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Three-dimensional Simulation of Hydrogen Detonations in the Olkiluoto BWR Reactor Building

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Abstract

This report describes the numerical simulations of hydrogen detonations in Olkiluoto reactor building room B.60.80 using the DET3D code. The code is developed at Forschungszentrum Karlsruhe (FZK) and uses the finite difference method based on three-dimensional Euler equations for a multicomponent reacting gas. DET3D is mainly developed for modelling of gaseous detonations initiated by a direct ignition. DDT phenomena are not treated.

The initial conditions of the detonation simulation were based on previous hydrogen spreading analyses carried out with the FLUENT code. DET3D calculations continued the previous, rough estimates of shock pressure loads performed with a simple DETO code. The DETO analyses were based on the strong ignition theory with oblique and normal reflection relations of the adiabatic shock waves. Shock waves were induced by point-like energy release without modelling of the propagating combustion front. In the DETO modelling, only the first shock reflection was treated. The approach of the DET3D code enables the more detailed assessment of detonation pressure loads in a real 3-D geometry.

The objective of the work was to assess the pressure loads on room structures under detonation conditions.

The initial conditions of detonation simulation were based on the previous hydrogen spreading analyses performed with the FLUENT code. Two sizes of leakage from the containment to the reactor building were considered: 2 mm^2, which corresponds to the nominal leakage of containment, and a large leak of 20 mm^2.

The DET3D simulation indicated that the highest pressure spikes occurred in the room corners due to reflections and superposition of the shock waves. The highest pressure maximum in all simulation cases was about 10.6 MPa. This value was obtained in the upper corner of the room beside the containment wall. The highest pressure impulses to structures during the 150 ms simulation were about 30 - 35 kPa-s.

Key words

severe accident, detonation, hydrogen, reactor building, DET3D, simulation

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THREE-DIMENSIONAL SIMULATION OF HYDROGEN DETONATIONS IN THE OLKILUOTO BWR REACTOR BUILDING

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EXECUTIVE SUMMARY

The containments of the Olkiluoto BWR units are inerted with nitrogen during normal operation, hence hydrogen burning has not been considered a major problem in severe accidents. However, significant release of hydrogen into a relatively small containment can occur in a severe accident. A hydrogen leakage from the containment into the surrounding reactor-building rooms cannot be ruled out. Because the atmosphere in the reactor building is normal air, the ignition and combustion of hydrogen is possible. The safety concern is whether the hydrogen in the reactor building can detonate and jeopardise the containment integrity from outside

Three-dimensional detonation simulation for a selected Olkiluoto reactor building room B.60.80 was carried out with the DET3D code developed at Forschungszentrum Karlsruhe (FZK). The code uses the finite difference method based on three-dimensional Euler equations for a multicomponent reacting gas. DET3D is mainly developed for modelling of gaseous detonations initiated by a direct ignition. DDT phenomena are not treated.
DET3D calculations continued the previous, rough estimates of shock pressure loads performed with a simple 1-D DETO code. The approach of the DET3D code enables the more detailed assessment of detonation pressure loads in a real 3-D geometry taking also into account the multiple shock reflections and superposition of shock waves.

The objective of the work was to assess the pressure loads on room structures under detonation conditions.

The initial conditions of the DET3D simulation were based on previous CFD-analyses carried out with the FLUENT code. Two sizes of leakage from the containment to the reactor building were considered: 2 mm^2 leakage, which corresponds to the nominal leakage of containment, and a large leak of 20 mm^2. Also the influence of ignition location and the numerical method (1. order versus 2. order) of the hydrodynamics solver of DET3D on the detonation loads were studied. The same computational grid was used in all simulation cases, having 778 320 cells with the cell size of 0.117 m.

Prior to actual detonation simulation for the Olkiluoto reactor building, the numerical parameters of DET3D were firstly verified against the theoretical Chapman-Jouguet values in one-dimensional geometry. The initial conditions in the verification calculations were selected to be similar to those used in actual simulation for the Olkiluoto reactor building. The test calculations with DET3D showed very good agreement with the C-J pressure and velocity. General conclusion from the test calculations was that the DET3D results were quantitatively accurate enough over a wide range of hydrogen concentrations to justify the use of the DET3D code for the hydrogen detonation assessment in the Olkiluoto reactor building.

The DET3D simulation for the Olkiluoto reactor building indicated that the highest pressure spikes occurred in the room corners due to reflections and superposition of shock waves. The highest pressure maximum in all simulation cases was about

10.6 MPa. This value was obtained in case of 20 mm^2 leakage in the upper corner of the room beside the containment wall. The highest pressure impulses on structures during the 150 ms simulation were about 30 - 35 kPa-s.
At the end stage of 20 mm^2 leakage, the gas concentration gradient in the reactor building room was very strong in the upper part of the room, and a hydrogen inerted layer existed near the room ceiling. Under these conditions, only a relatively small amount of hydrogen was burned during the first detonation wave. Later propagation of a slow combustion front to the still hydrogen rich upper region was predicted to lead to flame acceleration and a second detonation, now at a different location from the first one. In all other detonation simulation cases, the gas mixture above the level of leakage was initially relatively homogeneous and no hydrogen inerted layer existed in the room. In these cases, practically all hydrogen was burned during the first and single detonation.

DET3D proved to be a highly effective, best-estimate tool for assessment of detonation pressure loads in a real 3-D geometry.

Future work will include transfer of DET3D data to the ABAQUS code for structural analyses.

1 INTRODUCTION

The containments of the Olkiluoto BWR units (Fig. 1) are inerted with nitrogen during normal operation, hence hydrogen burning has not been considered a major problem in severe accidents. The BWR core contains a large amount of zirconium. Significant release of hydrogen into a relatively small containment can occur in a severe accident. Hydrogen leakage from a containment into the surrounding reactor-building rooms cannot be excluded. The atmosphere in the reactor building is normal air, making the ignition and combustion of hydrogen possible. The safety concern is whether the hydrogen in the reactor building can detonate and jeopardise the containment integrity from outside.

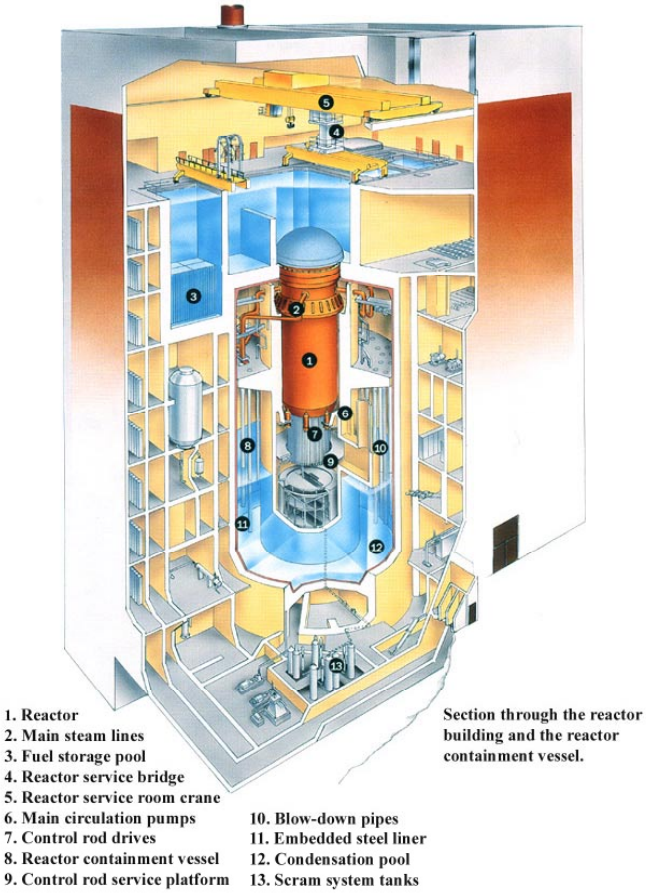


Figure 1. Olkiluoto BWR containment and adjacent reactor building rooms (Manninen et al. 2000)

Recent FLUENT calculations (FLUENT Inc. 1998) for selected reactor building rooms in Olkiluoto 1 and 2 BWR by Manninen and Huhtanen (1999) suggested that hydrogen accumulates up to the ceilings of rooms, leading to rather stable stratification. Very high hydrogen concentration was estimated in the upper parts of the rooms. Further assessment of FLAME acceleration and onset of detonation indicated that the criteria for flame acceleration and DDT were fulfilled in some cases under consideration

(Manninen et al. 1999). Due to simplification and limitations of the modelling, no definite conclusions could be drawn. However, the general conclusion was that the possibility of detonation in the reactor building during a severe accident could not be ruled out.

The purpose of this study is to assess the detonation pressure loads in Olkiluoto 1 and 2 reactor building room B.60.80 using the DET3D code (Breitung & Redlinger, 1994). DET3D is a finite difference code for numerical simulation of chemically reacting multicomponent gas flow in three spatial dimensions. DET3D solves the Euler equations of gas dynamics with additional source terms due to chemical reactions. The code is mainly developed for simulation of gaseous detonations assuming a direct ignition. DDT phenomena are not treated.

DET3D analyses are the extension of earlier detonation studies by a simple 1-D DETO code (Silde & Lindholm, 1999). The DETO analyses were based on the strong ignition theory with oblique and normal reflection relations of adiabatic shock waves. Shock waves were induced by point-like energy release without modelling of the propagating combustion front. Only the first shock reflection from a wall was modelled. The approach of the DET3D code enables the detailed assessment of detonation processes and consequential pressure loads in a real 3-D geometry taking into account the multiple reflections and superposition of shock waves.

The hydrogen leak rates from the containment into the reactor building were based on earlier analyses with the MELCOR code (Sandia National Laboratories, 1994). In these analyses a station blackout sequence with depressurisation of the reactor coolant system was assumed. One hundred percent of the zirconium was conservatively assumed to oxidise, leading to a total hydrogen release of 1900 kg within the containment. Two leakage sizes from the containment to the reactor building were considered: 2 mm^2 and 20 mm^2. The smaller leak corresponds to the nominal leakage of containment. The hydrogen spreading in the reactor building was analysed with the FLUENT code by Manninen and Huhtanen (1999). Three of these cases were selected as initial conditions for the detonation simulations with the DET3D code.

One aim of the DET3D analyses was also to provide input data for structural analyses, which will be carried out with the ABAQUS code (Saarenheimo 2000).

2 DESCRIPTION OF DET3D

2.1 PHYSICAL MODEL

Since gaseous detonations are very fast processes, the usual velocity of a hydrogen-air detonation wave is 1500 *m/s* or more. It is not necessary to include in the physical modelling effects like molecular diffusion, turbulence, radiation or heat conduction. It suffices to solve numerically the Euler equations of compressible gas dynamics for a mixture consisting of N chemically reacting gaseous components. Let ρ^k be the density of the *k*-th gaseous component, with $\rho = \sum_k \rho^k$ denoting total density, *p* total pressure, $u = (u_1, u_2, u_3)$ *the* velocity in 3 spatial dimensions, and $e = 1/2\,u^2 + \varepsilon$ the total specific energy with ε specific internal energy. Then these equations read in Cartesian coordinates x_j as follows ($k = 1, 2, \ldots, N$; lower indices *t* and x_j denote partial differentiation with respect to time and spatial coordinate x_j resp.; summation is over *j* from 1 to 3):

$$\rho_t^k + (\rho^k u_j)_{x_j} = S^k \qquad \text{Conservation of mass} \qquad (1)$$

$$(\rho u_i)_t + (\rho u_i u_j)_{x_j} + p_{x_i} = 0 \qquad \text{Conservation of impulse } (i = 1, 2, 3) \qquad (2)$$

$$(\rho e)_t + \left[(\rho e + p) u_j\right]_{x_j} = 0 \qquad \text{Conservation of energy} \qquad (3)$$

Here, the source term S^k in the mass equation models changes in the component densities due to the chemical reactions. The special form of this term as used in DET3D is described below.

The above conservation equations must be supplemented by an equation of state. In DET3D, each component *k* is assumed to be an ideal gas with temperature-dependent specific heat c_p^k and enthalpy h^k given by

$$h^k(T) = \int^T c_p^k(\tau)\, d\tau + Q_k \qquad (4)$$

with Q_k denoting the heat of formation of component *k* (assumed to be constant in the code). Tabulated values for the c_p^k and h^k can be found e.g. in (JANAF 1985), and the code uses interpolation polynomials to approximate these values. For the enthalpy, the polynomial is of degree 2, whereas for the specific heats interpolation polynomials of degree 9 are used.

The specific internal energy ε is then calculated as

$$\varepsilon = h - p/\rho \qquad \text{with} \quad h = \sum \frac{\rho^k}{\rho} h^k . \tag{5}$$

In DET3D, the source terms S^k are sums of simple chemical reactions of the form

$$\sum_{k=1}^{N} v_{jk} n_k = 0 \qquad \text{with rate } f_j \tag{6}$$

with n_k the molar concentration of species k and the v_{jk} denotes the stoichiometric coefficients of reaction j. The reaction rate is modelled by an Arrhenius law of the form (omitting the index j)

$$f \equiv \begin{cases} BT^n \exp(-E_{act}/RT) & \text{for} \quad T > T_{crit} \\ 0 & \text{else} \end{cases} \tag{7}$$

where B, n, E_{act} and T_{crit} are input variables. (R is the universal gas constant). Both the number of the gaseous components and the number of chemical reactions can be freely chosen by the user.

2.2 NUMERICAL SOLVER

Assuming

$$W = (\rho^1, \ldots, \rho^N, \rho u_1, \rho u_2, \rho u_3, \rho\varepsilon), \tag{8}$$

the above Euler equations can be written concisely as

$$W_t + \left[F_j(W)\right]_{x_j} = S(W) \tag{9}$$

This hyperbolic system is solved numerically by DET3D on a uniform Cartesian mesh using operator splitting and an explicit method. The solution algorithm can be sketched as follows:

- Starting value W^n (discretized, time t^n)
- Determine time step using CFL condition

$$\Delta t = \sigma \cdot \frac{\Delta x}{\max(c + |u_j|)}, \qquad \sigma < 1 \tag{10}$$

- Solve $W_t + (F_1)_{x_1} = 0_{|W^n} \rightarrow W_{(1)}$ (11)

- Solve $W_t + (F_2)_{x_2} = 0_{|W_{(1)}} \rightarrow W_{(2)}$ (12)

- Solve $W_t + (F_3)_{x_3} = 0_{|W_{(2)}} \rightarrow W_{(3)}$ (13)

- Solve $W_t = S_{|W_{(3)}} \rightarrow W^{n+1}$ (14)

- Repeat (with t^{n+1} instead of t^n).

To implement this solution approach, one needs to choose numerical solvers for the chemistry and the hydrodynamics. In DET3D, for the chemistry the simple Euler-Cauchy method is used with possible subcyling of the time step. (Note that the time step Δt is determined solely by the hydrodynamics.) As for the hydrodynamics solver, DET3D uses one of the modern shock capturing schemes, namely the method of Harten, Lax and van Leer (Harten et al. 1983, LeVeque 1990, Van Leer 1979).

