as regards to that complex phenomenon.

KEYWORDS
Hydrogen, combustion, experiments, simulation, lumped-parameter codes.

1. INTRODUCTION

The Fukushima accident (Japan, March 2011) had highlighted the consequences of hydrogen explosions on the plant buildings, as well as the significant capability of spreading radioactive pollutants to the outdoor environment [1].

During a severe accident in a light water reactor nuclear power plant (NPP), hydrogen could be first generated during degradation of the reactor core as a by-product of Zircaloy oxidation, and eventually later due to interaction between the molten core and the concrete (supposing that the core melts, the reactor pressure vessel fails and the core melt spills into the containment. If local hydrogen concentration is within the flammability limits, hydrogen combustion could occur, causing mechanical and thermal loads that could eventually cause containment failure, thus allowing the release of fission products into the environment [2]. Although the hydrogen explosions observed in Fukushima did not occur in the plant containments, they reminded of the real possibility of generation of sufficiently large quantities of it during severe accidents.

Indeed, the phenomenon of hydrogen explosion (fast deflagration) is modeled in severe accident codes through simplifying assumptions that can be managed with the lumped-parameter approach typically used for the thermal-hydraulics of severe accident computer codes [3]. Therefore, hydrogen deflagration in a containment should be adequately simulated although hydrogen deflagration models implemented in lumped-parameter codes do not reflect all the complexity of the combustion process.
Besides, the containments of actual NPPs are too much large to be simulated in case of accident using so-called Computational Fluid Dynamics (CFD) codes in a relatively short time.

A really more complex phenomenon is the flame propagation, mainly in case of an explosion, through obstacles and holes. The physical reason of that behavior is due to the complexity of flame thermo-fluid-dynamics, mainly when it is flowing through obstacles, which to be simulated need an effective modeling of physical and chemical characteristics of flame and of gas mixtures close to it [4].

In those cases lumped-parameter codes are really close (or beyond) their limits and the use of CFD codes, because of their intrinsic ability to better model the particulars of scenario, is very interesting.
So, it is expected, that performing simulations with the former numerical codes of experiments with explosion flame propagation is an effective way to assess the possibilities and limits of those codes and their improving needs.

The benchmark exercise to do that was organized by RSE (Ricerca sul Sistema Energetico), with the purpose to compare simulation results of hydrogen explosion flame propagation experiments, obtained with different lumped-parameter codes. The following organizations took part in the benchmark: Jozef Stefan Institute (JSI - Slovenia), Nuclear Regulatory Authority of the Slovak Republic (UJD SR - Slovakia), Lithuanian Energy Institute (LEI - Lithuania), Ricerca sul Sistema Energetico (RSE - Italy).

In the present paper, the results obtained with different codes (pressure, flame propagation) are compared to the experimental results, with the main purpose of assessing the general possibilities and limits of lumped-parameter modeling (open benchmark).

2. EXPERIMENTS

The experimental activity related to the benchmark was carried out at the University of Pisa by using the LargeView2 facility (the latest apparatus of the VIEW series) which was designed and built to study deflagrations of hydrogen and methane with air, and in particular, to understand flame behavior in a vented multi-compartment container during explosions (deflagrations) [5]. The vessel (Fig. 1) is a square parallelepiped made up of rectangular panels fastened to a steel framework (total inner volume of 1.48 m^3, inner dimensions of 0.68 x 0.68 x 3.2 m). One side and the upper panels are made of high-strength stratified glass (40 mm thick); the other panels are made of enhanced carbon steel. The ends are closed by two steel plates and the right-hand end has a large opening to allow safety venting during deflagration (it is closed with a plastic bag, open area approximately of 0.166 m^2).

As for the benchmark configuration, the vessel was divided into two parts by a steel diaphragm, with an orifice (always open) in the center that allows the flame to pass from the left-hand chamber (1 - where combustion ignition takes place) to the right-hand one (2). The ignition was constituted of an electrical spark placed close to the bottom of left chamber at the opposite side from the one with the diaphragm. In the benchmark configuration, the orifice diameter values were 50, 70, 100 mm and the diaphragm was placed 1.066 m far from the left-hand end, therefore the volume of the second chamber was twice the volume of the first chamber.

The apparatus was designed to withstand a maximum internal overpressure of about 300 kPa.
The concentrations of hydrogen were 10%, 10.5%, 11% in normal air and initial conditions of 293.15 K and 101325 Pa.

