VALIDATION OF FLACS-HYDROGEN CFD CONSEQUENCE PREDICTION MODEL AGAINST LARGE SCALE H_2 EXPLOSION EXPERIMENTS IN THE FLAME FACILITY

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ABSTRACT

The FLACS CFD-tool for consequence prediction has been developed continuously since 1980. The initial focus was explosion safety on offshore oil platforms, in recent years the tool is also applied to study dispersion, hydrogen safety, dust explosions and more. A development project sponsored by Norsk Hydro, Statoil and Ishikawajima Heavy Industries (IHI) was carried out to improve the modelling and validation of hydrogen dispersion and explosions. In this project GexCon carried out 200 small-scale experiments on dispersion and explosion with H_2 and mixtures with H_2 and CO or N_2. Experiments with varying confinement, congestion, concentration, and ignition location were performed. Since the main purpose of the tests was to produce good validation data, all tests were simulated with the FLACS-HYDROGEN tool. The simulations confirmed the ability to predict explosions effects for the wide range of scenarios studied. A few examples of comparisons will be shown. To build confidence in a consequence prediction model, it is important that the scales used for validation are as close as possible to reality. Since the hazard to people and facilities, and the risk, will generally increase with scale, validation against large-scale experiments is important. In the 1980s a series of large-scale explosion experiments with H_2 was carried out in the Sandia FLAME facility and sponsored by the US Nuclear Regulatory Commission. The FLAME facility is a 30.5m x 1.83m x 2.44m channel, tests were performed with H_2 concentrations from 7% to 30%, with varying degree of top venting (0%, 13% and 50%) and congestion (with or without baffles blocking 33% of the channel cross-section). A wide range of flame speeds and overpressures were observed. Comparisons are made between FLACS simulations and FLAME tests. The main conclusion from this validation study is that the precision when predicting H_2 explosion consequences with FLACS has been improved to a very acceptable level.

1.0 INTRODUCTION

The development of the CFD-simulator FLACS (FLame ACceleration Simulator) started in 1980. The initial motivation was to improve platform safety in the North-Sea, as it was recognized that the large offshore structures used for oil exploration were exposed to explosion hazards. In 1980-86 the first in a series of gas explosion programs (GEPs) was carried out with substantial support from sponsors BP, Elf, Esso (Exxon), Mobil, Norsk Hydro and Statoil. Numerous large-scale explosion tests were carried out, and the knowledge acquired was implemented in the CFD-tool FLACS-86. The improved tool from the next GEP, FLACS-89, included hydrogen as a gas. The series of continuous gas safety R&D programs ended in 2003. In the meantime the explosion group had demerged into Christian Michelsen Research (CMR) in 1992, and further into GexCon AS (Consultants in 1998, R&D-activity in 2001). To ensure the future of the FLACS-software with decreasing R&D-funding, FLACS was made commercially available in 1996. Today FLACS is used for consequence studies at about 30 offices worldwide (in addition to academic licenses).

In parallel to this development the nuclear industry has been focusing on hydrogen explosion hazards. Accidents like Three Mile Island [1] and in particular Chernobyl [2] increased the focus on the understanding of hydrogen safety within the nuclear industry. Compared to offshore oil exploration accidents, where consequences will be mainly local and highly visible, the consequences from nuclear accidents with its radiation can be more global and less visible. It is therefore of paramount importance to keep the confinement in case of an accidental hydrogen explosion. On behalf of US Nuclear Regulatory Commission Sandia National Laboratories constructed the FLAME facility

(FLame Acceleration Measurements and Experiments) and conducted a series of large-scale hydrogen explosion tests [3]. The dimensions of the channel were selected to be half-scale of the upper plenum region of an ice condenser PWR containment. Both the scale of the FLAME facility and the scenario variations studied in these tests make them very valuable for validation of consequence prediction tools.

2.0 DESCRIPTION OF FLACS

FLACS was initially developed to predict dispersion of gas leaks and subsequent explosions in offshore oil and gas production platforms. The conservation equations for mass, momentum, and enthalpy, in addition to equations for concentration of flammable species and flame progress, are solved on a Cartesian grid using a finite volume method. The equations are closed using the k-ε equations for turbulence. The SIMPLE pressure correction method [4] is applied, and extended for compressible flows with source terms for the compression work in the enthalpy equation. Hjertager [5,6] describes the basic equations used in the FLACS model. Early explosion experiments to develop and validate FLACS are also published [7,8].

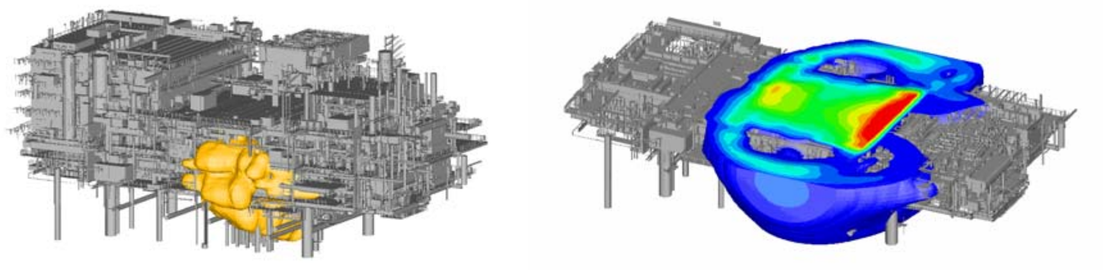

Figure 1. For explosion and dispersion studies representation of the detailed geometry is important for the quality of the predictions. In FLACS this is handled with a porosity concept.