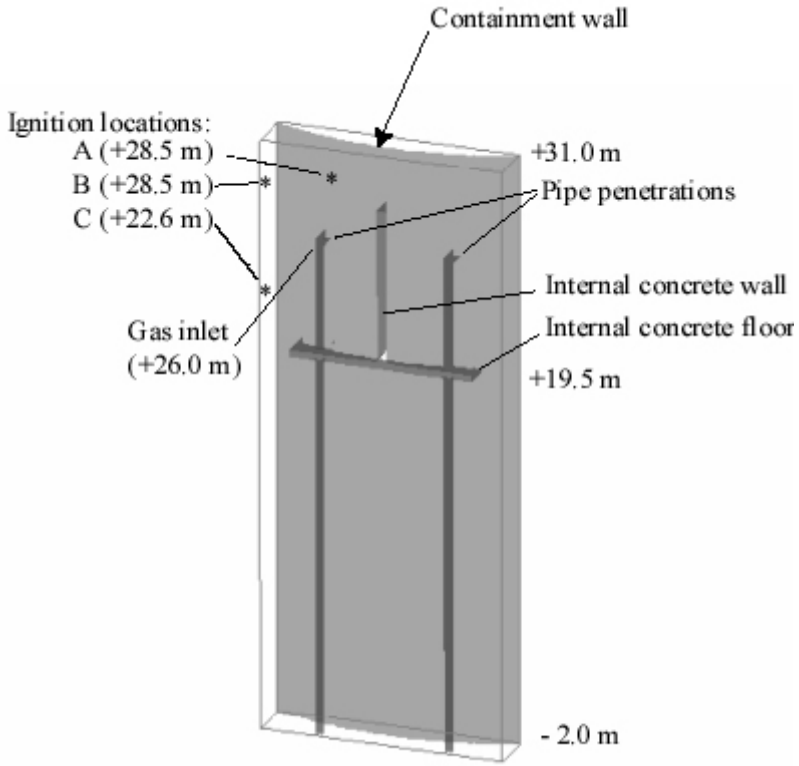
Thus when doing calculations with DET3D, the user is able to choose between a first and a second version of the HLL method. The second order one has the advantage of giving steeper shock fronts and a more detailed resolution of the reflections and interactions of the shock waves. On the other hand, compared to the first order scheme the calculation time rises significantly while these more detailed effects are usually not so important in large scale applications. It thus depends on the wishes and objectives of the user to decide which method he will employ.

3 SIMULATION MODEL

3.1 GEOMETRY OF ROOM B.60.80

The geometry of room B.60.80 in the Olkiluoto reactor building is illustrated in Fig. 2. The height of the room is 33 m (from level – 2.0 m to level + 31.0 m) and the width 13.4 m, making the room very narrow. The shortest distance between the containment wall and opposite concrete wall is only 1.4 m (Fig. 3). Free volume of the room is 897 m^3. An internal concrete floor at level +19.5 m divides the room into two vertical parts, but two flow paths exist on both sides of the floor, enabling the gas flow between the upper and lower parts of the room (Fig. 3, middle). An internal concrete wall is located from level +19.5 m to level +28.0 m separating the upper part of the room into two adjacent spaces.

Figure 2. Basic geometry of room B.60.80.



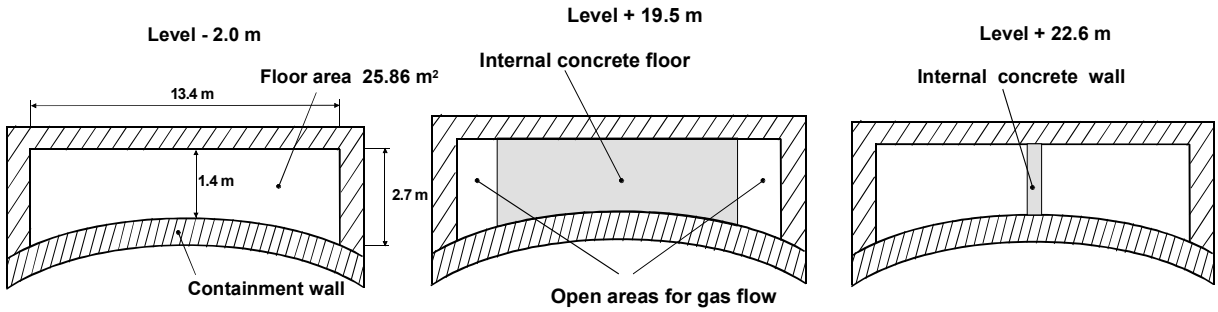


Figure 3. Cross-sectional pictures of room B.60.80 at three different elevations.

The computational model consisted of a uniform cartesian grid with 778 320 cells. The cell size was 0.117 m. The same grid was used in all simulation cases.

The concrete walls, floor and ceiling of the room were modelled as rigid boundary structures. The obstacles in the room were neglected. This is justified by the fact that the upper part of the room, where the hydrogen existed, is relatively open space. The influence of few obstacles in very fast detonation processes was therefore assumed to be insignificant.

Two pipelines and their penetrations in the containment were included in the model to generate data for future structural analyses. The pipes leave horizontally from the containment wall at level + 26.0 m, make a 90 degrees turn, and continue vertically to the bottom of the room (see Fig. 2). The pipes were modelled as rectangular shapes. A relatively small room, B4.43, connected to the room B.60.80 was not modelled in the simulation.

3.2 INITIAL CONDITIONS

The initial gas concentrations for the detonation simulations were based on the earlier CFD analyses carried out with the FLUENT code (Manninen et. al., 1999). Three gas compositions were selected as initial conditions for the detonation simulations. The FLUENT data could not be utilised directly as the grids used by the FLUENT and the DET3D models are different. Therefore curve fittings for the gas concentrations as a function of room height were first made from the FLUENT results. These fittings were then used in defining the initial gas concentrations on each room level for DET3D. In the DET3D model, the horizontal gas distribution on each level of the room was initially assumed to be homogeneous. Initial room pressure and temperature in the detonation simulation were supposed to be constant, corresponding to the average value in the detonable gas cloud according to FLUENT results.

All doors in room B.60-80 were supposed to be closed. The critical temperature for the solution of chemical reaction rate (T_{crit} in Eq. 7) was assumed to be 1000 K. Other input variables for the Arrhenius equation were: B = 10 000, n = 1.0, and E_{act} = 73 kJ/mole. The detonation was initiated by a direct ignition introducing a high pressure (6 MPa) and temperature (4000 K) into a relatively small space (≈1x1x1 m) in the desired

location in the computational grid. The duration of the simulation was 150 milliseconds.

The initial conditions of all simulation cases are summarised in Table 1. Two sizes of leakage were considered: 2 mm^2 and 20 mm^2. The ignition location and the numerical method for the hydrodynamics solver of DET3D were also varied in the simulations.

Table 1. Initial conditions in detonation analyses.

Case	H_2 mass [kg]	Start time *) [s]	Leak size [mm^2]	Pres. [MPa]	Temp. [K]	Density [kg/m^3] **)	HLL method	Ignition location	X_{AIR} [%] **)	X_{H2} [%] **)
1	1.428	13000	20	0.1274	307.7	1.4 / 0.4	1. order	+ 22.7 m, on narrow wall	98. / 18.	2. / 81.
2	3.15	7500	20	0.1052	302.5	1.2 / 0.8	1. order	+ 28.5 m, on narrow wall	100. / 66.	0. / 34.
3	3.15	7500	20	0.1052	302.5	1.2 / 0.8	1. order	+ 28.5 m, on wide wall	100. / 66.	0. / 34.
4	3.15	7500	20	0.1052	302.5	1.2 / 0.8	2. order	+ 28.5 , on narrow wall	100. / 66.	0. / 34.
5	1.4	12500	2	0.1035	300.4	1.2 / 1.0	1. order	+ 28.5 m, on narrow wall	100. / 82.	0. / 18.

*) Calculated from start of hydrogen leakage to reactor building
**) At level +19.5 m / + 31.0 m.

Case 1:

Case 1 corresponded to the end state of the FLUENT simulation of 20 mm^2 leakage (13 000 s from the start of accident). At that time, a very strong concentration gradient existed in the upper part of the room (Fig. 4). The mole fraction of hydrogen close to the ceiling was very high, about 80% (Fig. 5), and the mole fraction of oxygen at the same location was below 2%. The gas space near the ceiling was hydrogen inerted. The ignition of detonation was assumed to occur on level + 22.6 m where nearly stoichiometric conditions existed (31.9% H_2, 13.1% O_2). The ignition started in the middle of the narrow end wall of the room (Fig. 2, ignition location C).

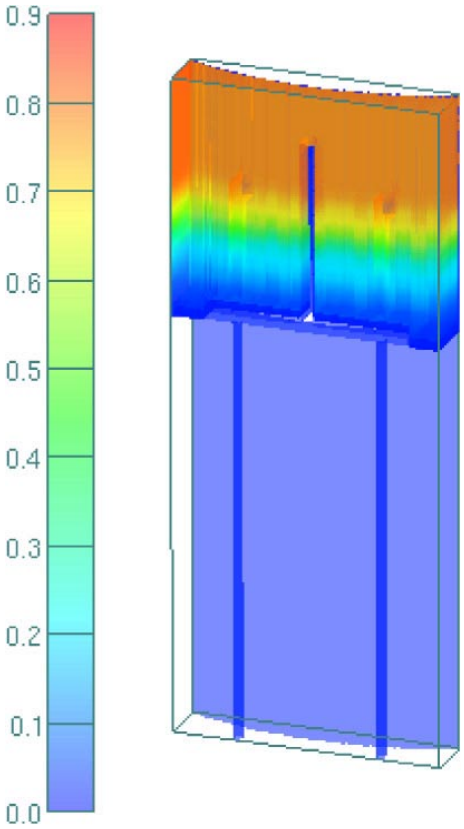


Figure 4. Initial mole fraction profile of hydrogen in Case 1.

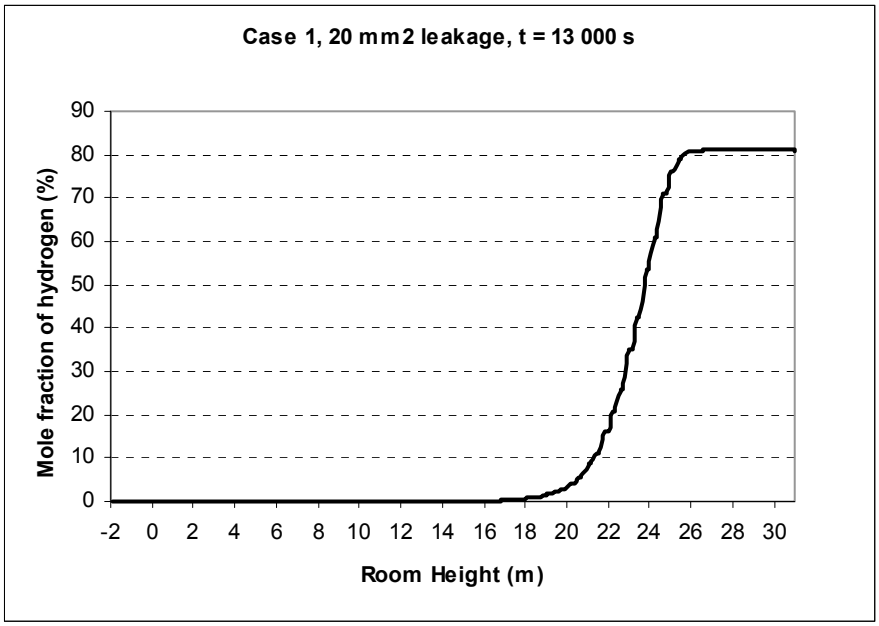


Figure 5. Vertical profile of the mole fraction of hydrogen in room B.60.80, Case 1.

Case 2:

Case 2 corresponded to the earlier instant of time of the 20 mm^2 leakage (t = 7500 s) when the gas concentrations above level + 28 m were roughly stoichiometric (Fig. 6). The maximum mole fraction of hydrogen near the ceiling was about 35%. The detonation was ignited on level + 28.5 m, where there is a fluorescent lamp (Fig. 2, ignition location B). The ignition occurred in the middle of the end wall as in Case 1.

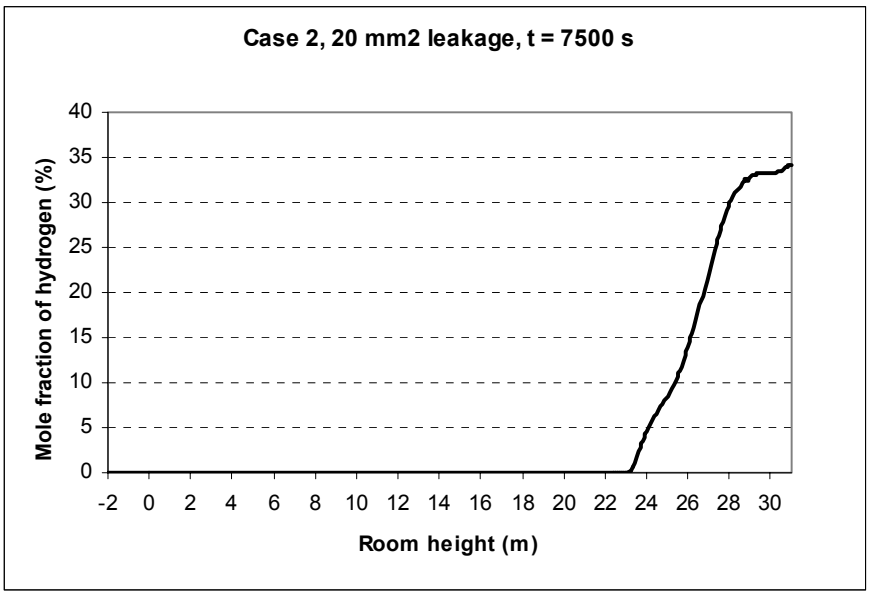


Figure 6. Vertical profile of the mole fraction of hydrogen in room B.60.80, Case 2.

Case 3:

Case 3 was similar to Case 2, except that the location of ignition was on the wide concrete wall on the opposite side of the containment wall (Fig. 2, ignition location A). The ignition occurred on level +28.5 m as in Case 2.

Case 4:

In all other simulation cases, a first-order version of HLL method for the hydrodynamics solver of DET3D was used, but in Case 4 the more accurate second-order HLL method was used. The second order method gives steeper shock fronts and a more detailed resolution of the reflections and interactions of the shock waves (see chapter 2).

Case 5:

Case 5 corresponded to the 2 mm^2 leakage (t = 12 500 s) where the mole fractions of hydrogen and oxygen were both roughly 17 - 18% above the level of the leakage (Fig. 7). The location of ignition (level +28.5 m) was as in Case 2.

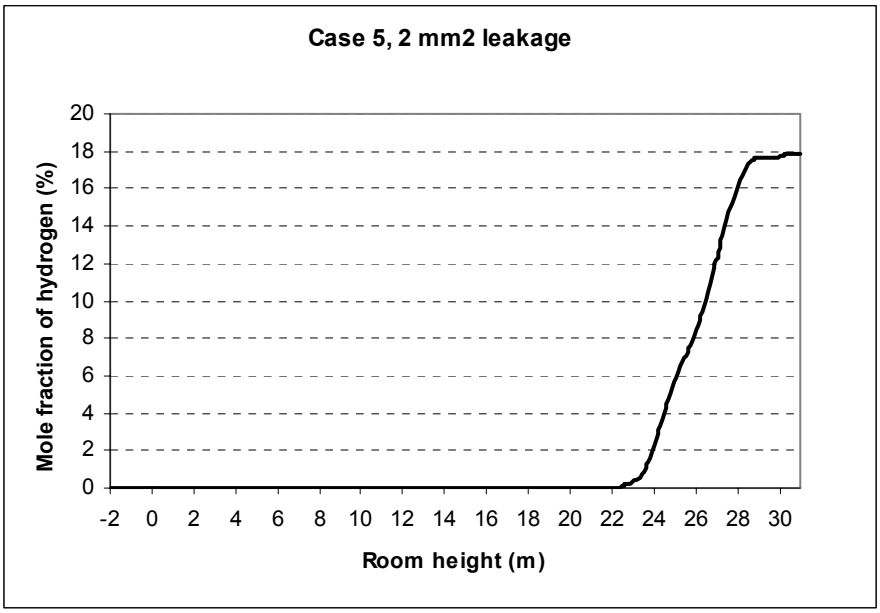


Figure 7. Vertical profile of the mole fraction of hydrogen in room B.60.80, 2 mm^2 leakage, Case 5.

3.3 VERIFICATION OF NUMERICAL PARAMETERS

As is well known, the numerical solution of hyperbolic differential systems can produce non-physical solutions. Thus in the case of DET3D so called weak detonation waves could appear (see Berkenbosch et. el., 1998). Computational results of DET3D also depend on the proper choice of some essential input parameters. Verification of the numerical input parameters is therefore necessary and always recommended before actual simulation. A simple way to do this is to compare the calculational results with the theoretical values (e.g. to Chapman-Jouguet) in one-dimensional geometry.