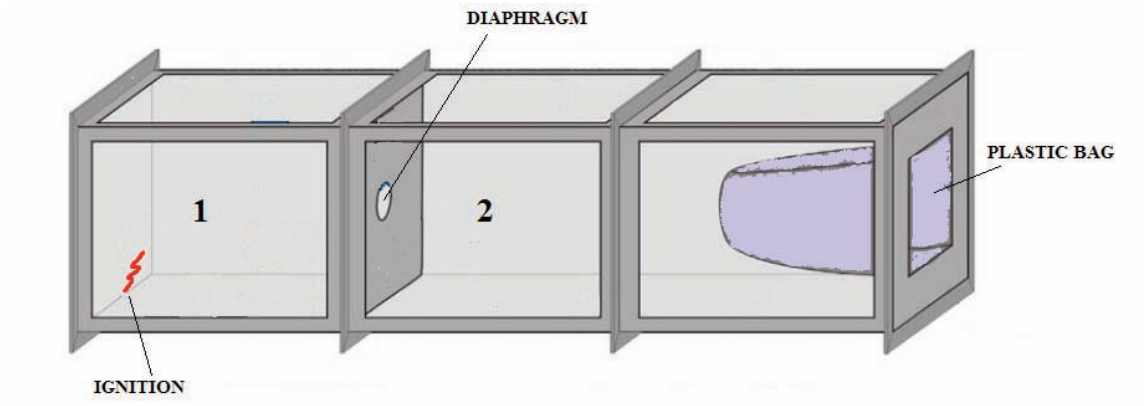

Figure 1. LargeView2 apparatus vessel.

The tests carried out and utilized in this benchmark are:

- Test 90: C_{H2}= 11% (vol.), ignition time t_{ign}= 0.2 s, orifice diameter= 100 mm;
- Test 47: C_{H2}= 10.5% (vol.), ignition time t_{ign}= 0.2 s, orifice diameter= 70 mm;
- Test 06: C_{H2}= 10% (vol.), ignition time t_{ign}= 0.2 s, orifice diameter= 50 mm.

(Ignition time: time when electrical spark strikes).
The tests we considered have different features (C_{H2}, orifice diameter) because of results of every performed test have not yet been published and, among those present in references, it was not possible referring to some with only a feature varied [5] (because of same reason, other issues and limitations have been encountered about uncertainties of performed measurements).

The deflagration transients obtained in these tests were of three typologies, with three different pressure transients:

- Transients in which the ignition jet occurs as soon as the flame has reached the orifice and the hot gases flow into the second room (Test 90, pressure transient is shown in Fig. 2).
- Transients in which the ignition jet takes place a certain time after the flame has reached the orifice (delayed jet, Test 47, pressure transient is shown in Fig. 3).
- Transients in which jet ignition does not occur (Test 06, pressure transient is shown in Fig. 4).

(The rupture of the plastic bag happened approximately as follow: test 90 (0.43 s), test 47 (0.53 s), test 06 (0.83 s)).
As highlighted before, the physical reason for these different behaviors is due to the complex phenomenon of the jet ignition, which is related to physical and chemical characteristics of the flame (concentration of free radicals) and to thermo-fluid-dynamics of gas mixtures flowing through the orifice

(mainly speed and temperature of gases) [4]. In our cases the main reason for the delay of propagation (test 47) and then of his absence (test 06) should be the size of the orifice that was gradually reduced.