Compared to general CFD flow calculations, further challenges exist for an explosion model. A model for development of the flame that describes how the local reactivity of the flame changes with parameters like gas concentration, temperature and pressure, turbulence, interaction with obstructions and other factors is required. A good description of geometry and the geometry/flow/turbulence/flame coupling are key elements in the modeling. General conservation equations and numerical methods will not be described here, as these are similar for most CFD-tools.

In FLACS a “beta” flame model is applied in which the reaction zone becomes 3-5 grid cells thick. The burning velocity is primarily controlled by diffusion of reaction products. A flame library will decide the laminar burning velocity as function of gas mixture, concentration with air, pressure, temperature, oxygen concentration in air and more. Initial “quasi-laminar” flame wrinkling will increase the burning velocity with distance. With increasing turbulence a turbulent burning velocity will replace the quasi-laminar. A development to include models for DDT and detonation propagation of flames is ongoing. Models for the effect of inerts (nitrogen, water vapor and CO_2) also exist.

The real flame area has to be described. For a finite thickness of the reaction zone (in FLACS this is 3-5 grid cells), the flame area needs to be corrected for curvature at these scales and smaller. All flame wrinkling at scales less than the grid size must be represented by sub-grid models (and this is important for flame interaction with objects of the grid size or less). As a consequence of the necessary modeling, completely grid independent flame models for deflagrations in 3D do not exist.

The representation of geometry using a distributed porosity concept is one of the key advantages with FLACS compared to several other CFD-tools. The geometry is represented with area and volume porosities, as well as “wake generating” sub-grid object areas in 6 flow directions (positive and negative x, y and z). The FLACS porosity concept models the blockage, drag formulation, sub-grid turbulence generation and flame folding coefficients to obtain good simulation results despite coarse grid resolutions. For other CFD-models without sub-grid representation of geometry it becomes unrealistic to properly describe complex industry plants with 100.000 objects or more.

For turbulence modeling the k-ε model is used. In addition to the modeled generation of turbulence behind sub-grid objects, some further modifications are added [9]. Despite the known limitations of the k-ε model, it is a powerful model for industrial applications. With the close coupling between sub-grid modeling and turbulence model, it is not believed that replacing k-ε with a more advanced turbulence model with more equations and constants will give much added value for the typical simulations carried out with FLACS.

Deflagration calculations are challenging due to the strong feedback loop with flames generating expansion flow, producing turbulence, and accelerating the flames again (Schelkin mechanism). Small errors in the representation of geometry, flame area or other parameters can lead to significant errors in flame speed and consequence predictions. Therefore validation against a widest possible array of experiments is important. For natural gas deflagration calculations several hundred experiments were simulated as part of validation exercises [10] in the 1990s, some of the more important are the British Gas (Advantica) 180m^3 box [11], CMR (GexCon) 3D-corner (27m^3), CMR (GexCon) M24 module (50m^3) [7,8], Shell SOLVEX chambers (2.5m^3, 550m^3), MERGE (TNO and British Gas 1m^3-250m^3) [12], BG (Advantica) BFETS [13]/ HSE Phase 3A [14]/ Phase 3B full-scale tests (1600-2700m^3) [15].

Grid independency studies as well as more basic validation studies (shock-tube, transport of passive scalar, turbulence generation behind object with different grids, etc.) are important parts of a validation study. Similar studies are also performed for far-field blast propagation from deflagrations [16, 17], dispersion of flammable gas and ignition of non-homogeneous gas cloud relevant for QRA-studies towards offshore oil and gas industry [18], dispersion of tracer gas [9, 19] and dust explosion simulations with DESC, a tool based on FLACS [20].

Despite some sporadic explosion tests at GexCon (CMI) with hydrogen before 1990, the main focus was natural gas explosions. Through the 1990s when the validity of FLACS for natural gas dispersion and explosion predictions improved, the limitations when simulating hydrogen became more visible. This particularly applied for lean concentrations of hydrogen, for which the reactivity of FLACS was far too low and lower flammability limit (LFL) too high. With increasing interest in hydrogen safety in recent years an effort has been done to learn more about hydrogen explosions and improve FLACS. Hydrogen safety aspects were studied in projects on inert gas dilution [21] and transformer safety [22], as well as consulting activities.

3.0 FLACS-HYDROGEN VALIDATION PROJECT

From 2001 to 2004 a dedicated R&D project was carried out to improve the validation basis for FLACS-HYDROGEN. The original project received support from Norsk Hydro and Statoil. Later the activity was extended with additional funding from IHI. A primary objective was to increase the validation database for FLACS for explosion and dispersion calculations, see Figure 3. Since large-scale tests require much more resources than small-scale tests, and funds were limited, it was decided only to carry out small-scale tests. Numerous small-scale explosion and dispersion tests were carried out.