In this work, the verification calculations were carried out in an arbitrary defined geometry: a 130 m long and 0.12 m width rectangular channel. The ignition was assumed to occur at one (closed) end of the pipe. The cell size of the grid and the initial gas pressure and temperature were selected to be similar to those used in actual simulations for the Olkiluoto reactor building. The test calculations were carried out with four different initial gas compositions. These compositions corresponded to the existing conditions on the ignition level of the simulation model for the Olkiluoto reactor building. In addition, one test calculation was performed in a very rich hydrogen

mixture (about 50% H_2). The detonation was initiated by introducing a high pressure (6 MPa) and temperature (4000 K) into a 1.0 m long region at the end of the channel.

Comparison of the test calculation and the theoretical Chapman-Jouguet (C-J) values is illustrated in Table 2. Simulated detonation pressure and the velocity are denoted by p_s and v_s , respectively. Theoretical C-J pressure and velocity are detonated by p_{C-J} and v_{C-J} , respectively. Initial pressure and temperature are expressed as p_i *and* T_i, respectively.

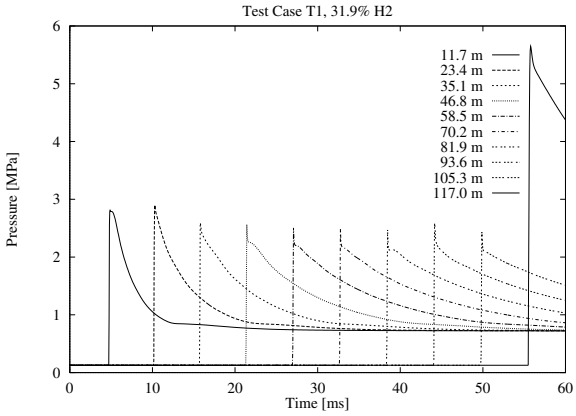
Table 2. Comparison of simulated and theoretical detonation values.

CASE	**INITIAL CONDITIONS**					**RESULTS**			
	H_2 [%]	**O_2** [%]	**N_2** [%]	**p_i** [MPa]	**T_i** [K]	**p_s** [MPa]	**v_s** [m/s]	**p_{C-J}** [MPa]	**v_{C-J}** [m/s]
T1	31.9	13.1	55.0	0.127	307.7	2.1	2060	1.92	1995
T2	31.4	12.9	55.7	0.105	302.5	1.8	2045	1.60	1980
T3	17.5	16.7	65.8	0.104	300.4	1.4	1650	1.23	1617
T4	49.8	8.9	41.3	0.127	307.7	1.7	2090	1.54	2078
T5[*)]	31.4	12.9	55.7	0.105	302.5	1.7	2055	1.60	1980

[*)] Second-order method.

The calculated pressure histories at different distances from the ignition location in each test case are shown in Figs. 8 ... 10. The calculated C-J velocity (v_s) and pressures (p_s) were estimated according to these figures using the following method:

The arrival of a detonation front at each location is detected as a sudden pressure jump. Simulated detonation velocity was evaluated by dividing the distance between two selected locations in the channel with the time interval of the pressure spikes. Note that the last and relatively high pressure spike in some plots was caused by the reflection pressure from the closed end of the channel, but was not considered important in this context. The calculated, steep pressure spike in Figs. 8 ... 10 may be arbitrarily higher than the C-J value, laying somewhere between the C-J value and the Neumann spike. Therefore the value at the pressure decrease-expansion point is the better approximation than the maximum pressure spike for the calculated C-J value (Fig. 11). This point was approximated from the calculational results in Figs. 8 ... 10 and is denoted by value p_s in Table 2.



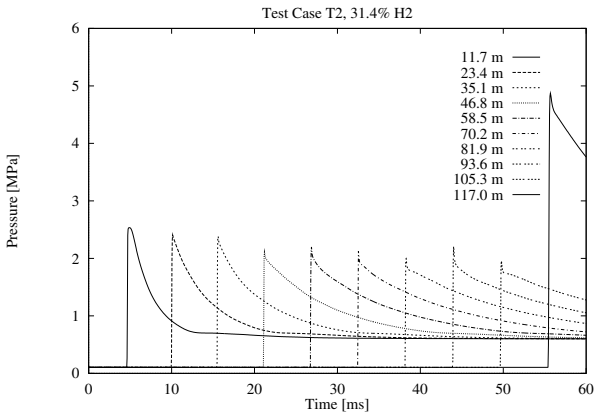
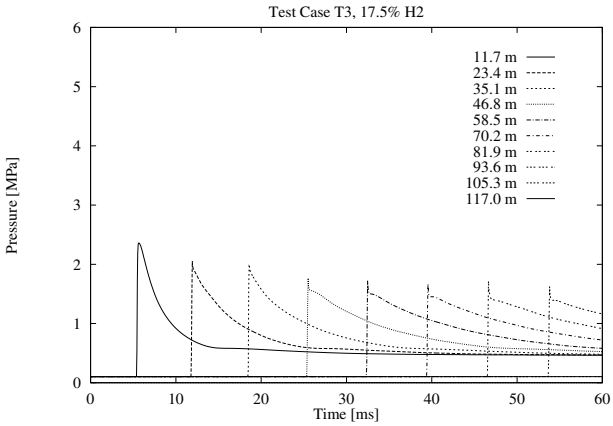


Figure 8. Simulated pressures in test calculations T1 and T2.



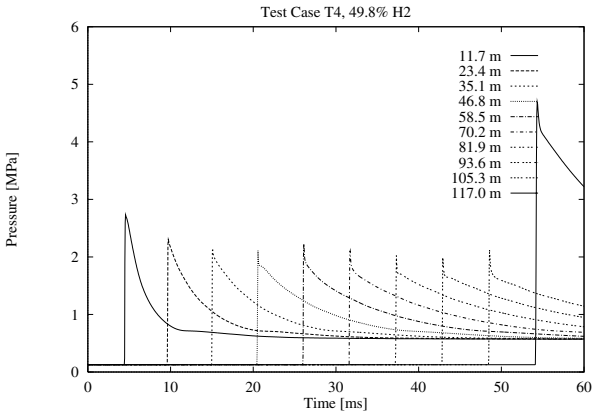


Figure 9. Simulated pressures in test calculations T3 and T4.

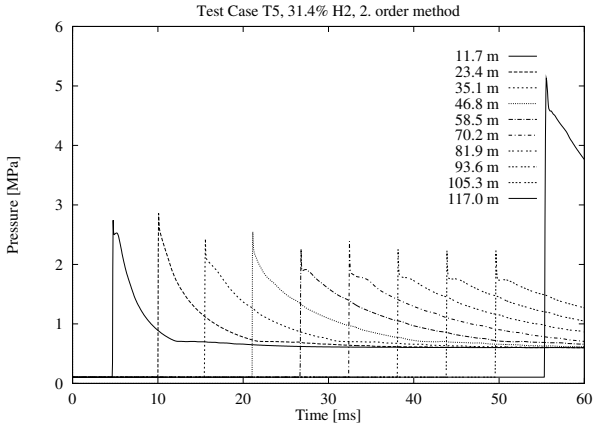


Figure 10. Simulated pressures in test calculation T5.

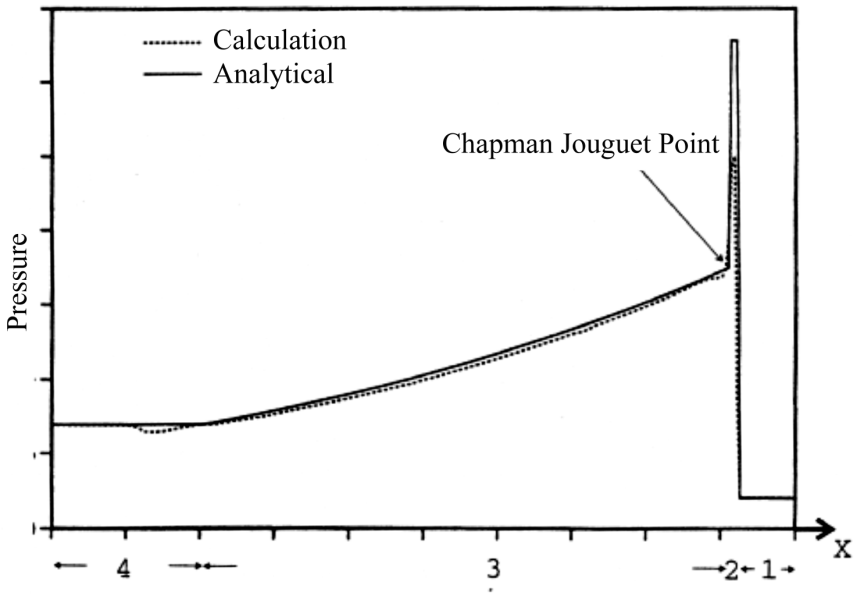


Figure 11. Illustration of C-J points in simulated and analytical detonation pressure curves (Redlinger 2000).

The test calculation with DET3D showed very good agreement with the C-J pressure and velocity. Simulated detonation pressures were maximally about 15% higher and the flame speed about 3% higher than the theoretical values. The simulated results were on the conservative side in each test case. General conclusion from the test calculations was that the DET3D results were accurate enough over a wide range of hydrogen concentrations to justify the use of the DET3D code for the hydrogen detonation assessment in the Olkiluoto reactor building.

General information about the validation work of the DET3D code has been described by Breitung and Redlinger (1994).

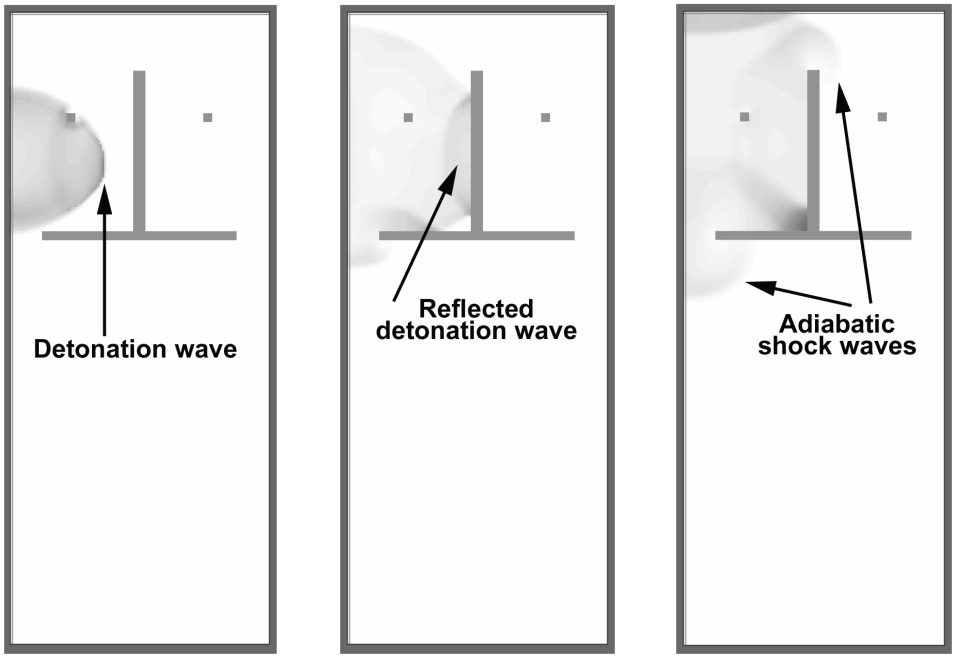
4 RESULTS

4.1 CASE 1

Case 1 was characterised by a strong concentration gradient of hydrogen in the upper part of the containment (see Fig. 5). A relatively thin, roughly 3.5 m high gas cloud from level + 21.5 m to + 25.0 m was assumed to be detonable (Manninen et al. 1999). The cloud was divided into two separate sections in the upper part of the room isolated by the internal concrete wall. An open area of about 4 m^2 for gas flow between these sections exists above the wall near the room ceiling. At that location the gas space was initially inerted by excess hydrogen (≈ 80% H_2). The ignition was assumed to occur in the upper part of the room at level + 22.6 m where the gas composition was nearly stoichiometric (see Fig 2, ignition location C). The detonation was initiated on surface of the narrow end wall. Structure surfaces promote the flow-structure interaction increasing the probability of generation of detonation wave.

Contours of pressure at selected instants of time are illustrated in Appendix A. Initially spherically expanding detonation was observed just after the ignition (Fig.12). Due to very high vertical concentration gradient of hydrogen, the horizontal velocity of the detonation wave was higher than the vertical, resulting in a flattened form of the wave (Fig. 12, left). The pressure in the horizontally propagating detonation wave (≈ 1.65 – 1.8 MPa) and the wave speed (≈ 1900 m/s) were close to the C-J values.

Figure 12. Illustration of pressure waves in room B.60.80 during the first detonation at three different instants of time: 2.0 ms (left), 4.0 ms (middle), and 6.0 ms (right), Case 1.



The strong detonation front could not propagate to the hydrogen inerted region above level + 24 m or to the lean hydrogen mixture below level + 21.5 m. However, the adiabatic shock waves expanded both to very rich and lean hydrogen mixtures. The detonation wave impacted against the internal concrete wall at t ≈ 2.5 ms (Fig. 12, middle). The decaying shock waves reached the concrete floor almost simultaneously at level +19.5 m, and the ceiling of the room a few milliseconds later. The detonation wave was wholly decayed roughly 5 ms after ignition. The detonation phase was followed by a weak combustion mode in the upper part of the room. The detonation induced shock waves propagated throughout the room reflecting of the structures in different parts of the room. Roughly 40 ms after ignition the shock waves reached the bottom of the room.

Combustion of hydrogen during the first detonation was very incomplete in the upper part of the room due to a very strong gas gradient and hydrogen inerted gas layer near the ceiling. The detonation was, therefore, restricted to one side of the upper part of the room (Fig. 12, right). The internal wall and the hydrogen inerted gas layer at the top of the room prevented the detonation from propagating to another side of the room. After the first detonation ceased to exist, the mole fraction of hydrogen near the ceiling was still about 80% and the mixture on the right-hand upper part of the room remained detonable (Figs. 13).

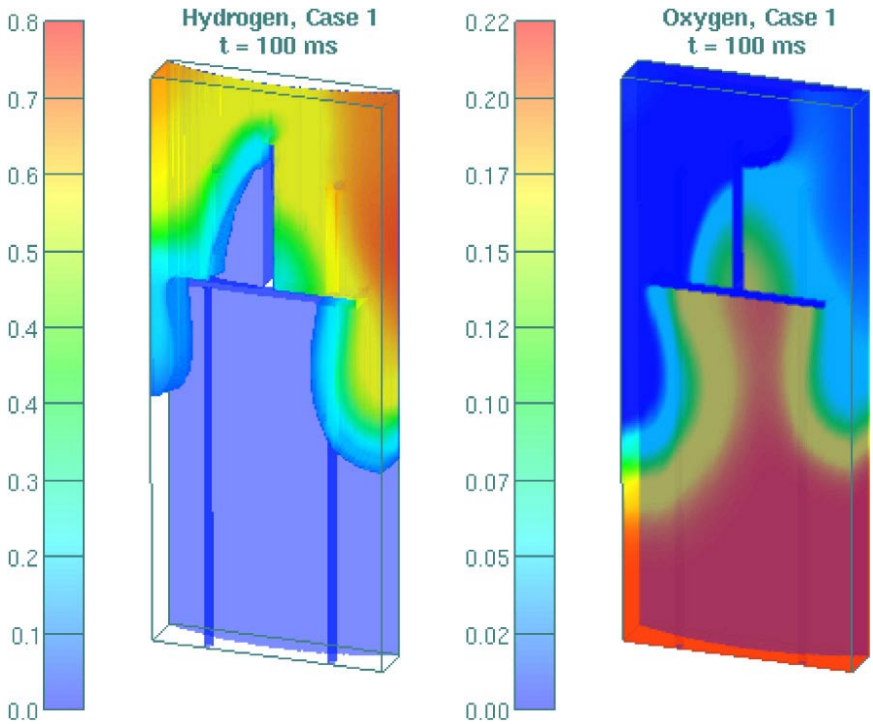


Figure 13. Mole fraction of hydrogen (left) and oxygen (right) at t = 100 ms, Case 1.