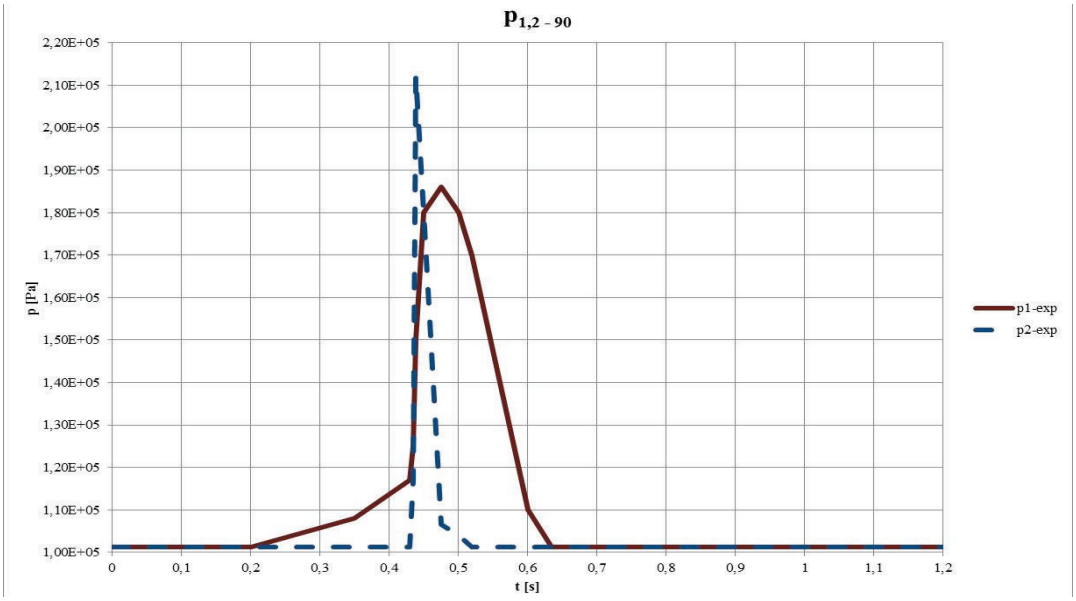

Figure 2. Pressure transient of test 90.

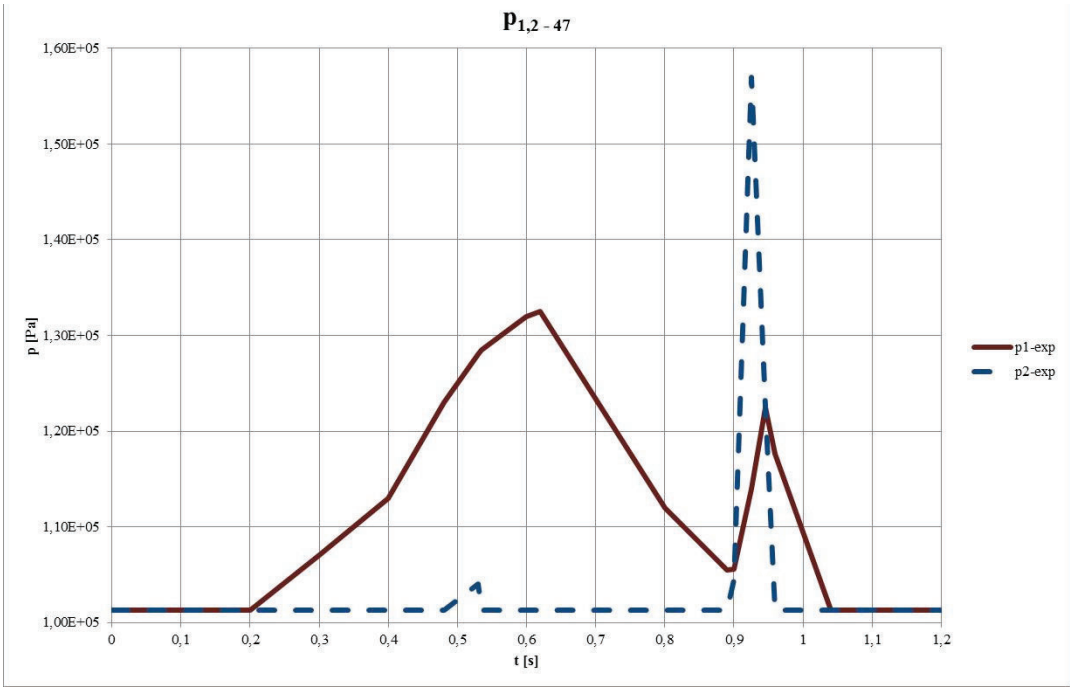

Figure 3. Pressure transient of test 47.