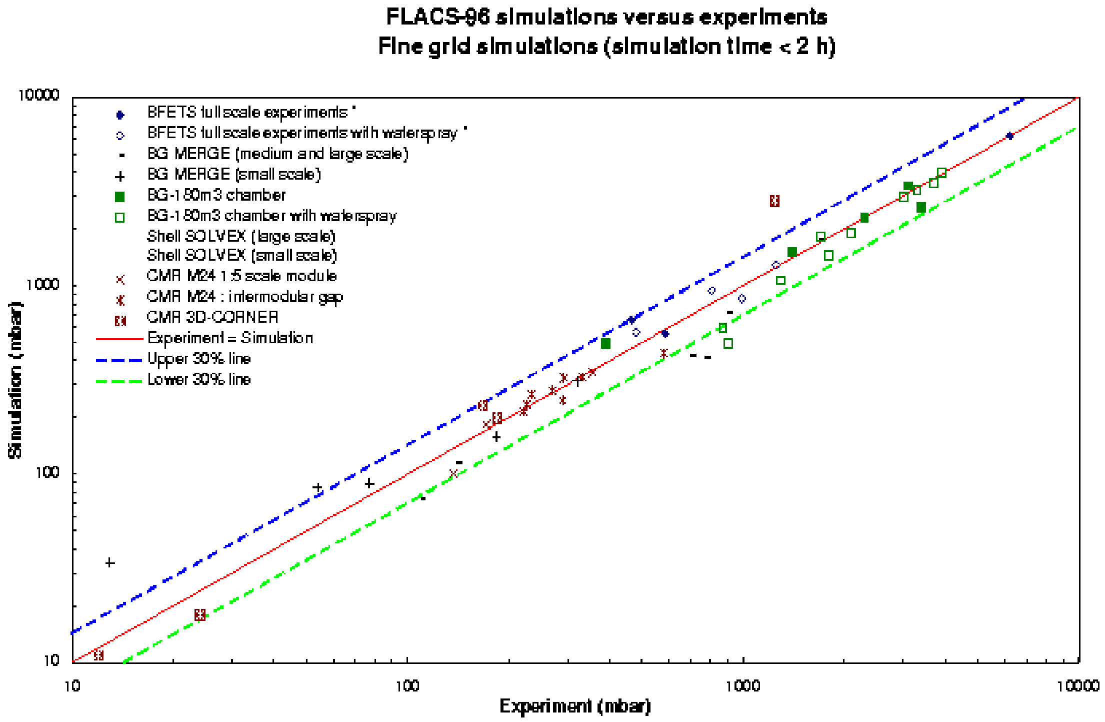

Figure 2. Validation of FLACS for deflagrations, plot from 1997 showing some of the comparisons between simulationand experiments performed for deflagrations for natural gas [10].

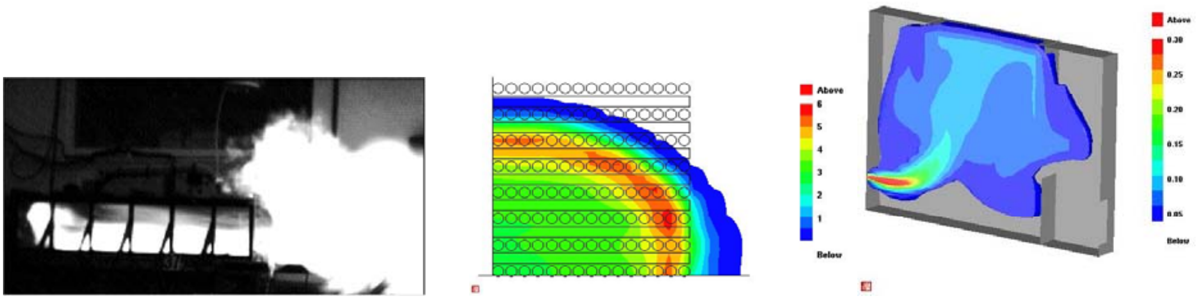

Figure 3. Picture and plots illustrating test series from the hydrogen safety project 2001-2004, explosion in the 1.4m channel (left), simulated pressure distribution (barg) of one of the 3D-corner tests (centre) and volume fraction H_2 in a dispersion test (right).

A short description of the different test series follows. In addition to tests with hydrogen, some tests with mixtures of hydrogen with N_2 or CO were also carried out for all test configurations:

- Small-scale 3D-corner tests (obstacle array of 37x37x37cm) with 3 different obstruction densities, 2 ignition locations and 3-6 H_2 concentrations.
- GexCon channel (1.4x0.30x0.30m) experiments with 3 different baffle configurations, 2 ignition locations, 3-6 H_2 concentrations.
- GexCon dispersion chamber (1.2x0.20x0.90m), low and high momentum releases in 3 different geometry configurations. Transient gas concentrations were measured at 12 different locations.

A significant number of tests were carried out. This gave valuable test data for FLACS to investigate;

- Effect of gas concentration for a range of test geometries: This helped identify weaknesses in previous versions of FLACS. Lower flammability limit has been lowered, and the significant difference in flame wrinkling between lean flames and rich flames is taken care of. A weakness in the mixing rules for flammable gases involving CO was also identified and improved.

- Effect of obstruction density and flame acceleration: Tests with varying number of baffles or obstruction density have provided valuable data for flame acceleration through obstructions.