The topmost layer of hydrogen in the room mixed gradually with oxygen. Later on, according to the simulation, a slow combustion front propagated to the still hydrogen rich upper region on the other side of the room. The flame started to accelerate downwards, now on the right-hand side of the room (Fig. 14, left). The flame acceleration and impact of the flame front on the concrete floor at level +19.5 m led to formation of a new detonation wave (Fig 14, middle). The detonation expanded towards the opening in the concrete floor (level +19.5 m) and propagated also into the region below it (Fig 14, right).

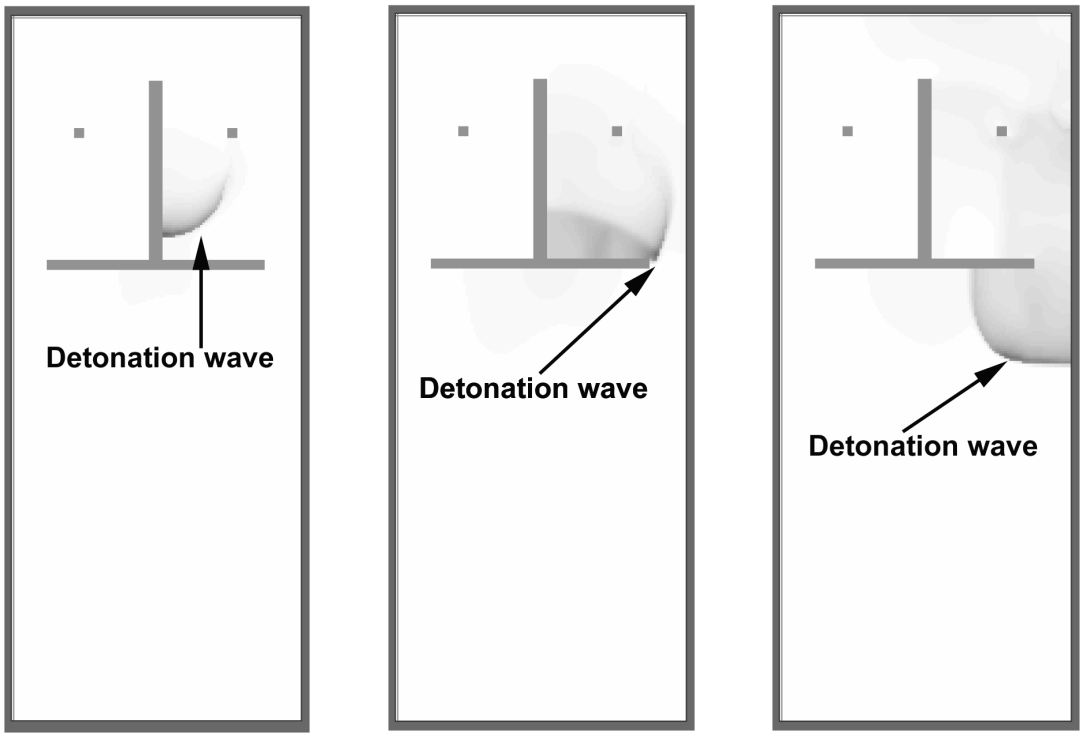


Figure 14. Illustration of pressure waves during the second detonation in Case 1 at three different instants of time: 112.0 ms (left), 114.0 ms (middle), and 117.0 ms (right).

The maximum pressure in each part of the room during the 150 ms simulation is illustrated in Fig. 15. Note that the maximum pressure titled in Fig. 15 and indicated in dark red is intentionally higher than the maximum value in the legend. The DET3D simulation indicates that the highest pressure spike of about 5.5 MPa occurs in the corner of the room near the ignition site of the first detonation (Fig. 16). The pressure of the incident detonation wave just before the reflections is about 1.65 MPa.

Figure 16 illustrates a typical pressure history near structure surface. The pressure history is characterised by a high and short (order of a few milliseconds) peak type pressure transient caused by the shock reflection of the detonation wave. In the corners, the spike is affected by the superposition of the shock waves. The first pressure spike is followed by a relatively slowly decreasing pressure. The pressure fluctuations after the first spike are caused by the later interaction of shock waves and their reflections from the room structures and walls.

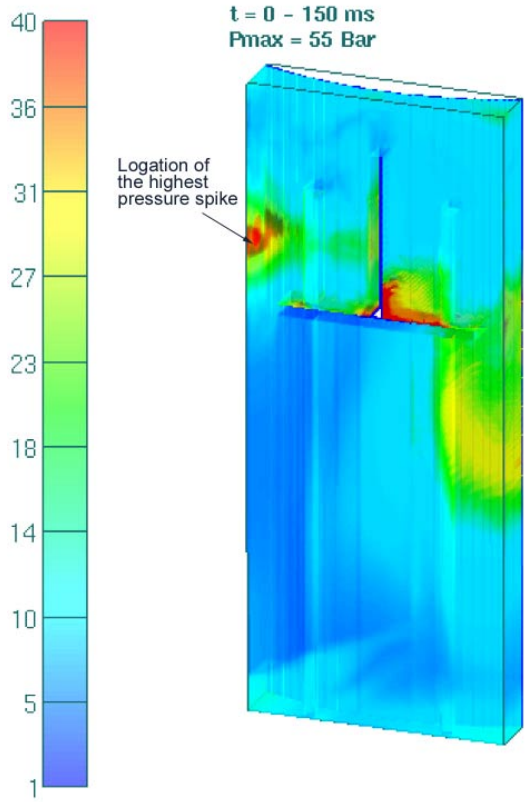


Figure 15. Contours of pressure maximum (Bar) in each part of room B.60.80 during the 150 ms simulation. Case 1.

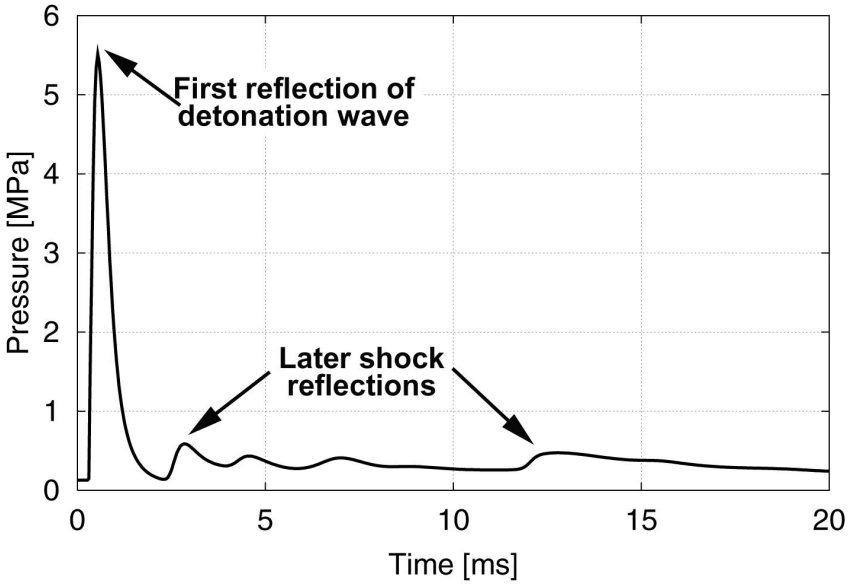


Figure 16. Pressure in the corner of room B.60.80 close to the ignition site. Case 1.

The pressures near structure surfaces on three different selected locations in the room are illustrated in Fig. 17. Corresponding pressure impulses are shown in Fig. 18. The maximum pressure (5.5 MPa) near the ignition is reached very soon (t ≈ 0.5) after the ignition of the first detonation. The maximum pressure of about 1.5 - 2.0 MPa at the floor level and near the ceiling of the room occurred relatively late at t ≈ 120 – 140 ms caused by the second detonation. The highest pressure impulses to the wall structures during the 150 ms simulation are about 20 - 25 kPa-s.

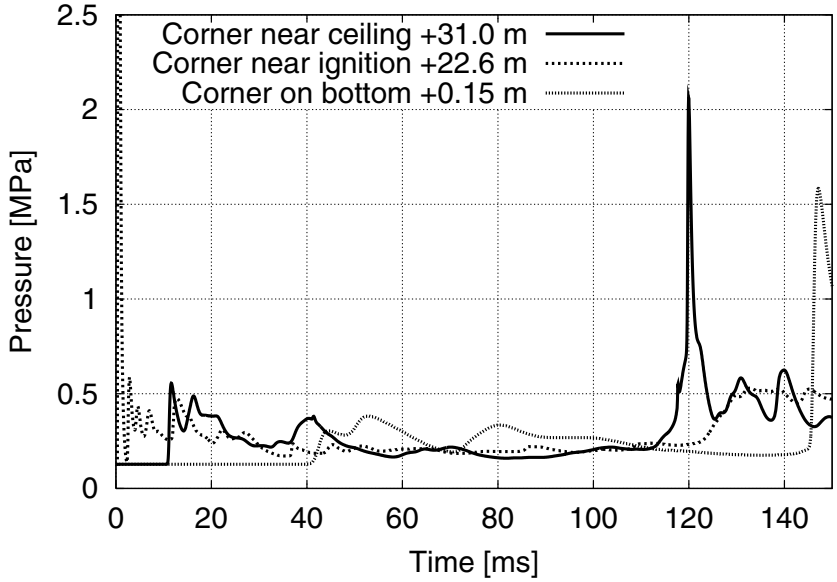


Figure 17. Simulated pressures at three different elevations, Case 1 (first spike at level +22.6 m is shown more detailed in Fig. 16).

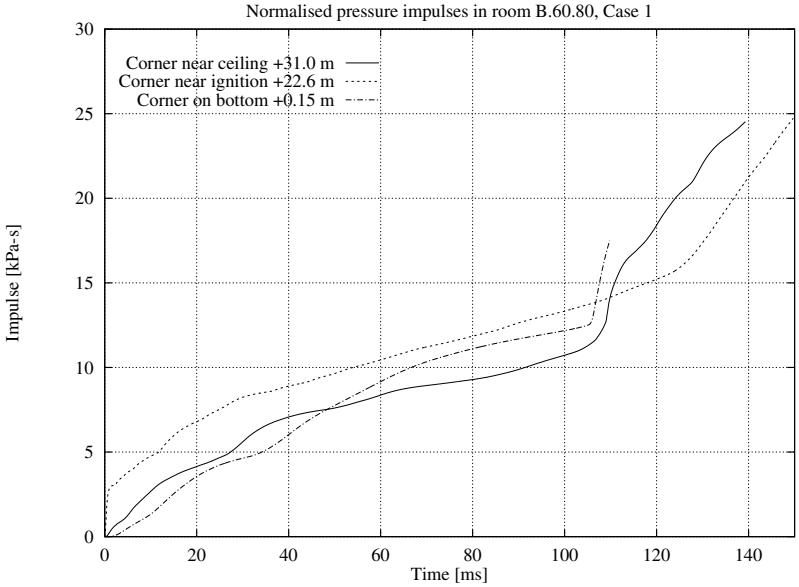


Figure 18. Normalised pressure impulses at three different elevations during the 150 ms simulation, Case 1.

The pressure loads at four different points around the pipe penetrations in the containment wall at level + 26.0 m are shown in Figs. 19 and 20. Corresponding

pressure impulses are shown in Figs. 21 and 22. The highest pressure loads are observed in the penetration, which is closest to the ignition site of the first detonation (Figs. 19 and 21).

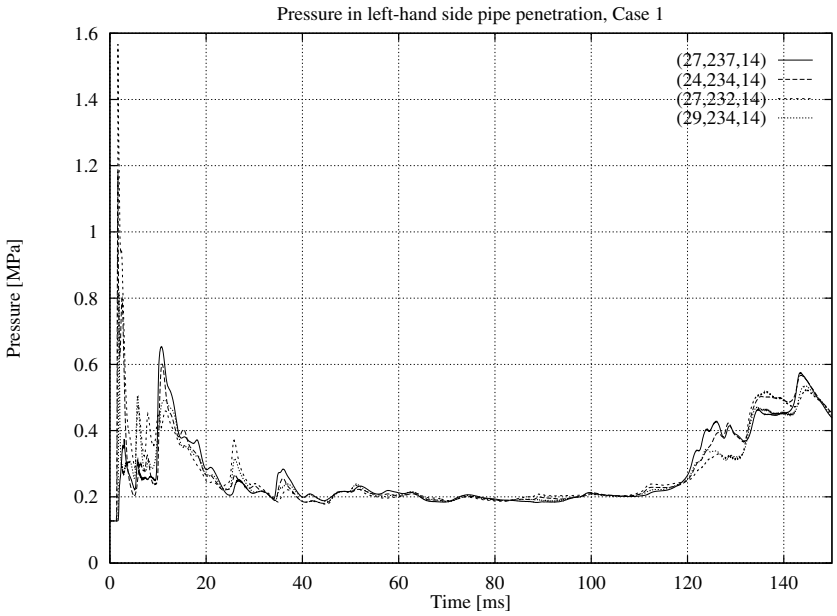


Figure 19. Simulated pressures at four points around the pipe penetration near the first ignition, Case 1.

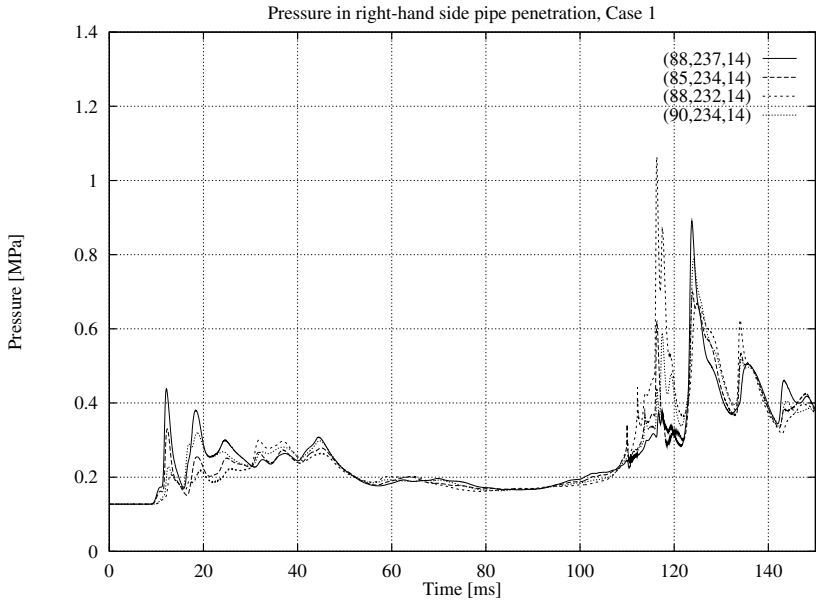


Figure 20. Simulated pressures at four points around the pipe penetration farther from the first ignition, Case 1.

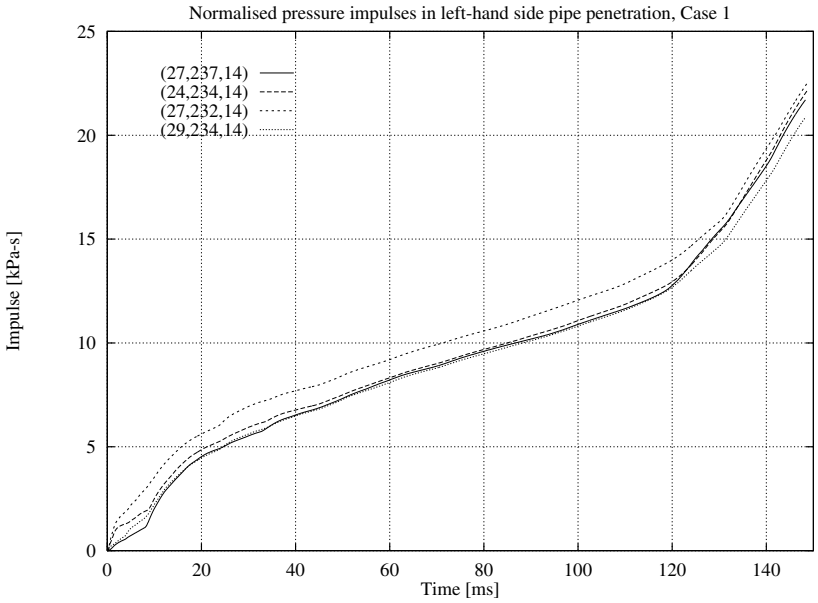


Figure 21. Normalised pressure impulses at four points around the pipe penetration near the first ignition, Case 1.