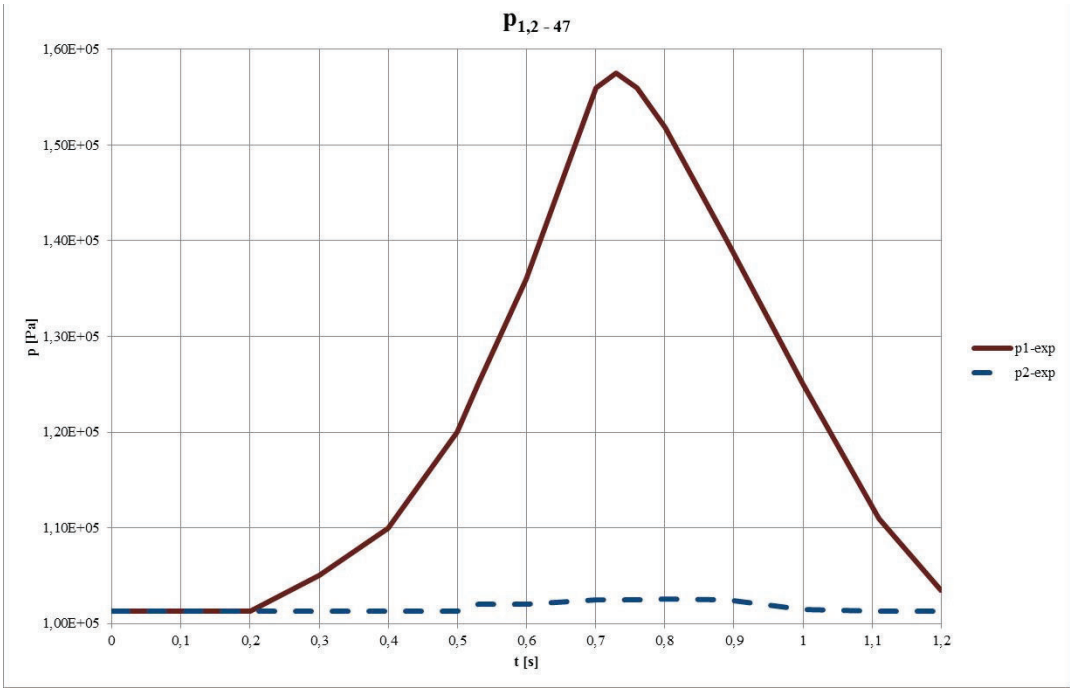

Figure 4. Pressure transient of test 06.

3. PARTICIPANTS AND LUMPED-PARAMETER CODES

The participants of this benchmark were: Jozef Stefan Institute (JSI - Slovenia) using ASTEC code, Nuclear Regulatory Authority of the Slovak Republic (UJD SR - Slovakia) using COCOSYS code, Lithuanian Energy Institute (LEI - Lithuania) using ASTEC code, Ricerca sul Sistema Energetico (RSE - Italy) using ECART code.

Here a brief description of the combustion modelling in each code is provided. Detailed descriptions may be found in the code documentations.

The ASTEC code [6] is being jointly developed by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN – France) and the Gesellschaft für Anlagen und Reaktorsicherheit (GRS – Germany). The ASTEC code has two different models to simulate hydrogen deflagration: the FRONT model and the PROCO model. The same FRONT model is available also in the COCOSYS code developed by GRS [7]. There are other combustion models in the COCOSYS code, which have not been used and/or tested within the benchmark.
The FRONT model calculates the flame propagation from one control volume into adjacent ones. The flame propagation takes place within the junction of the system (flow connections between the volumes). The combustion of the gas mixture takes place in the volumes and is calculated by a combustion model. In addition to the simplified combustion model, a checking is performed, whether the gas mixture in a volume is ignitable or not (that is, whether ignition criteria are fulfilled according to the well-known ternary Shapiro diagram). The boundary conditions for possible flame propagations and its directions are checked as well based on the ternary diagram. In case the ignition is possible, it occurs instantaneously or by user controlled boundary conditions – by time or hydrogen concentration. After the combustion completeness criteria are reached, the combustion stops. Burning velocity is calculated according to the Liu-MacFarlane correlation [8]. Turbulent flame front velocity is calculated via the Peters correlation [9].

The flame propagates through junctions. At the end of each junction, it is checked whether the conditions in the target zone are prone to ignition.
In the PROCO model, the conditions for combustion are evaluated in a similar way. However, the essential difference is that combustion is sequential, which means that a mixture in a volume starts to burn when combustion in the former volume is completely finished.

The ECART computer code [10] was originally created to calculate the concentration of airborne radiotoxic substances inside nuclear power plants in the case of a severe accident. The code is developed by a pool of Italian research institutions. The ECART H_2Ex model is dedicated to air–hydrogen mixture fast deflagrations and is internally divided into two sub-models relating, respectively, to the outdoor (open spaces) and indoor (confined spaces) explosions. Both sub-models consist of a set of correlations that provide the values of temperature and pressure required for calculating a first approximation of the explosion effects, in order to allow a realistic analysis of the overall accident scenario, either nuclear or conventional. In particular, the indoor explosion sub-model calculates pressure and temperature as a function of time by means of the interaction between thermal – hydraulics and chemical modules.

4. INPUT MODELS AND SIMULATIONS

About inputs of the simulations carried out, the main items were as follows.

ASTEC code (ASTEC-IK, JSI)
Nodalization: chamber 1 simulated by 1 control volume; chamber 2 simulated by 1 control volume; outdoor environment.
Test 90: the simulation used the FRONT combustion model.
Test 47: the simulation used the PROCO combustion model.
Test 06: no simulation.
Rupture junction to the environment (representing "bag" failure) simulated by overpressure.