- Inward versus outward burning flames: Inward burning flames and flame impact of pressure oscillations from venting are challenging to model compared to expansion driven flames.

In general, the experiments are well simulated with FLACS. Compared to natural gas explosion simulations it seems more important to follow guidelines on proper grid embedding when simulating hydrogen. This may be a result of the higher reactivity of hydrogen, and that a certain grid resolution is needed to pick up the faster oscillations and transients. In particular behind baffles and obstacles it seems necessary to resolve across the wake with a minimum of 2-4 grid cells.

At this stage most details of the comparisons cannot be made available as test results are still of confidential nature. In Figure 4 one of the comparisons between FLACS and experiments is shown. The scenario shown is with 24% H_2 in air, ignition in the inner end of the 1.4m channel equipped with 4 baffles (17% blockage). A grid resolution of 1.67cm is applied (3 grid cells across height of baffle, 18 across channel). Four pressure traces are shown, with position inner end (1), center (2), outer part (3), and outside vent (4) of channel. Most aspects with the simulated pressure traces correspond very well to the observed (maximum pressures, time of arrival, development of pressure and more). The scenario shown is a typical outward propagating flame scenario with ignition in one end and venting in the opposite end. The performance of FLACS when simulating this type of scenarios seems generally good, in particular if the baffle obstructions are properly resolved on the grid.

If the ignition is moved to the outer half of the channel closer to the vent opening, the physics get more complicated. Initially the flames propagate towards the vent opening, after a moderately strong external explosion, the pressure drops. The resulting pressure oscillations in the channel, the flow, and generated turbulence in the wake behind the objects give rise to enhanced flame acceleration into the inner end of the channel with strong reflected pressures in the inner end. In Figure 5 a comparison can be seen between FLACS and the experiment. The only changes from previous tests are that concentration is increased to 30% and ignition is moved 2/3 towards vent opening. This time the simulation over-predicts the explosion pressures by about a factor of 2 (both initial phase and reflected pressure in inner end of channel). In this kind of more challenging scenario, one will often see some grid dependency in simulation results.

The main missing elements in the generated test matrix are large-scale tests to investigate how well scaling and explosions at large-scale are handled. A 20m diameter hemispherical deflagration test from Fraunhofer-ICT [23] has been simulated with good results, this was done as a benchmark activity within the HYSAFE Network of Excellence. This experiment is valuable investigating the acceleration of flames with no obstacles present. For more realistic geometries at large-scale, simulations in the FLAME facility has been carried out [3]. The results will be described in the following sections.

4.0 SANDIA FLAME FACILITY

The Sandia FLAME facility was constructed in the years 1981-1983 with support from the US Nuclear Regulatory Commission [3]. In the aftermath of Three Mile Island accident, the purpose of building the test facility was to study the physics in connection to hydrogen flame acceleration potential in nuclear plants. The facility is therefore meant to represent a 1:2 scale down of the upper plenum of an ice condenser PWR containment. The geometry is a 30.5m long channel with closed or partly open ceiling (13% or 50%), and either no obstructions or repeated vertical baffles (33% blockage). In addition to being relevant for nuclear plant safety, the tests are also highly relevant for situations involving major releases in tunnels.

Twenty-nine large-scale experiments were carried out and described in the data report [3]. Removing tests where problems were experienced as well as some tests with (almost) repeated gas concentrations, a total of 23 scenarios in 5 categories remain. These 5 categories are closed ceiling with (2 scenarios) and without baffles (6 scenarios), 13% open ceiling without baffles (5 scenarios), and 50% open ceiling with (5 scenarios) and without (5 scenarios) baffles.