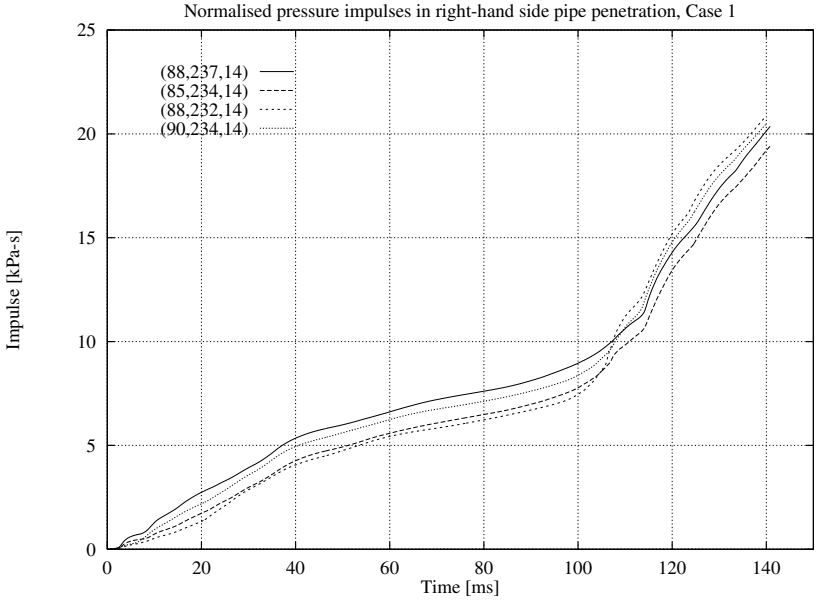


Figure 22. Normalised pressure impulses at four points around the pipe penetration farther from the first ignition, Case 1.

After the 150 ms simulation, a lot of unburned hydrogen still existed in the upper part of the room. Mole fraction of hydrogen near the ceiling was still nearly 60% (Fig. 23). However, by that time there was no longer oxygen in the hydrogen area.

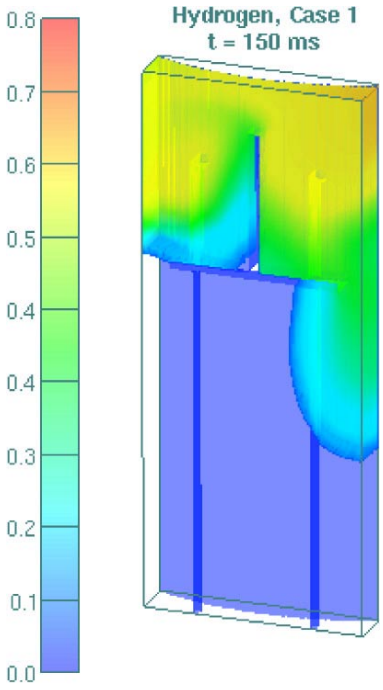


Figure 23. Mole fraction of hydrogen at t = 150 ms in Case 1.

4.2 CASE 2

The gas mixture above level + 26 m in Case 2 was supposed to be detonable. The mole fraction of hydrogen above level + 28 m is about 30 - 34%. At the same location the mole fraction of oxygen was about 12 - 13%.

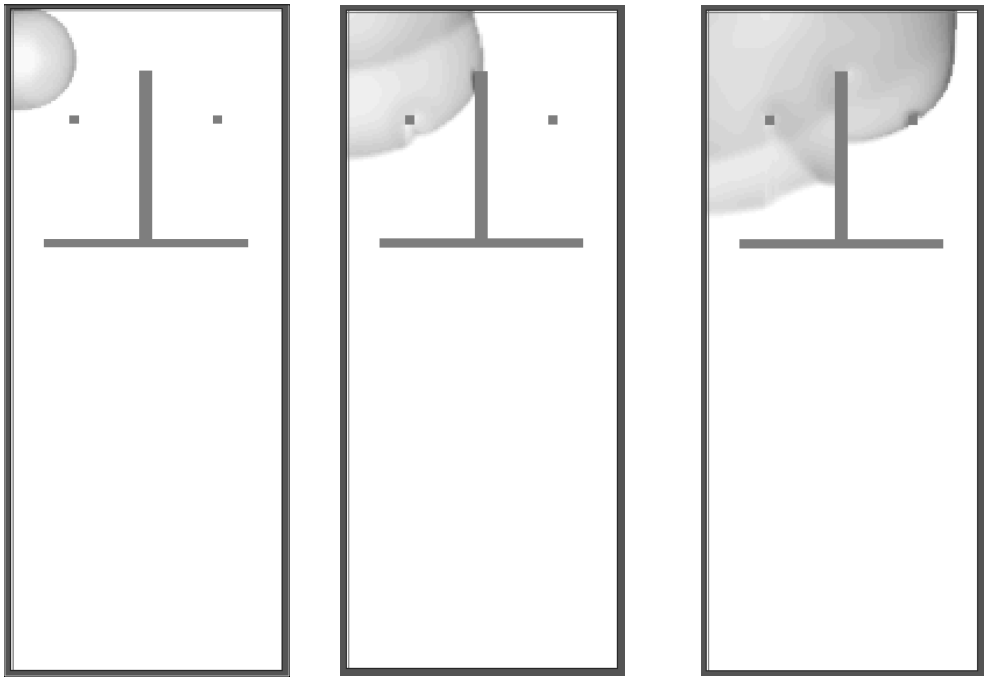
The ignition of detonation was assumed to occur at level + 28.5 m on surface of the narrow end wall, where there is a fluorescent lamp (Fig. 2, ignition location B). The mole fractions of hydrogen and oxygen at the ignition level were 31.4% and 12.8%, respectively.

Contours of pressure at selected instants of time are illustrated in Appendix B. A spherically expanding detonation wave is observed just after ignition (Fig 24, left). The detonation wave could not propagate below the level around + 26 m, where a lean hydrogen mixture existed (< 15% H_2). However, detonation-induced shock waves propagated throughout the room reflecting from the structures. The pressure of the incident detonation wave (1.5 – 1.65 MPa) and the wave speed (≈ 1900 m/s) agree well with the theoretical C-J values. The detonation wave reached the room ceiling at t ≈ 1 ms and the internal concrete wall t ≈ 3 ms (Fig. 24, middle). The wave propagated further through the open area above the wall at the other side of the room (Fig. 24, right).

Roughly 12 ms after ignition the shock waves had proceeded throughout the upper part of the room (above level + 19.5 m). By that time, all hydrogen had burned off below level + 26 m and the mole fraction of hydrogen near the ceiling was roughly 10%. At t ≈

45 ms the shock waves reached the bottom of the room. After the 150 ms simulation no hydrogen existed below level + 27.5 m and the mole fraction of hydrogen near ceiling was roughly 2 – 4% (Fig. 25).

Figure 24. Illustration of pressure waves during detonation in Case 2 at three different instants of time: 1.0 ms (left), 3.0 ms (middle), and 6.0 ms (right).



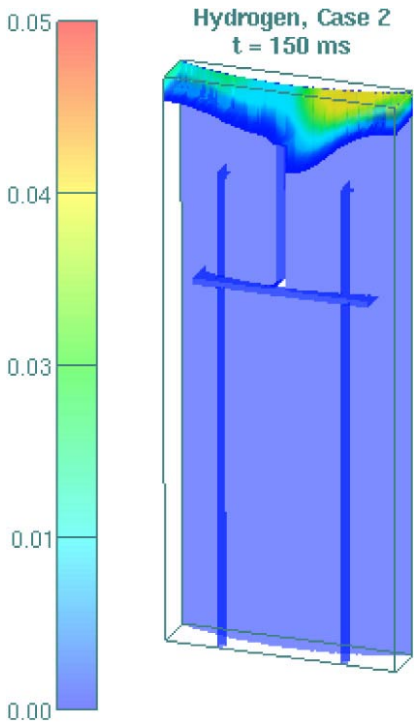


Figure 25. Mole fraction of hydrogen at t = 150 ms in Case 2.

The maximum pressure in each cell of the computational domain during the 150 ms simulation is illustrated in Fig. 26. A maximum pressure spike of about 7.0 MPa was observed in the upper corner of the room beside the containment wall. The pressure histories in this corner and at 0.7 m from the corner are illustrated in Fig. 27. The pressure before and after the reflection at 0.7 m from the corner is about 1.7 MPa. The reflection pressure in the corner was about 7 MPa affected by superposition of the shock waves.

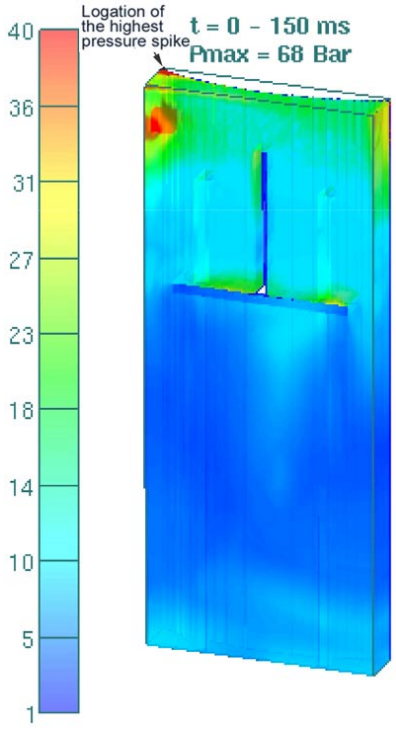


Figure 26. Contours of pressure maximum (Bar) in each part of room B.60.80 during the 150 ms simulation. Case 2.

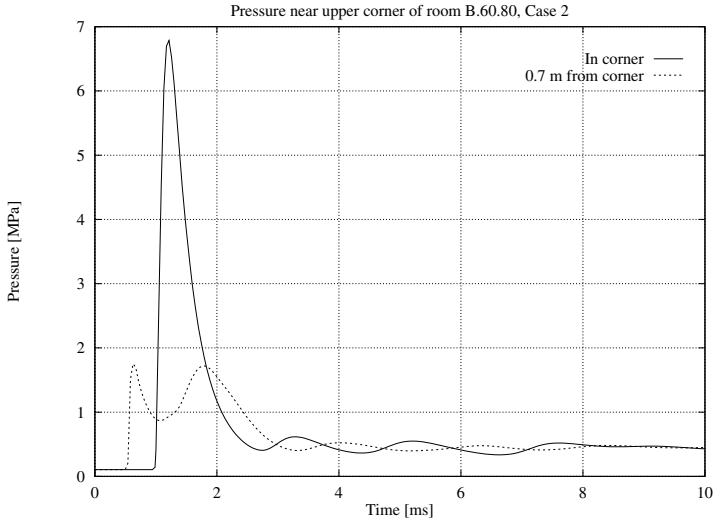


Figure 27. Pressure near the upper corner of room B.60.80. Case 2.

A relative high pressure maximum (≈ 5.5 MPa) was also observed in the corner near the ignition site at level + 28.5 m (Fig. 28). The pressure maximum at the bottom of the room was only about 0.8 MPa caused by the later reflection of decaying shock waves. The highest pressure impulses on wall structures during the 150 ms simulation were about 30 - 35 kPa-s (Fig. 29).

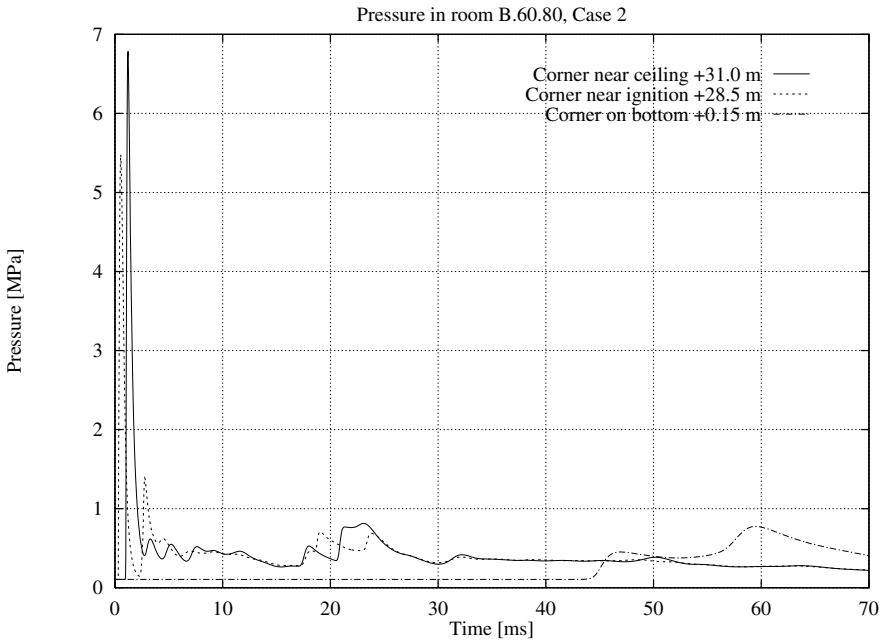


Figure 28. Simulated pressures near structure surfaces at three different elevations in room B.60.80. Case 2.

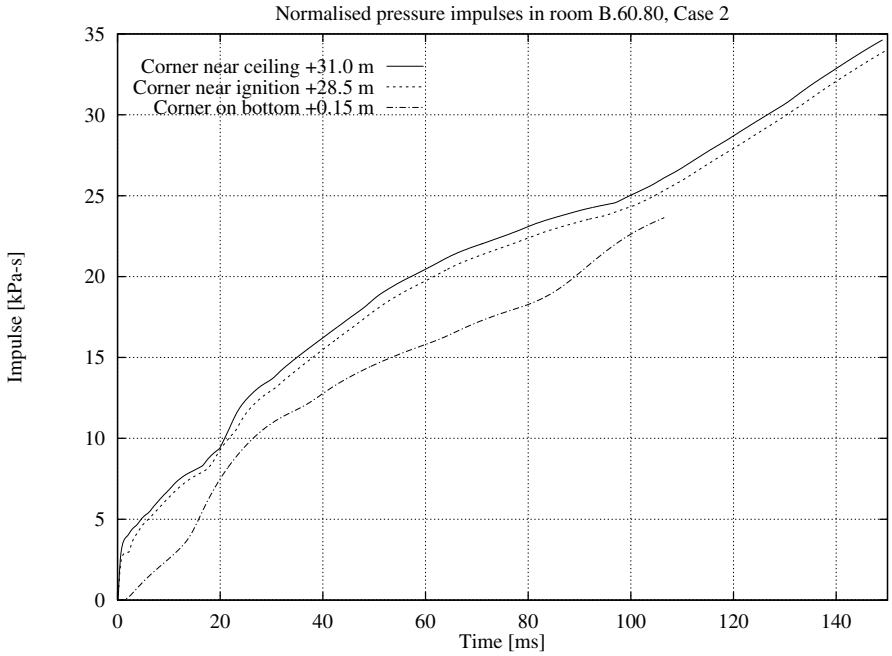


Figure 29. Normalised pressure impulses at three different elevations in room B.60.80. Case 2.

The pressure loads at four different points around the pipe penetrations in the containment wall at level + 26.0 m are shown in Figs. 30 and 31. Corresponding pressure impulses are shown in Figs. 32 and 33.