COCOSYS code (COCOSYS, UJD)
Nodalization: chamber 1 simulated by 2 control volume (a small one from the left side with the length of 0.1 m and a big one in the remaining part); chamber 2 simulated by 2 control volumes (a small one from the left side with the length of 0.1m and a big one in the remaining part); outdoor environment.
Rupture junction to the environment (representing "bag" failure) simulated by overpressure.
Test 90: the simulation used the FRONT combustion model.
Test 47: no simulation results (FRONT combustion model unsuccessful).
Test 06: the simulation used the FRONT combustion model.

ASTEC code (ASTEC-MP, LEI)
Nodalization: chamber 1 simulated by 9 control volume (equal); chamber 2 simulated by 2 control volume (equal); outdoor environment.
Rupture junction to the environment (representing "bag" failure) simulated by overpressure.
Test 90: the simulation used the FRONT combustion model.
Test 47: the simulation used the FRONT combustion model.
Test 06: the simulation used the FRONT combustion model.

ECART code (ECART, RSE)
Nodalization: chamber 1 simulated by 1 control volume; chamber 2 simulated by 1 control volume.
Explosion in chamber 2 happens or not by user choice (Yes, it happen; Not, it not happen) and, about the time of explosion, the values were (imposed by user choice): test 90: t_{ex2}= 0.513 s; test 47: no Ex; test 06: no Ex.
Plastic bag rupture time as input data: test 90: 0.43 s; test 47: 0.53 s; test 06: 0.83 s.

(The simulations were stopped at bag rupture times).

Moreover, although the experimental results were already known at the time of inputs preparation, the considerable remaining uncertainties have caused that it was considered more convenient not to do any kind of tuning of such inputs, with the aim to better understand what approach would allow to achieve results more realistic about the propagation of combustion.

5. RESULTS AND DISCUSSION

Main results (pressure of chamber 1 – p_1; pressure of chamber 2 – p_2) are summarized in the figures following (Fig.5, 6, 7).

(exp: experimental values,
ASTEC-IK: I. Kljenak - Jozef Stefan Institute, Slovenia,
COCOSYS: L. Kubišova - Nuclear Regulatory Authority of the Slovak Republic, Slovakia,
ASTEC-MP: M. Povilaitis - Lithuanian Energy Institute, Lithuania,
ECART: G. Manzini - Ricerca sul Sistema Energetico, Italy).

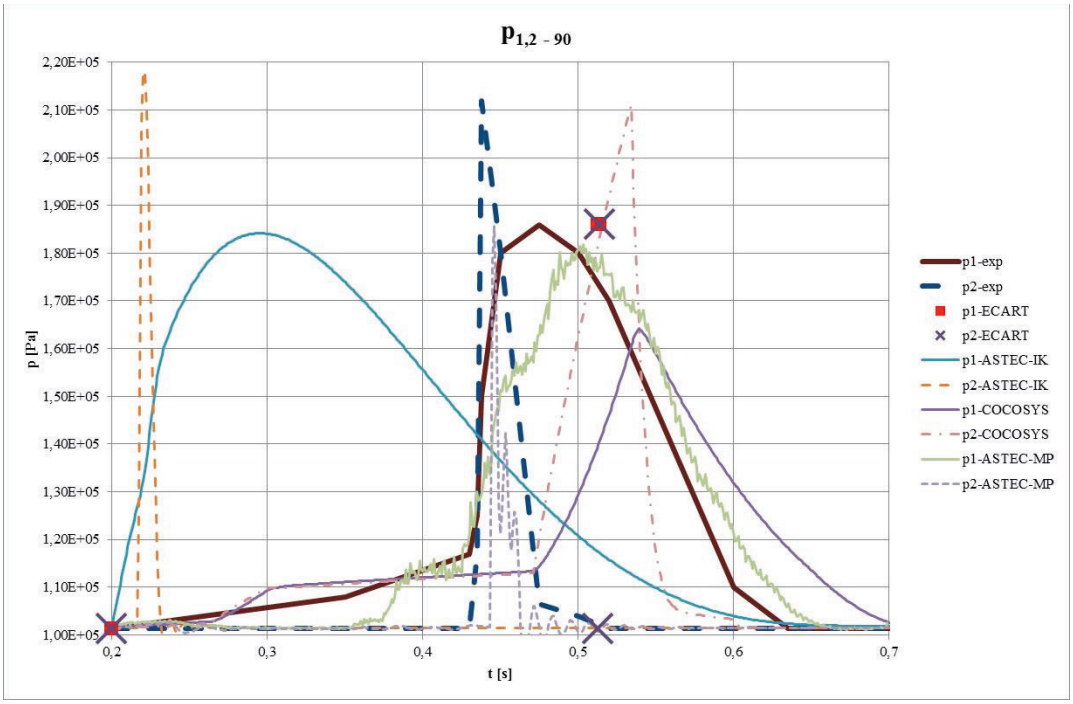

Figure 5. Pressure transients (test 90: exp. and simulations results).