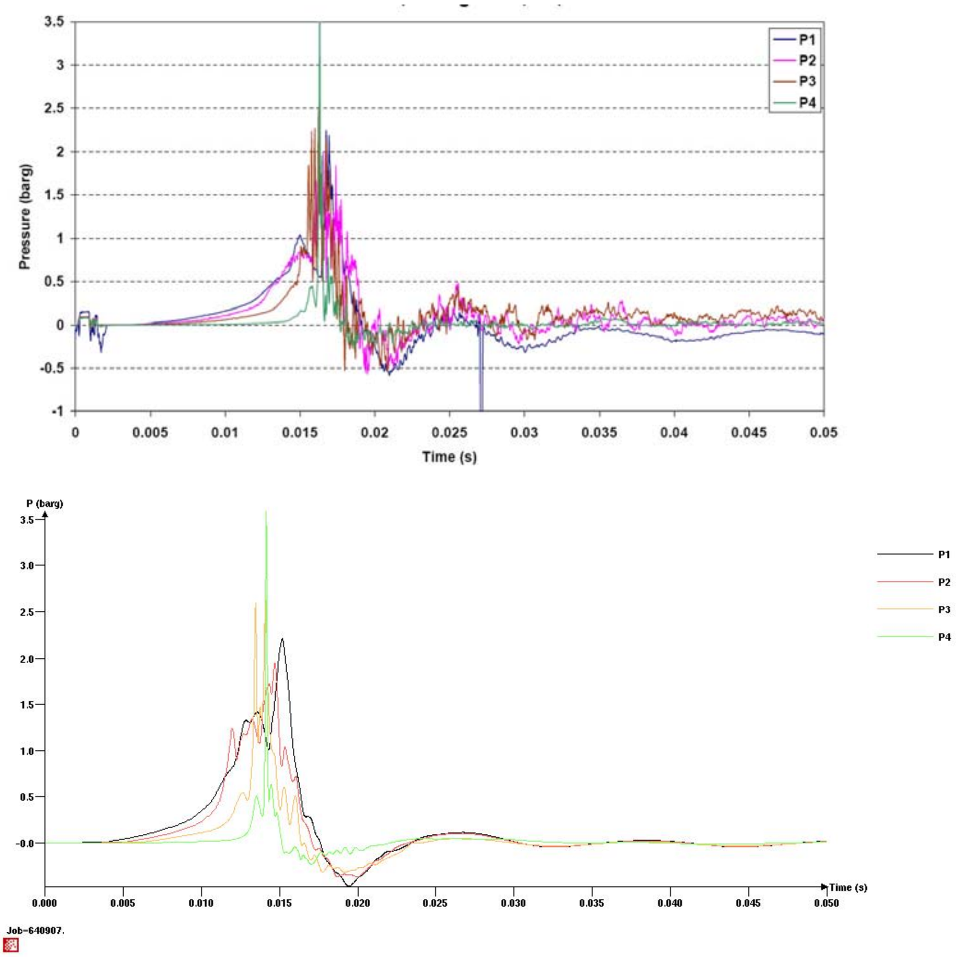

Figure 4. Experiment (top) and FLACS simulation (lower) compared, 24% H_2 in GexCon 1.4m channel with 4 baffles (17% blockage) and ignition in closed end. Pressure monitors are located in inner end (P1), middle (P2), outer end (P3) and outside (P4) channel.

The first step in the preparation process for FLACS simulations is geometry building. For this kind of simple test geometry with walls, floor, ceiling with vents and repeated obstacles a user can define each of the geometries within minutes. In Figure 6 the test geometry with baffles (ceiling removed) is shown. A computational grid must thereafter be defined. FLACS user guidelines require cubical grid cells inside the channel, further a minimum of 5-6 grid cells across is required for the situations with closed ceiling. For the situations with venting upwards at least 10-12 grid cells in vertical direction is required to conform with the FLACS user guidelines. To avoid unphysical influence from boundaries, the guidelines also require a significant distance to external boundaries in the case of top venting. For simplicity, all simulation scenarios were performed with the same grids.

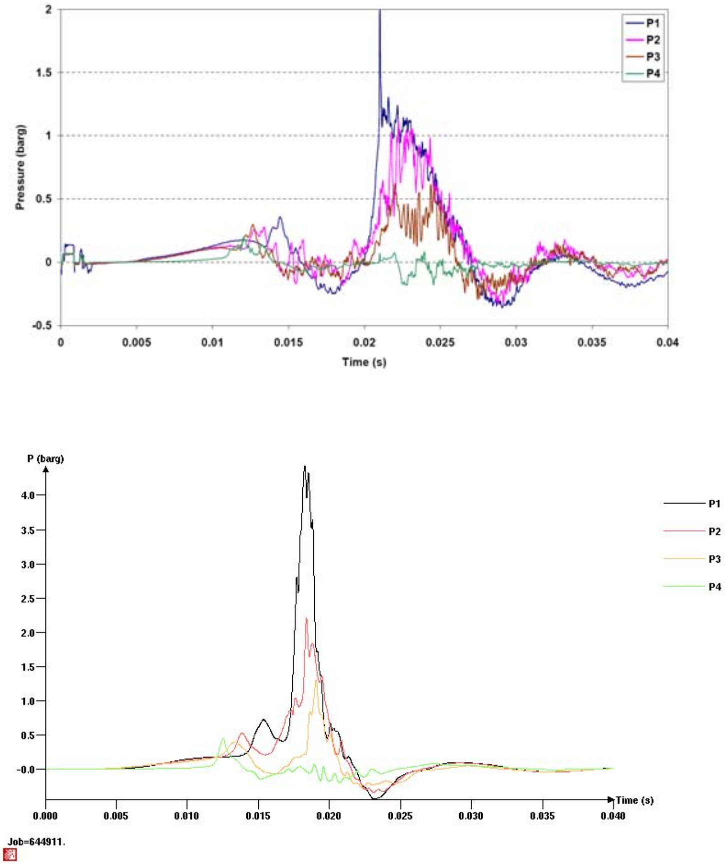

Figure 5. Experiment (left) and FLACS simulation (right) compared, 30% H_2 in GexCon 1.4m channel with 4 baffles (17% blockage) and ignition 2/3rd towards open end. Pressure monitors are located in inner end (P1), middle (P2), outer end (P3) and outside (P4) channel.