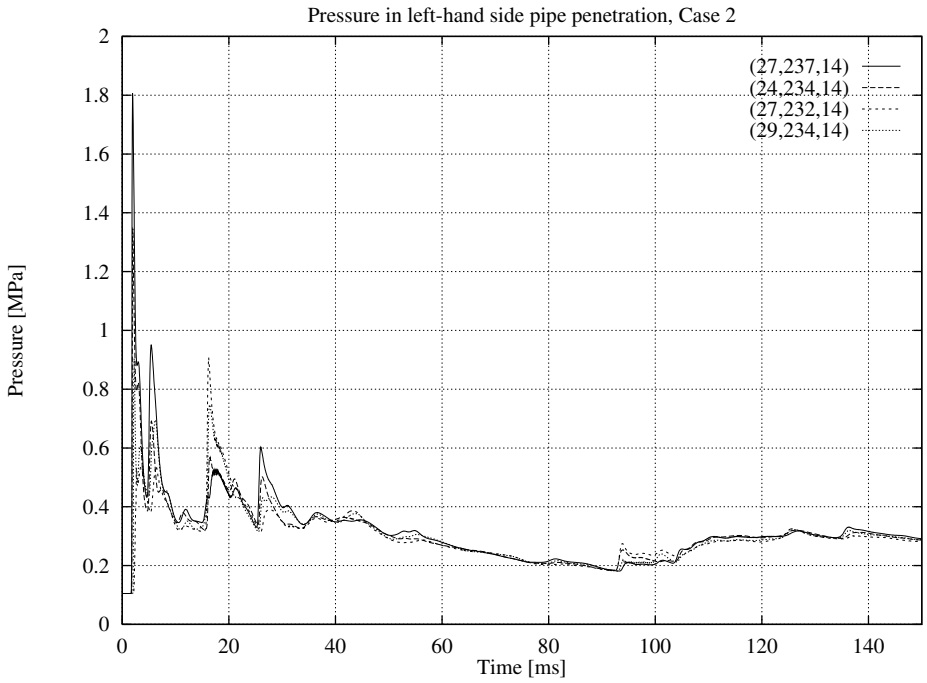


Figure 30. Simulated pressures at four points around the pipe penetration near the ignition site, Case 2.

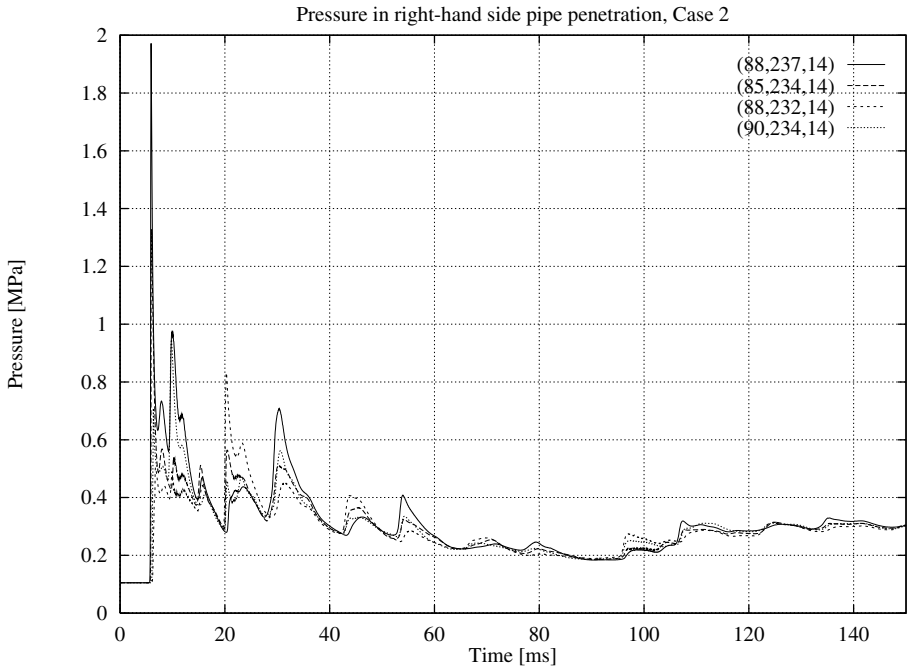


Figure 31. Simulated pressures at four points around the pipe penetration farther from the ignition site, Case 2.

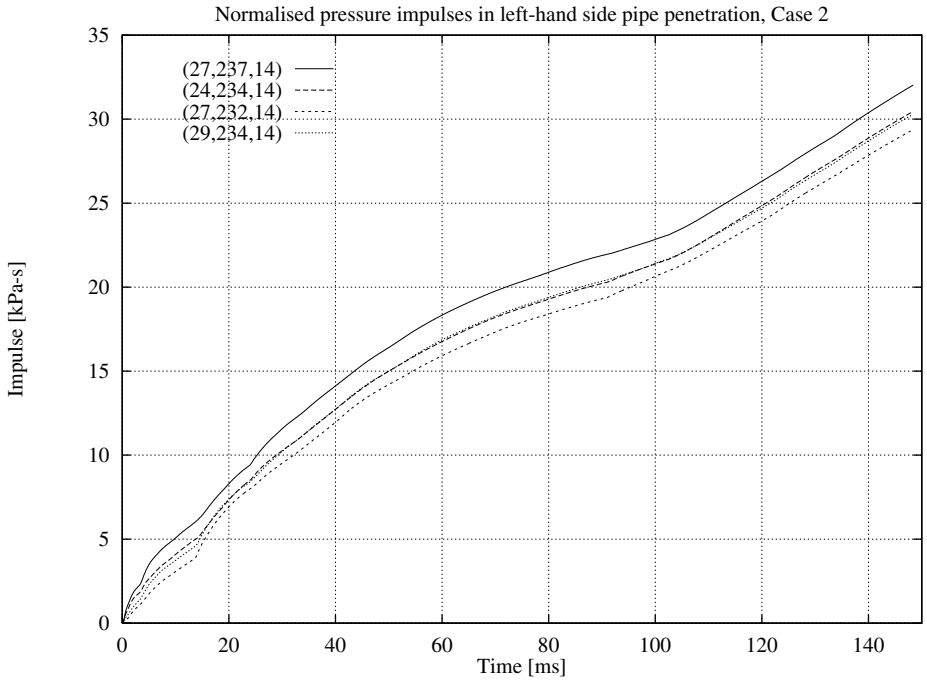


Figure 32. Normalised pressure impulses at four points around the pipe penetration near the ignition site, Case 2.

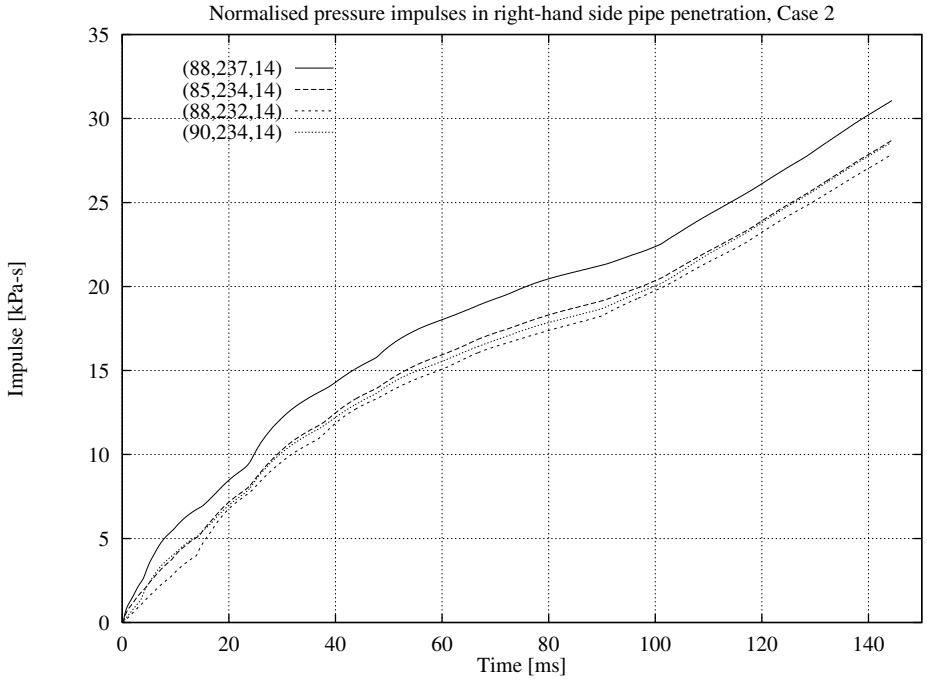


Figure 33. Normalised pressure impulses at four points around the pipe penetration farther from the ignition site, Case 2.

4.3 CASE 3

Case 3 was carried out to study the influence of ignition location on pressure loads. Ignition was set at the wide concrete wall of room B.60.80 opposite the containment wall (Fig. 2, ignition location A). For comparison, in Case 2 ignition occurred at the narrow end wall of the room (Fig. 2, ignition location B). In both cases, ignition was at the same level of + 28.5 m.

Comparison of pressure loads near structure surfaces at three different elevations with two different ignition locations is shown in Figs. 34 ... 36. Naturally, the point of ignition affects the timing of the pressure spikes in different parts of the room. In the simulation cases, the difference between the pressures seems to be highest near the ignition (Fig. 35). Farther from the ignition the differences are smaller (Fig. 34) and at the floor level nearly unnoticeable (Fig. 36). Comparison of pressure impulses near the ignition site, where the highest difference in pressure existed, is shown in Fig. 37. Generally, the differences in the pressure impulses are small, and can be considered insignificant.

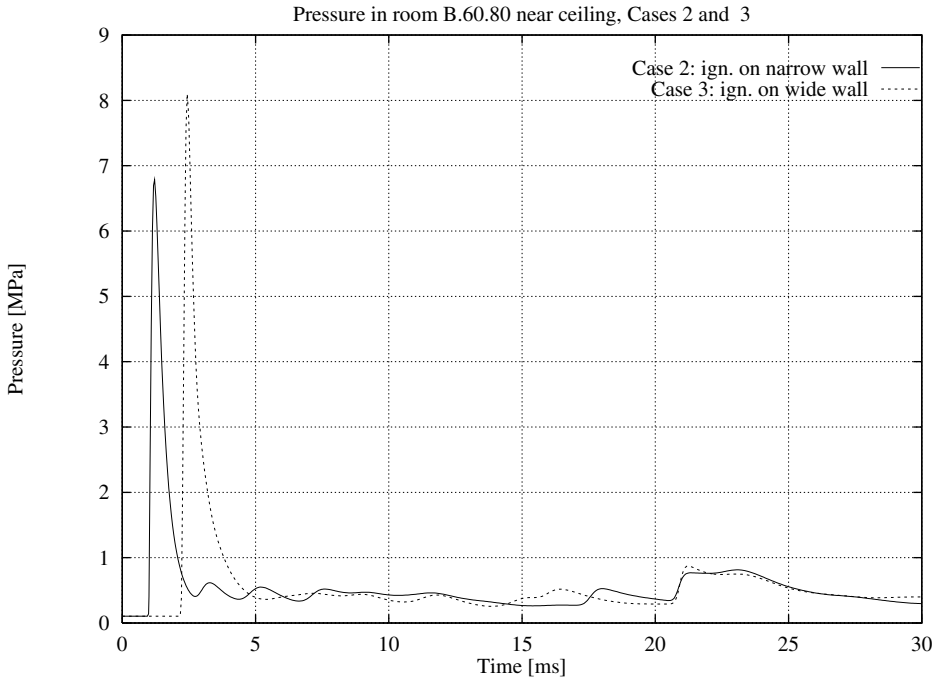


Figure 34. Pressure history near the room ceiling in Cases 2 and 3.

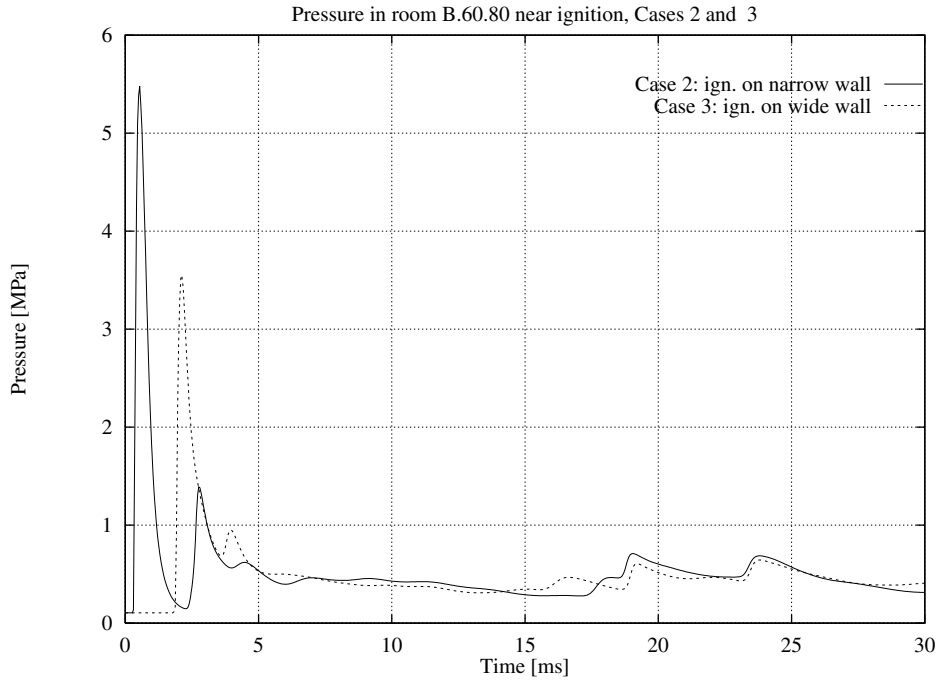


Figure 35. Pressure history near the ignition site in Cases 2 and 3.

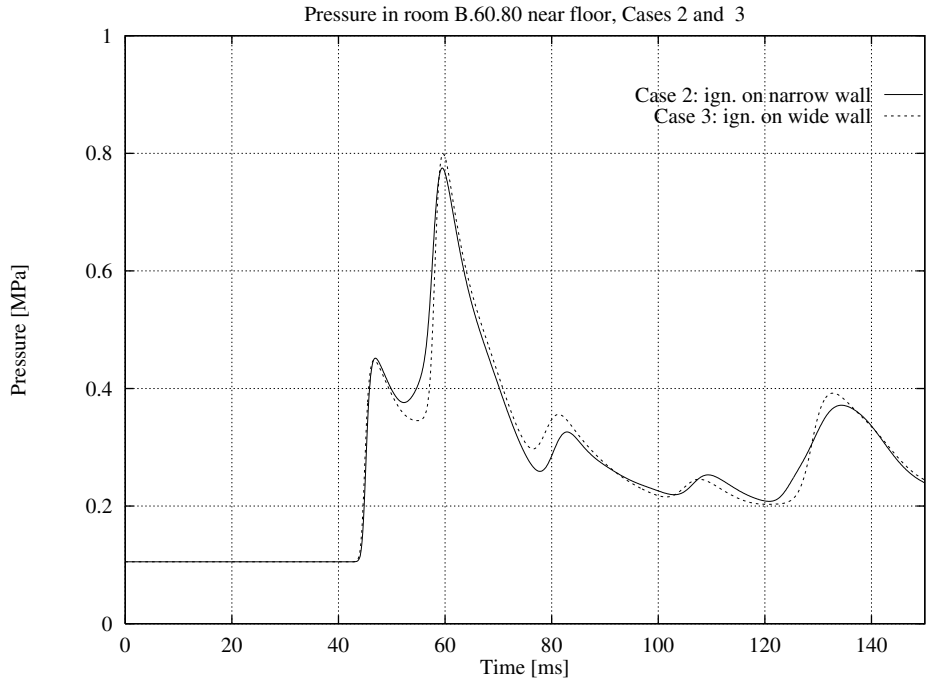


Figure 36. Pressure history near the room floor in Cases 2 and 3.