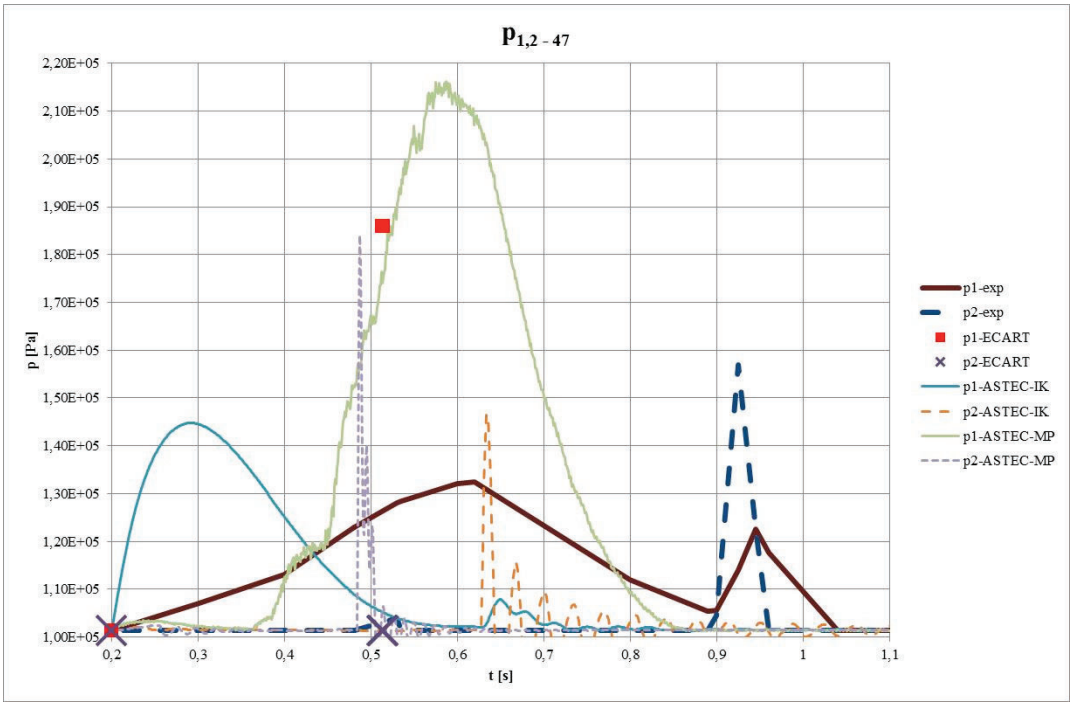

Figure 6. Pressure transients (test 47: exp. and simulations results).