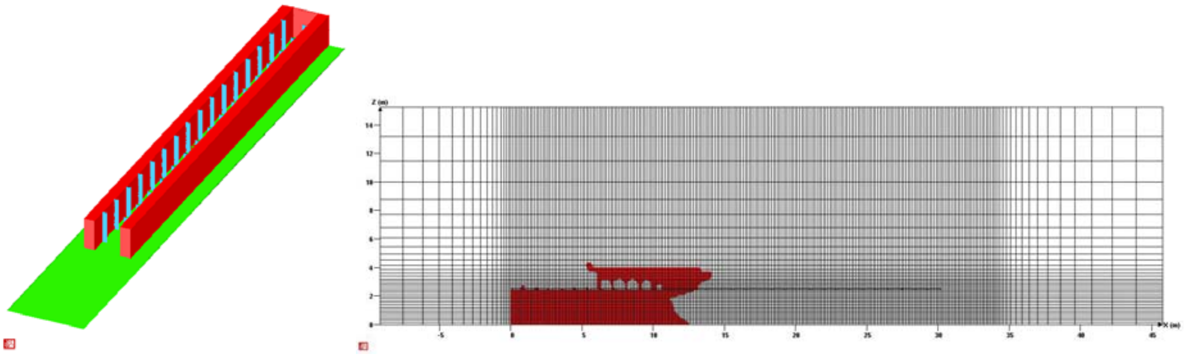

Figure 6. In left picture one geometry configuration in the 30.5m long Sandia FLAME facility experiments is seen (roof made invisible). In the right picture the simulation grid is shown together with a flame plot from one of the scenarios with 13% top venting.

It was decided to apply 2 different grid resolutions for the simulations, one coarse grid for screening calculations with 6 cells across the channel width (only 1 grid cell across baffle), and one normal grid with 12 cells across channel width (2 across baffle). The coarse grid is not acceptable according to the guidelines, but is still expected to provide decent results for a range of situations due to the porosity model and sub-grid models. The degree of scatter in results between simulations with coarse and normal grid can indicate confidence level in the predictions (large scatter means low confidence). The normal grid used for the simulations is shown in Figure 6. Simulation time was around 30 minutes for the screening grid, and 3-10h for normal grid.

Scenario parameters like ignition point and gas cloud and concentration must be defined prior to the simulation. In the top-vented experiments, it was observed that the plastic foil confining the gas, had some influence on the flame propagation in some of the scenarios. It was therefore decided to represent this in FLACS with a PLASTIC panel defined on top of the geometry. This will start venting when 20 mbarg is reached. The scenario definition is done in the dedicated visual pre-processor, CASD. Once the setup has been defined for one scenario, it is quickly copied and modified to another scenario. Before simulations are started, the porosity calculation program must be run for each of the grid/geometry configurations.

Table 1. Comparisons between experiments and FLACS. The screening column shows FLACS results with a coarse grid resolution, the FLACS column show results with recommended grid resolution. Comments to certain results from the experimental report [3] are left out.

Test	% H2	Baffles	Top vent	Pressure (barg)			Flame speed (m/s)		
				Exp.	FLACS	Screening	Exp.	FLACS[d]	Screening[d]
2	19.7 %	No	50 %	0.028	0.044	0.062	54	20	17
3	20.8%	No	50 %	-	0.072	0.085	65	26	19
4	28.0 %	No	50 %	0.2	0.18 / 0.28[a]	0.23 / 0.48[a]	126	55	77
5	12.6 %	No	50 %	0.009	0.020	0.020 / 0.006[c]	4	12	12 / 3
6	15.5 %	No	50 %	0.034	0.022	0.032	19	19	17
7	12.0 %	No	0	0.012	0.019	0.027	16	15	19
8	18.4 %	No	0	0.26	0.33	0.26	170	250	250
9	6.9 %	No	0	-	0.001	0.001	1.2	6	6
11	12.9 %	No	0	0.045	0.026	0.032	30	16	19
12[e]	24.7 %	No	0	0.95 / 11[b]	1.5 / 2.8[b]	1.5 / 3.2[b]	374	410	460
14[e]	30.0 %	No	0	2.5 / 21[b]	2.2 / 3.8[b]	1.6 / 3.2[b]	932	740	740
15	15.4 %	No	13 %	0.031	0.029	0.043	50	22	20
16	17.6 %	No	13 %	0.10	0.068	0.14	75	31	35
18	18.1 %	No	13 %	0.36	0.083	0.17	136	33	37
19[e]	24.8 %	No	13 %	0.65 / 8.5	0.47	0.62	160	100	160
20	20.7 %	No	13 %	0.78	0.18	0.30	483	50	60
22[e]	15.0 %	Yes	0	31	3.2 / 5.3[b]	2.5 / 2.7[b]	700	520	520
23	14.5 %	Yes	0	12	2.8 / 4.2[b]	2.0 / 2.0[b]	540	500	480
24	15.5 %	Yes	50 %	-	0.02 / 0.06[a]	0.03 / 0.04[a]	46	91	62
25[e]	19.7 %	Yes	50 %	15	0.05 / 0.19[a]	0.07 / 0.05[a]	890	114	70
27	13.1 %	Yes	50 %	0.09	0.02 / 0.04[a]	0.02 / 0.03[a]	15	70	62
28	14.9 %	Yes	50 %	0.09	0.02 / 0.06[a]	0.03 / 0.04[a]	33.4	85	60
29	18.5 %	Yes	50 %	0.23	0.04 / 0.12[a]	0.05 / 0.05[a]	130	90	70

[a] First peak appears early before top venting, second peak after new flame acceleration along channel.