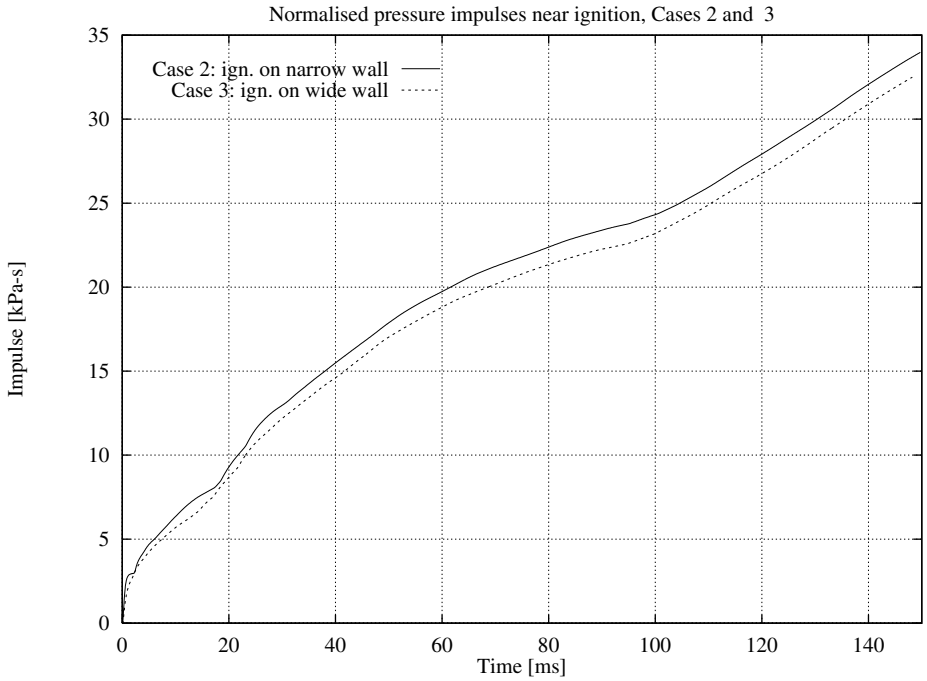


Figure 37. Normalised pressure impulses near the ignition site in Cases 2 and 3.

According to calculational results in Cases 2 and 3, the location of ignition had an effect on the timing of the pressure spikes, especially in the upper part of the room. The ignition location also had an influence on the angle between the incident detonation wave and the structure surfaces affecting the pressure after oblique shock reflection. In Case 4, only the influence of two different ignition locations was studied at selected points in the room. The differences between the results were relatively small and, in respect of pressure impulses insignificant. It is, however, noteworthy that the ignition position both in Case 2 and 3 was at the same room elevation, where the composition of the gas mixture was similar. A change of gas composition near the ignition would have a direct effect on the pressure and velocity of the incident detonation wave.

4.4 CASE 4

In all other simulation cases except in Case 4, the hydrodynamics solver of DET3D used a first-order version of the HLL method. Case 4 was carried out using the more accurate second-order method, which gives steeper shock fronts and a more detailed resolution of the reflections and interactions of the shock waves

Comparison of the pressures near structure surface at two different room elevations as predicted with the first and second order methods is shown in Figs. 38 and 39. Corresponding pressure impulses are shown in Figs. 40 and 41.

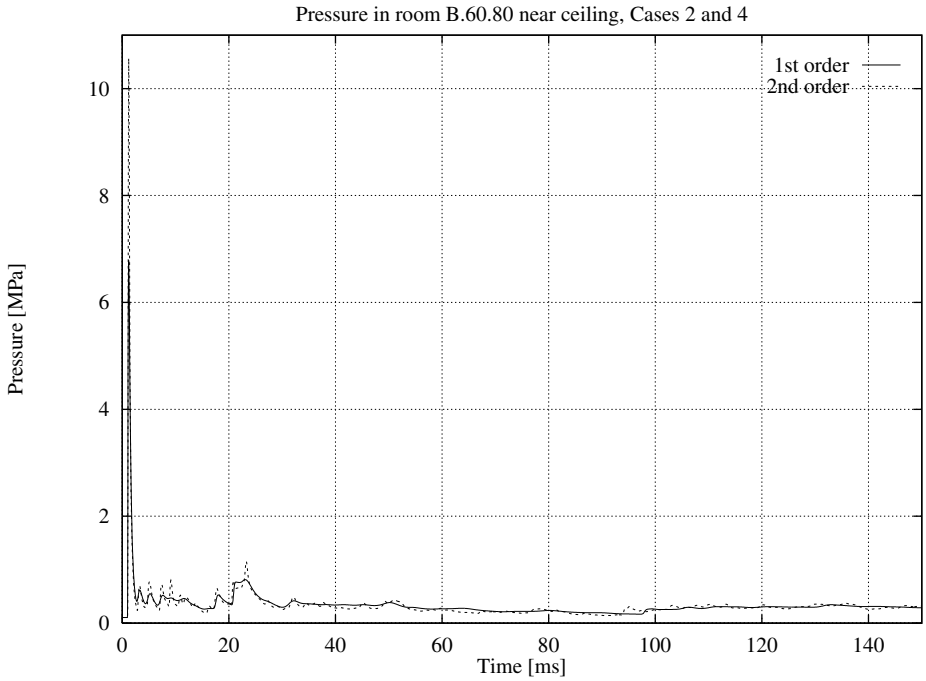


Figure 38. Pressure history near the room ceiling in Cases 2 and 4.

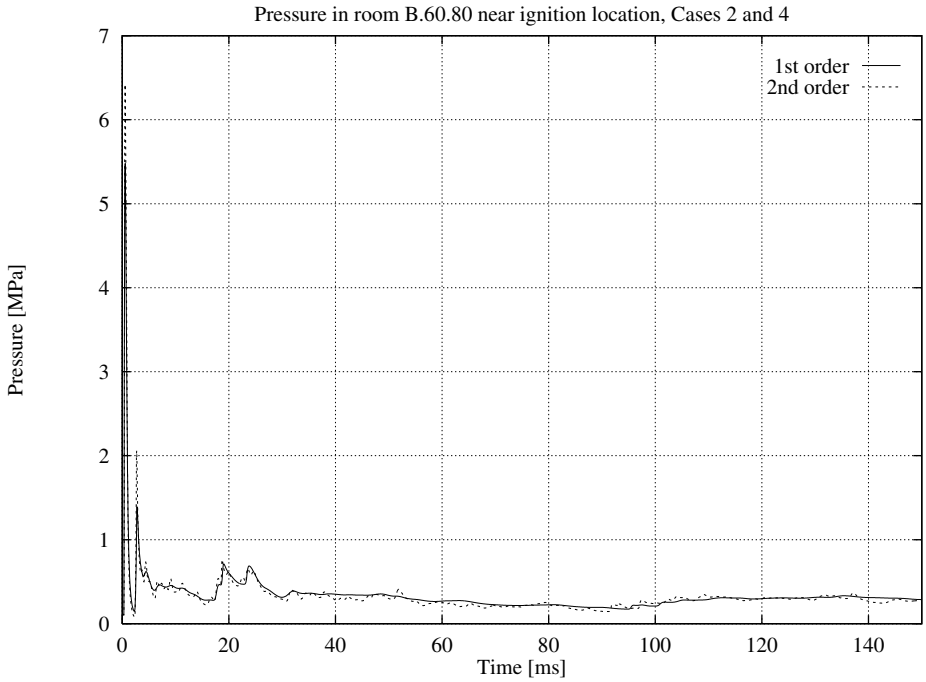


Figure 39. Pressure history near the ignition site in Cases 2 and 4.

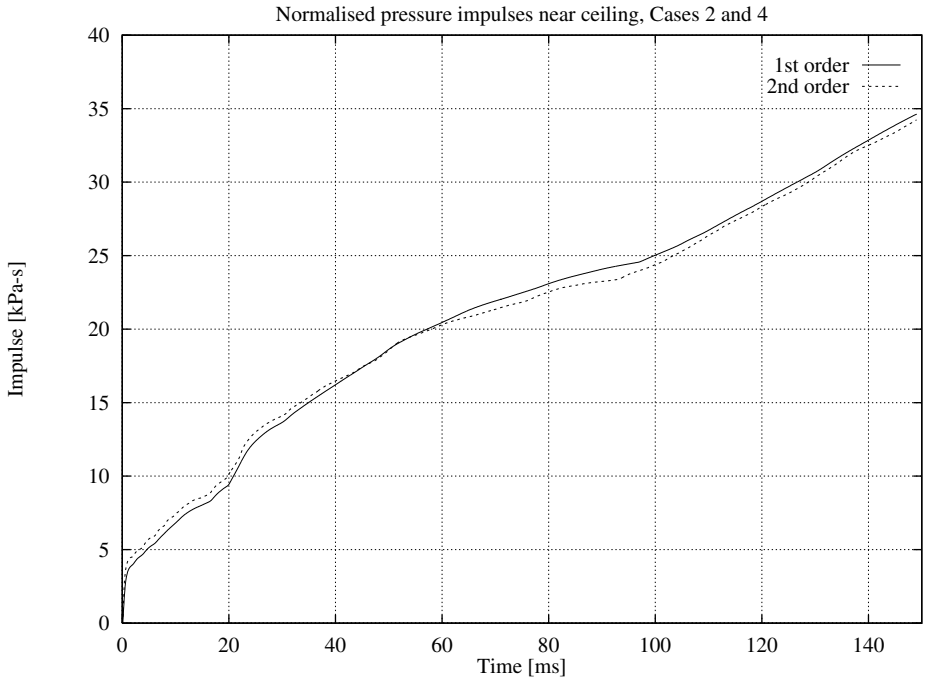


Figure 40. Normalised pressure impulses near the room ceiling during the 50 ms simulation, Cases 2 and 4

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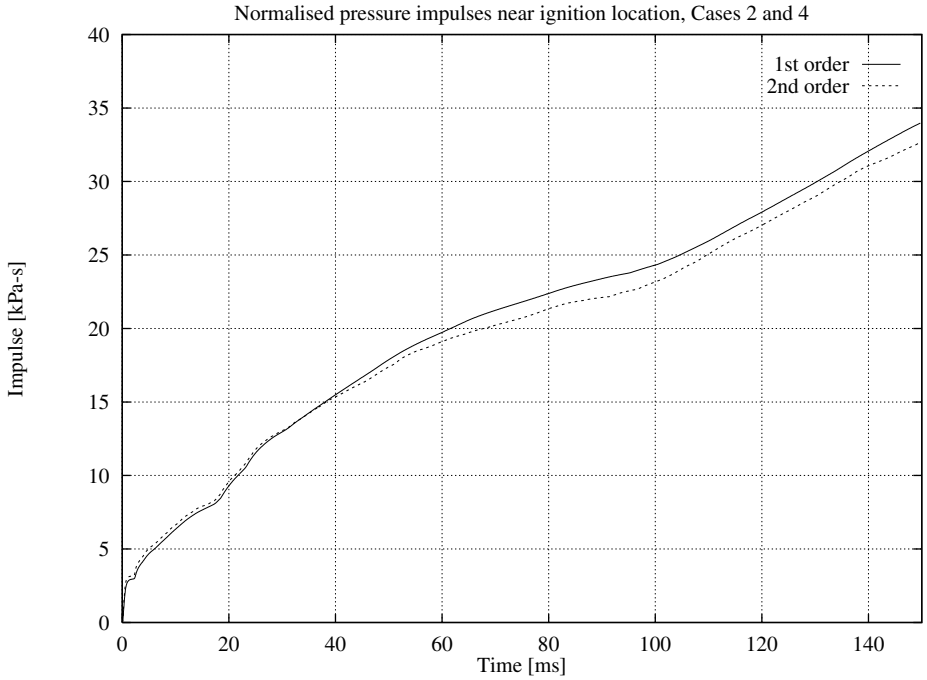

Figure 41. Normalised pressure impulses near the ignition site during the 50 ms simulation, Cases 2 and 4.

The second-order method gives maximally a roughly 30% higher value for the pressure spike after the first shock reflection than the first-order method (Figs. 38 and 39), but the differences in pressure impulses are insignificant (Figs. 40 and 41). The maximum pressure using the second-order method was about 10.6 MPa at the same location as

observed in Case 2 (Fig. 26). This value is the highest pressure observed in all simulation cases. On the lower level of the room near the ignition site, the differences in results are smaller.

The second order calculation was found to give occasionally higher pressure spikes than the first-order method. However, the differences were relatively small, especially in pressure impulse, which is the most important factor in respect of structural integrity. Because highly detailed effects are seldom important in large-scale applications, and because the second-order method requires much more CPU time, the choice of method must be always made based on the objective of the work.

4.5 CASE 5

Case 5 corresponded to a 2 mm^2 leakage (t = 12 500 s) where the mole fractions of hydrogen and oxygen were both roughly 17 – 18% above the level of leakage (Fig. 7). The location of ignition was the same as in Case 2. The mole fractions of hydrogen and air at the ignition level were 17% and 83%, respectively.

Contours of pressure at selected instants of time in Case 5 are illustrated in Appendix C. The general behaviour of the incident detonation wave in Case 5 was similar to Case 2. However, in Case 5 the mole fraction of hydrogen was lower and the wave propagated more slowly than in Case 2 (compare Figs. 24 and 42). A spherical detonation wave impacted on the ceiling at t ≈ 1.2 ms and the internal concrete wall at t ≈ 4.5 ms (Fig. 42). Because the initial mole fraction of hydrogen was less than 15% below the level + 27.5 m, the detonation wave could only propagate about one meter downwards from the ignition level. Detonation-induced shock waves propagated throughout the room.

The pressure of the incident detonation wave is about 1.2 – 1.3 MPa and the wave speed approximately 1500 m/s. These values agree well with the C-J values. At 17 ms from ignition, the shock waves had proceeded through the whole upper part of the room (above level + 19.5 m). By that time practically all the hydrogen had burned off. At t ≈ 45 ms the shock waves reached the room bottom.

The maximum pressure in each cell of the computational domain during the 150 ms simulation is illustrated in Fig. 43. The maximum pressure spike of about 6.2 MPa was observed in the upper corner of the room beside the containment wall (level + 31.0 m). The site of the pressure maximum in the room was roughly similar to Case 2.

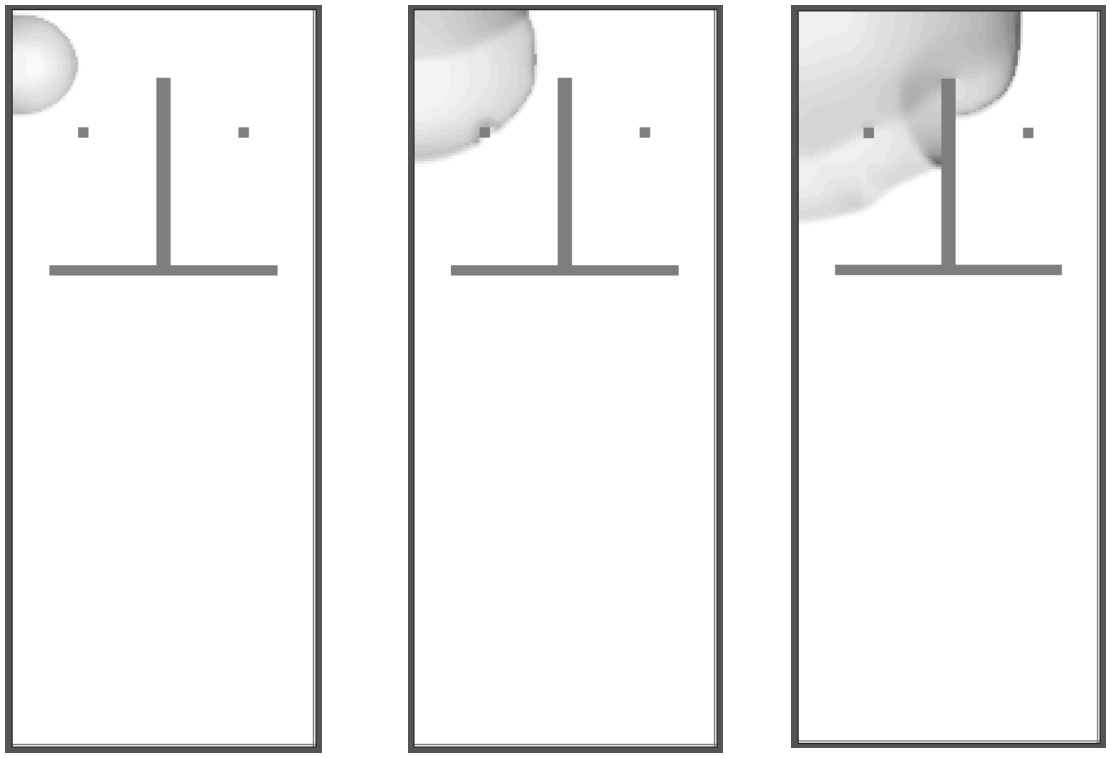

Figure 42. Illustration of pressure waves during detonation in Case 5 at three different instants of time: 1.0 ms (left), 3.0 ms (middle), and 6.0 ms (right).