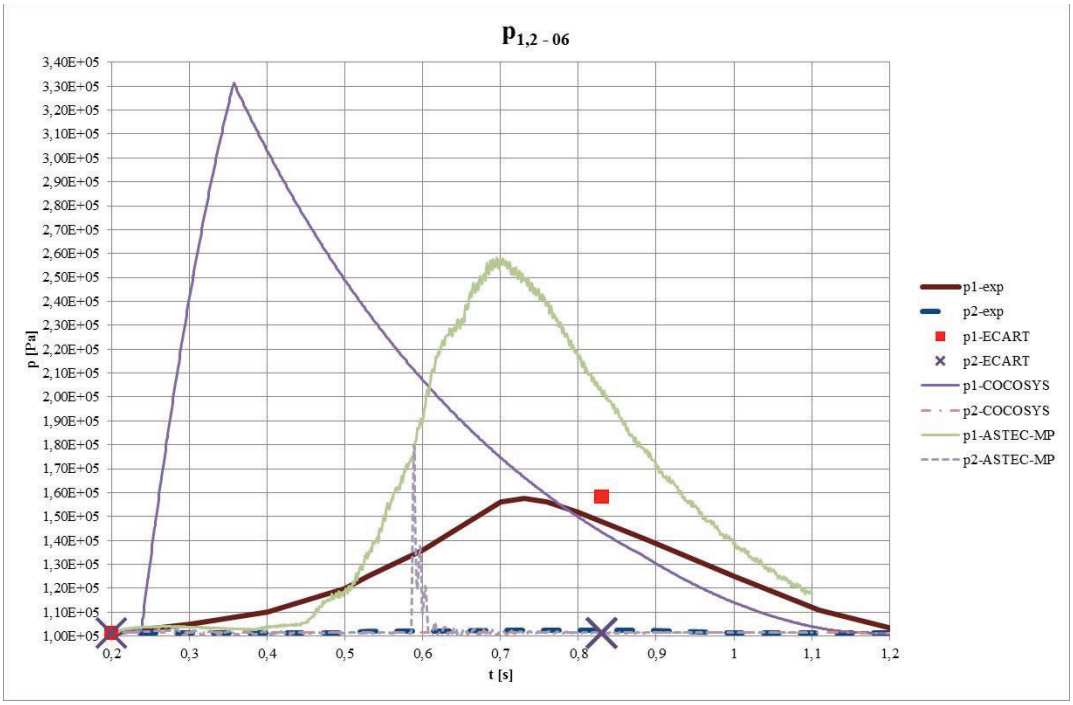

Figure 7. Pressure transients (test 06: exp. and simulations results).

About the main values, the tables (Tab. I, II, III) are summarizing maximum pressures (exp. and simulations results), temperatures (simulations results) and times when the flame is at the diaphragm orifice.

Table I. Main values – test 90 (exp. and simulations results).

90	t	p_{1Max}	t	p_{2Max}	t	T_{1Max}	t	T_{2Max}	t	Flame at the orifice
	Time [s]	Pressure [Pa]	Time [s]	Pressure [Pa]	Time [s]	Temperature [K]	Time [s]	Temperature [K]	Time [s]	
EXP	0.475	186000	0.438	212000					0.425	YES
ECART	0.513	185953	0.514	185953	0.513	543	0.514	543		NN
ASTEC-IK	0.295	184159	0.220	218206	1.200	1072	0.518	1138	0.217	YES
COCOSYS	0.539	164139	0.534	211033	0.539	391	0.602	1128	0.261	YES
ASTEC-MP	0.503	181811	0.446	185727	0.549	1140	0.576	1156	0.443	YES

Table II. Main values – test 47 (exp. and simulations results).

47	t	p_{1Max}	t	p_{2Max}	t	T_{1Max}	t	T_{2Max}	t	Flame at the orifice
	Time [s]	Pressure [Pa]	Time [s]	Pressure [Pa]	Time [s]	Temperature [K]	Time [s]	Temperature [K]	Time [s]	
EXP	0.620	132500	0.925	157000					0.570	YES
ECART	0.513	185953		101325	0.513	543		293		NN
ASTEC-IK	0.295	144773	0.634	146577	1.200	1019	0.671	836	0.217	YES
COCOSYS										
ASTEC-MP	0.587	216252	0.487	184100	0.630	1162	0.666	1142	0.484	YES

Table III. Main values – test 06 (exp. and simulations results).

06	t	p_{1Max}	t	p_{2Max}	t	T_{1Max}	t	T_{2Max}	t	Flame at the orifice
	Time [s]	Pressure [Pa]	Time [s]	Pressure [Pa]	Time [s]	Temperature [K]	Time [s]	Temperature [K]	Time [s]	
EXP	0.730	157500	0.800	102550					0.640	YES
ECART	0.830	158195		101325	0.830	461		293		NN
ASTEC-IK										
COCOSYS	0.357	331339	0.261	103009	0.357	1263	1.142	542		NN
ASTEC-MP	0.695	258363	0.588	179635	0.724	1180	0.820	1107	0.585	YES

ASTEC-IK. For the results obtained by JSI, it may be noticed that the qualitative agreement for test 90 (that is, the shape and arrangement of curves representing the pressure in both chambers) is quite good. Also, the maximum values of both calculated pressures agree quite well with measured values. This was achieved by an adequate tuning of adjustable parameters of the combustion FRONT model. The major discrepancy is the time shift of about 0.25 s. For test 47, this qualitative agreement is less good, the major discrepancy being the shorter combustion time in the left-hand chamber. Also, the agreement between calculated and measured maximum pressures is not as good as in test 90, but still acceptable. Again,

parameters of the combustion PROCO model were adjusted to obtain these results. The start of combustion in the right-hand chamber only after combustion in the left-hand chamber has stopped, as was also observed in the experiment, is the consequence of the modelling in the PROCO model.