[b] Second pressure peak is showing pressures of short duration (typical detonation pressure shape)

[c] Second pressure peak is without simulated plastic panel (20 mbar)

[d] Flame velocities are very approximate estimates and are recorded towards end of channel

[e] DDT observed

For the discussion we will only consider the pressure values, as there can be significant uncertainties in the estimate of flame speeds, both experimentally and in the simulations. Considering the pressure results in Table 1, it can be concluded that with a few exceptions simulations reflect the observed explosion characteristics to a certain degree. FLACS is still not a tool that can simulate shock-ignition seen for detonations (work in progress), and therefore it is expected that cases with DDT/detonation pressures are underpredicted. It is seen that in most cases the grid dependency is moderate despite the use of very coarse grid for the screening calculations. For some of the tests with top venting a very distinct second phase of flame acceleration establishes in some of the situations.

In Figure 7 a comparison between pressure curves from simulation and experiment F-12 can be seen, this is a situation with 24.7% hydrogen, without top venting and with no baffles. In this case DDT was observed, and a significant deviation of maximum pressure is reported in Table 1. From Figure 7 it can be seen that even if some maximum pressures recorded in connection to the detonation deviates, the general shape of the pressure curves at other locations is reasonable.

Largest deviation between experimental pressure and simulation is seen for test 25. The predicted maximum overpressure is two orders of magnitude too low compared to the data. A standard (at least highly recommended) part of simulation is a grid dependency study. If the results show significant grid dependence, this is an indication that higher uncertainty estimates are required. Of all 23 scenarios, the highest grid dependency is seen for test 25. The second peak seen for flame acceleration towards the end of the channel is 4 times higher with normal grid compared to screening grid (It can be mentioned that the grid dependency predicting the first peak prior to venting is low). Such an observation will normally lead to additional simulations either to understand the reason for the grid dependency or to increase confidence in either of the results. In this case we decided to perform a simulation with an even finer grid resolution (4 grid cells across the baffle, 24 across the channel width). The first pressure peak before the upward venting starts is very similar to the two previous simulations. The flame acceleration and pressure build-up towards the end of the channel is much higher with the finer grid. In Figure 8 pressure curves near ignition and near the end of the channel are compared with experimental values. A competent and cautious FLACS user would therefore manage to identify the potential for strong flame acceleration even in this case. In Figure 8 3D plots showing the flame and pressure just before flame exit is also shown, one can here observe a number of pressure waves inside the channel. Test 25 is a difficult scenario in that small changes in hydrogen concentration result in large changes in outcome. In test 29 only slightly lower gas concentrations was used (18.5% versus 19.8%) and no DDT was observed.

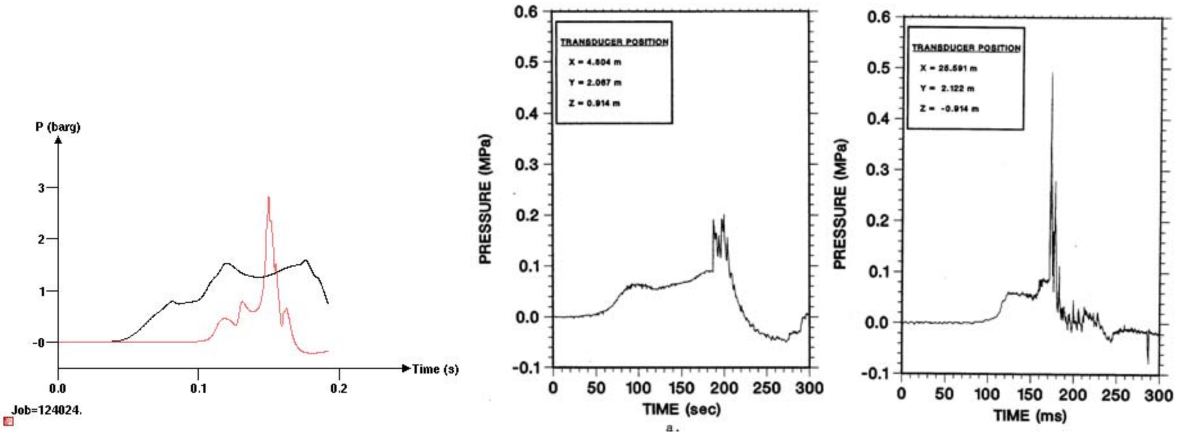

Figure 7. Test F-12, 24.7% H_2, no baffles or top venting. Pressure traces 5m from ignition and near the exit of pipe are shown, from left FLACS simulation and experiment (Unit conversion 100 kPa=1 barg).