COCOSYS. There were some limitations in availability of information on experimental boundary conditions. In the modelling, UJD focused on capturing the timing and maximum values of pressure in both chambers. Relatively good agreement of these parameters was achieved for test 90, although the shape of the pressure curves deviates comparing to the experimental results, and the calculated peak in chamber room 1 is lower. Selection of the appropriate nodalization seems to be the most important parameter influencing the calculated results. In case that some unknown details of experimental boundary conditions are available (e.g. pressure resistance of the plastic bag and/or its volume), further improvements of the modelling could be expected, too.
Modelling of the delayed jet ignition is problematic with the FRONT model. Once the flame front reaches the neighboring zone (zone 2), i.e. the end of junction, and there are flammable conditions in the zone, hydrogen combustion starts there. There is a possibility to exclude the respective junction from flame propagation and to control start of the ignition in the zone 2 by time definition. Using of this option with combination of lower overpressure for “bag” failure was to some extend helpful for modelling the test 06 without jet ignition. But capturing of the delayed pressure peak in zone 2 of the test 47 has not been successful.

ASTEC-MP. LEI results of the test 90 simulation show good qualitative agreement with the experiment. Quantitatively, maximum pressure peak, reached in the right-hand chamber, is underestimated by almost 0.3 bar. Pressure in the left-hand chamber reaches similar value, however calculated pressure rise is steeper than in the experiment. Results for the other two tests are distorted by the combustion in the right-hand chamber. In the experiment 47 jet ignition is delayed and in the experiment 6 it does not occur at all. In the calculations combustible mixture in the right-hand chamber ignites as soon as the flame reaches it through the orifice junction, because there is no model to account for the flame quenching and delayed ignition. In the test 47 simulation right-hand chamber ignition is calculated to occur ~0.4 s earlier than observed, leading to a significant overestimation of pressure (by up to ~0.9 bar) in the left-hand chamber. However, additional calculations showed that without right-hand chamber ignition pressure in the left-hand chamber would still be overestimated, but by the smaller values of up to ~0.5 bar. This overestimation may be caused by a faster calculated combustion than observed in the left-hand chamber. The same description is valid for the test 6 simulation results - ignition in the right-hand chamber, which does not occur in the experiment, causes significant overpressure of up to ~1 bar compared to the experiment. Without this ignition overpressure would reach ~0.6 bar.

ECART. The results are approximately good for test 90 case (maximum values of p_1 and p_2 and instants of time to reach the peak values). With regard to the other cases (tests 47, 06), the simulations are not particularly meaningful because the code has not the models capable of an effective simulation of combustion propagation between the different control volumes, yet.

The results of the simulations show that the delay with which occurs the sharp rise of pressure in the chamber 2 is reproduced in the simulations employing ASTEC and COCOSYS, although with timing sometimes distant from those of the experimental results.
About the differences between the results obtained, it seems that nodalizations with an improved number of control volumes, also well distributed in order to represent more realistically the geometry and phenomena inside (ignition, combustion propagation through the diaphragm orifice, see par. 4), have led to more precise results. This is mainly concerning the timing of phenomena development and the combustion propagation between the two chambers.
Otherwise no significant difference appears to be due to different combustion models used (FRONT, PROCO).

6. CONCLUSIONS

Some of the explosion propagation experiments, performed in the LargeView2 facility at University of Pisa (Italy), were simulated with lumped-parameter codes within an organized benchmark exercise. The calculated results show that, despite a few relatively large discrepancies, the lumped-parameter codes used in the benchmark exercise are able to provide quickly useful predictions, even if only in principle (first approximation), about hydrogen explosion and propagation in a lab-scale vessel facility in case of immediate – fast propagation between chamber 1 (ignition chamber) and chamber 2. This is, at least, in case of the adoption of a refined nodalization for codes of this type. While, in cases with a rough nodalization, the discrepancies compared with reality are considerable.
Furthermore, in case of more slow propagation of combustion or without any propagation, the calculated results are quite different compared with measured ones.

Therefore it seems that there are still needs for improvements of models used in lumped-parameter codes for simulating the complex phenomena of explosion propagation. This is mainly in case of complex scenarios like those involving nuclear reactor containments.

In relation to that, it appears to be interesting to carry out other tests, by trying additional nodalizations and / or modeling options, different combustion models available in the lumped-parameter codes used in this benchmark, or consider the option of using CFD codes.

ACKNOWLEDGMENTS

Special thanks are due to prof. M.N. Carcassi (University of Pisa) to have carried out the experiments with a lot of experience and also passion and for allowing us the using of some results for the benchmark.

The work performed by JSI was financed by the Slovenian Research Agency (research programme "Reactor engineering").

The license for using COCOSYS V2.4v3 by UJD has been kindly provided by GRS.

About RSE: this work has been financed by the Research Fund for the Italian Electrical System under the Contract Agreement between RSE S.p.A. and the Ministry of Economic Development - General Directorate for Nuclear Energy, Renewable Energy and Energy Efficiency in compliance with the Decree of March 8, 2006.

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