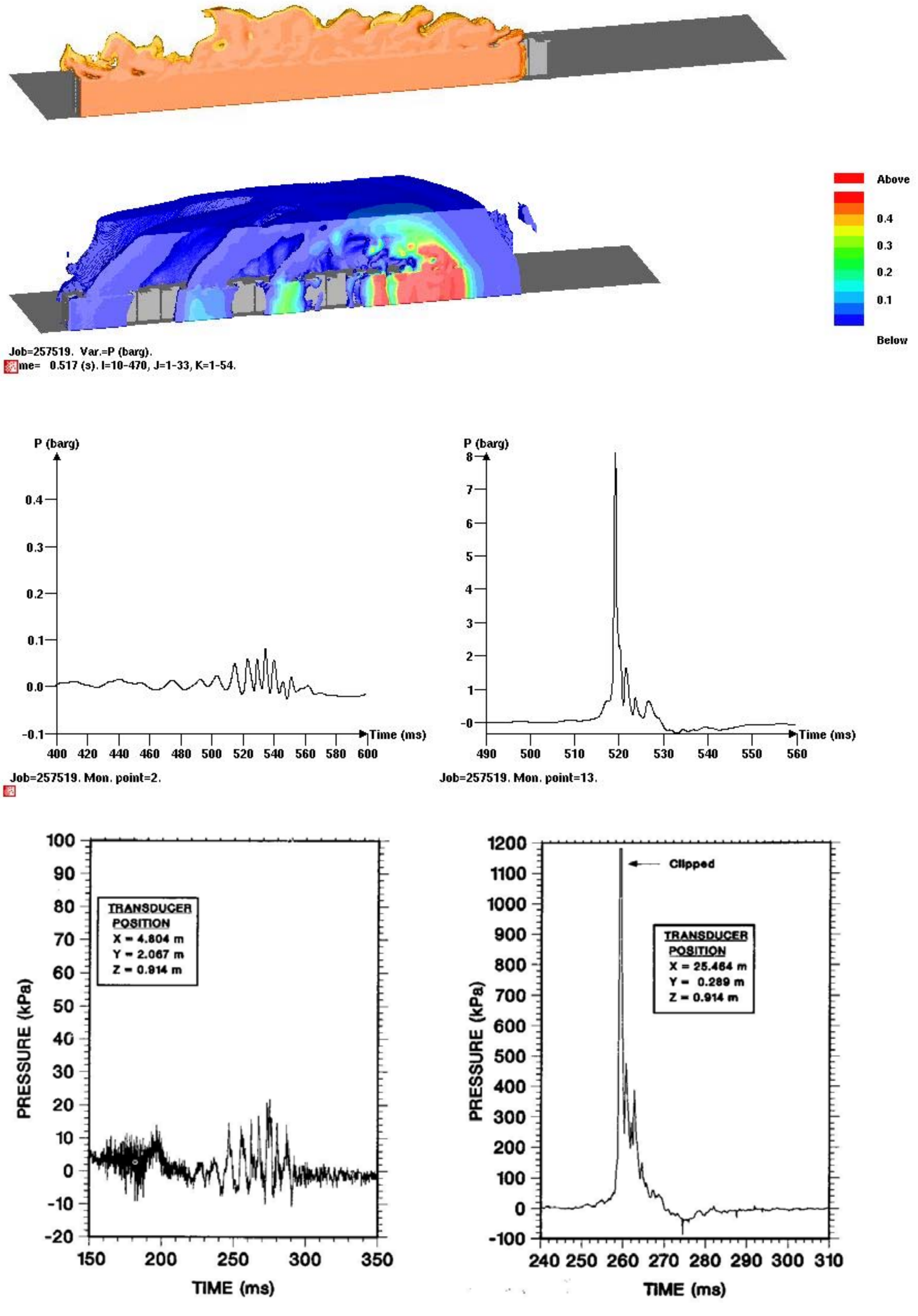

Figure 8. Test F-25; Top pictures show 3D flame (top) and pressure plot when flame is near end of channel. Below pressure traces from simulation 5m from ignition (left) and near the exit of pipe (right), for simulations (top) and experiments (below). Time window is 250 ms shifted for simulations, (conversion factor for unit is 100 kPa=1 barg).

5.0 CONCLUSIONS

As a result of a dedicated effort towards hydrogen safety the CFD-tool FLACS can now demonstrate an improved performance and validation simulating hydrogen explosions. Numerous small-scale experiments have been simulated. In this paper a validation study against large-scale tests in the Sandia FLAME facility is presented. Work is ongoing to improve capabilities to predict and simulate DDT and detonations. FLACS is a commercial CFD-tool for simulation of dispersion and explosion consequences to be used in risk assessments and consequence evaluations for the industry.

All simulations presented in this paper are performed using the most recent commercially available version of FLACS, FLACSv8.1 (issued March 2005) and following user guidelines for grid embedding and more. For some scenarios prediction will deviate from experiment, but no general trend of under-prediction or over-prediction can be observed. A grid sensitivity study can often indicate level of confidence in the results, as the difficult scenarios to predict are also more likely to show grid dependency. An experienced FLACS user doing blind simulations of the FLAME facility tests (including grid sensitivity study) should not be surprised by any of the experimental findings. Since FLACS is not constructed or validated only with FLAME facility in mind, the same performance as observed for the FLAME facility simulations should be expected in any real geometry of similar (or even different) scale and congestion level.

6.0 ACKNOWLEDGEMENTS

GexCon is grateful to R&D partners (oil and gas companies, chemical industry, Norwegian Research Council, the European Commission and more) having contributed supporting the development of the FLACS CFD-tool and the generation of explosion knowledge at GexCon. The same accounts for companies and institutions that have purchased or are leasing the FLACS software. Special thanks to Norsk Hydro, Statoil and IHI supporting the recent validation study of FLACS-HYDROGEN. GexCon also appreciates the positive attitude at Sandia National Laboratories giving access to the FLAME facility test data. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

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