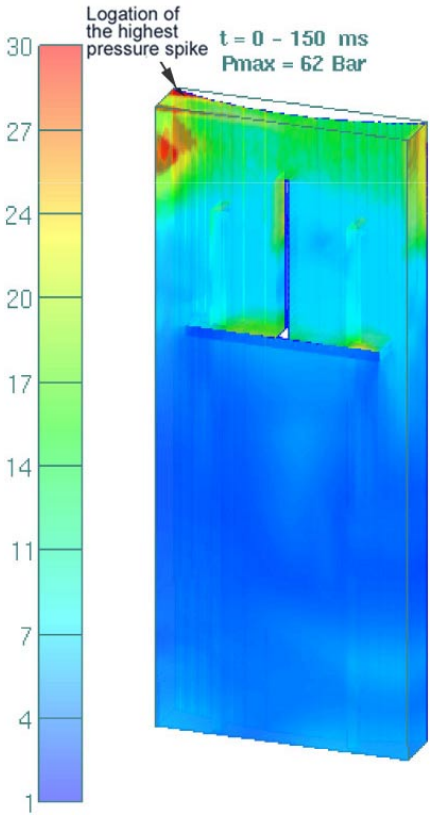

Figure 43. Contours of pressure maximum (Bar) in each part of room B.60.80 during the 150 ms simulation. Case 5.

Pressure histories near structure surfaces at three different levels in the room are illustrated in Fig. 44. Corresponding pressure impulses during the 150 ms simulation are shown in Fig. 45. The highest pressure spikes occurred in the corner near the ceiling and the ignition site. The pressure maximum at the bottom of the room was only about 0.5 MPa caused by reflections of decaying shock waves. The highest pressure impulses on wall structures during the 150 ms simulation were about 20 - 25 kPa-s.

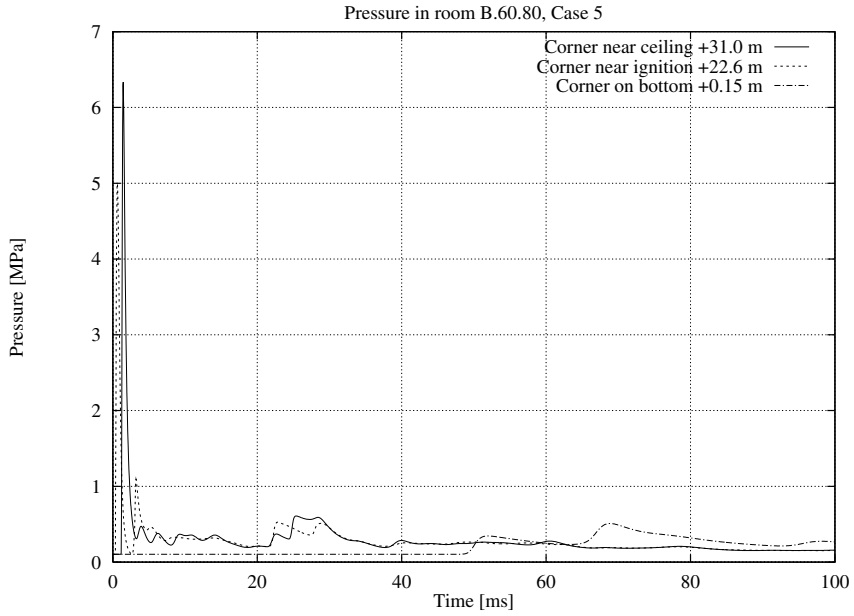

Figure 44. Simulated pressures at three different elevations in room B.60.80. Case 5.

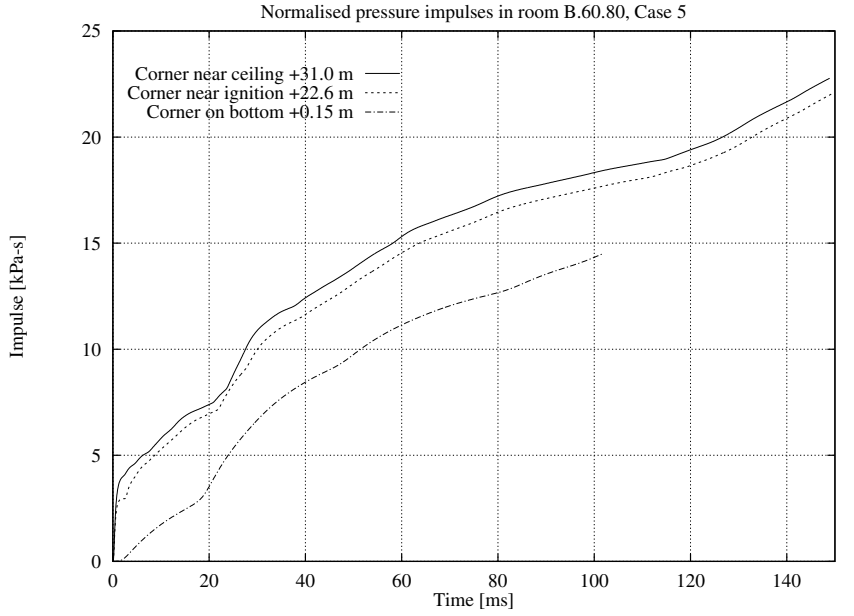

Figure 45. Normalised pressure impulses at three different elevations in room B.60.80. Case 5.

The pressure loads at four different points around the pipe penetrations on level + 26.0 m are shown in Figs. 46 and 47. Corresponding pressure impulses are shown in Figs. 48 and 49.

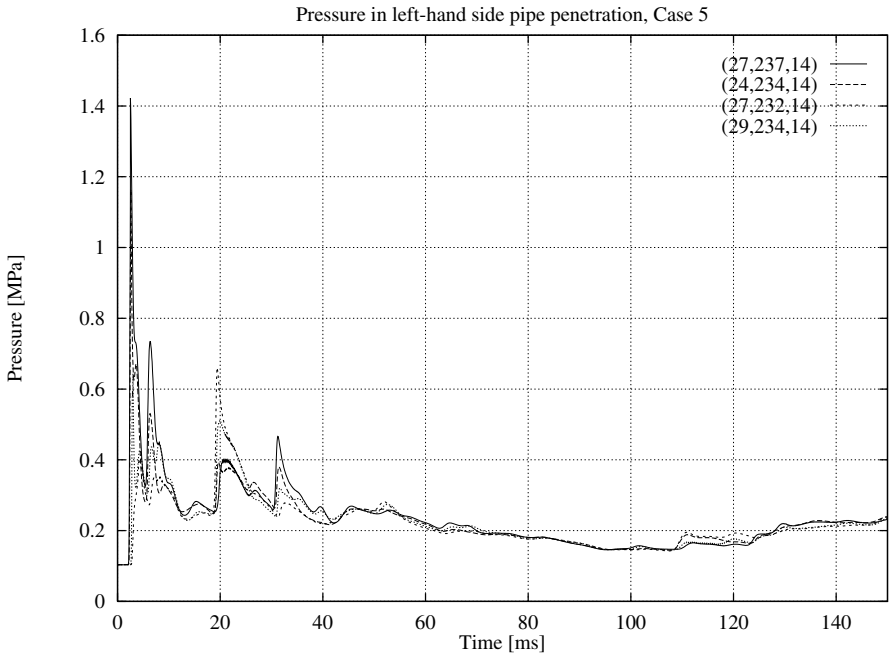

Figure 46. Simulated pressures at four points around the pipe penetration near the ignition site, Case 5.

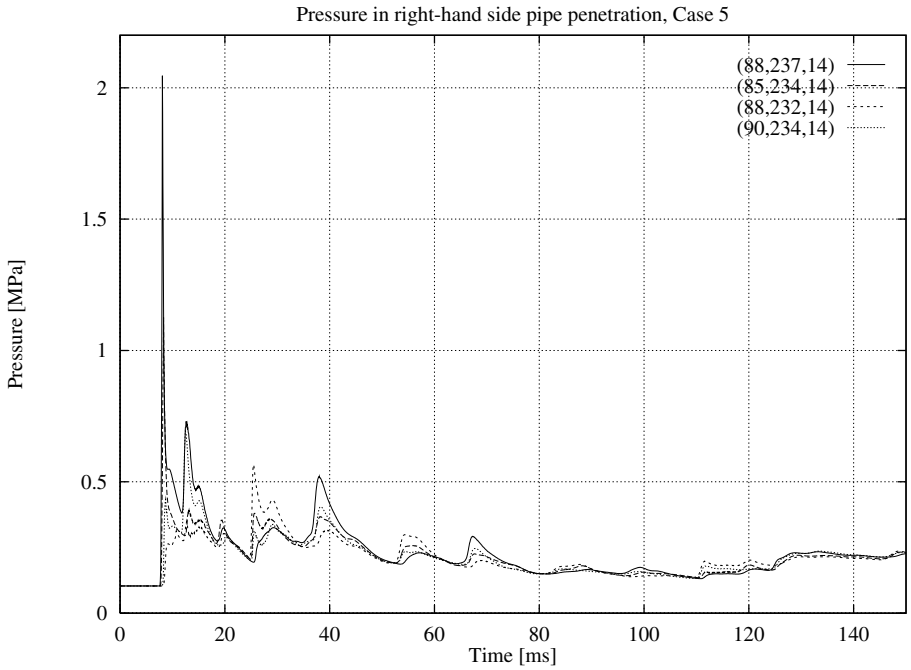

Figure 47. Simulated pressures at four points around the pipe penetration farther from the ignition site, Case 5.

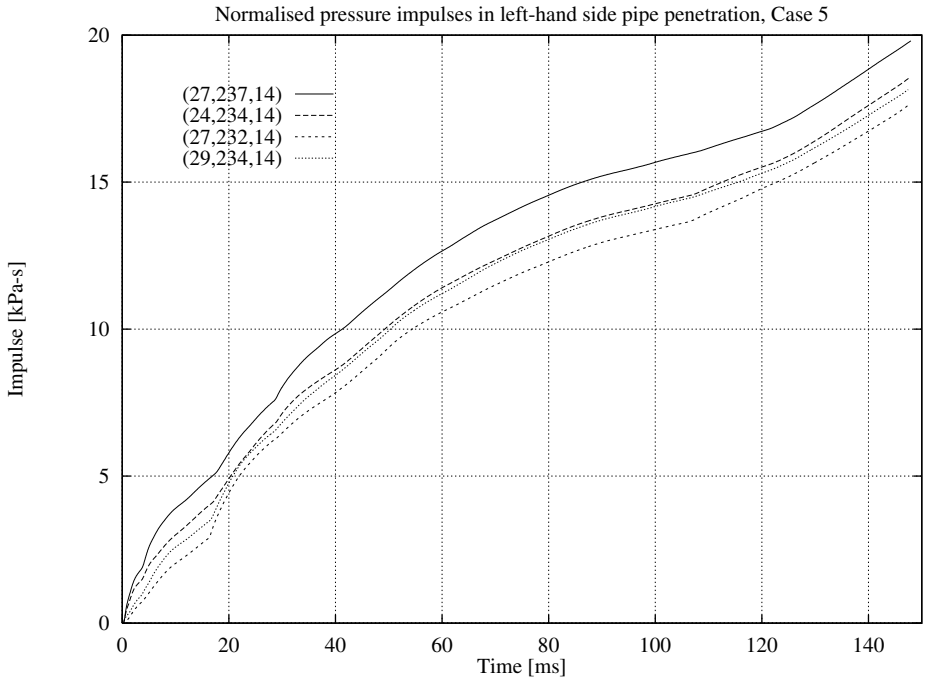

Figure 48. Normalised pressure impulses at four points around the pipe penetration near the ignition site, Case 5

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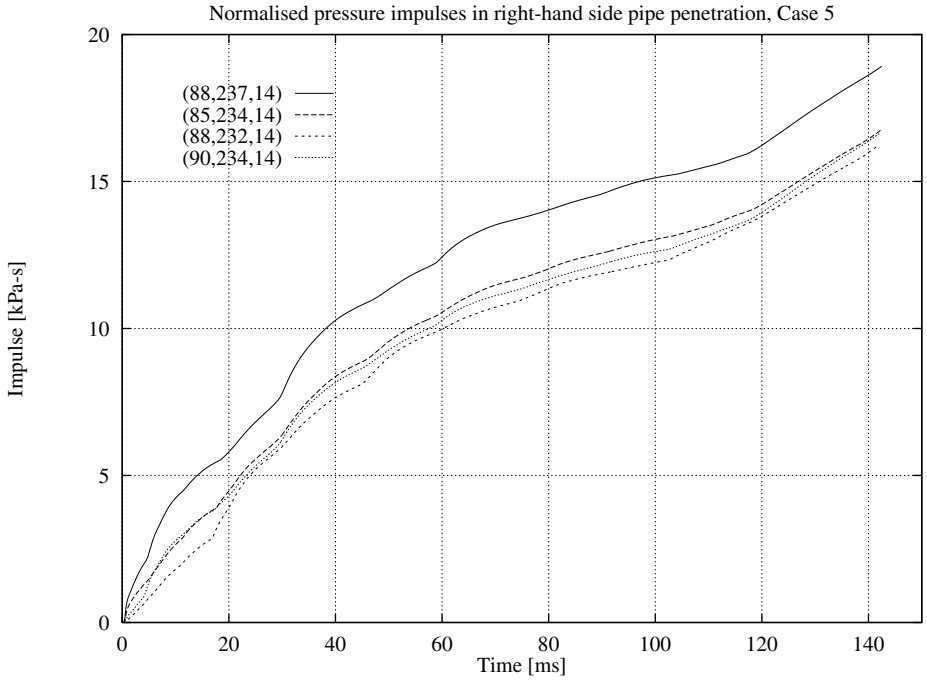

Figure 49. Normalised pressure impulses at four points around the pipe penetration farther from the ignition site, Case 5.

5 SUMMARY AND CONCLUSIONS

Three-dimensional simulations of hydrogen detonations in an Olkiluoto reactor building room during a severe accident were carried out with the DET3D code. The hydrogen leak rates from the containment into the reactor building were based on earlier analyses with the MELCOR code. In these analyses, a station blackout accident sequence with depressurisation of the reactor coolant system was assumed. One hundred percent of zirconium was conservatively assumed to oxidise, leading to a total hydrogen release of 1900 kg to the containment.

Two different leakage sizes from the containment to the reactor building were considered. The hydrogen spreading in the reactor building was analysed with the FLUENT code. Three different situations from the FLUENT analyses were selected as initial conditions for the detonation simulations. Also the influence of ignition location and the numerical method of the hydrodynamics solver of DET3D on the detonation loads were studied.

The DET3D simulation indicated that the highest pressure spikes occurred in the room corners due to reflections and superposition of shock waves. The highest pressure maximum in all simulation cases was about 10.6 MPa. This value was obtained in the upper corner of the room beside the containment wall. The highest pressure impulses on structures during the 150 ms simulation were about 30 - 35 kPa-s.

In Case 1, the initial gas concentration gradient was very strong in the upper part of the room and a hydrogen inerted layer existed near the room ceiling. Only a relatively small amount of hydrogen was burned during the first detonation. Later propagation of a slow combustion front to the still hydrogen rich upper region was predicted to lead to flame acceleration and a second detonation, now at a different location from the first one.

In all other simulation cases, the gas mixture above the level of leakage was relatively homogeneous and no hydrogen inerted layer initially existed in the room. In these cases, practically all hydrogen was burned during the first and single detonation.

The DET3D code proved to be a highly effective, best-estimate tool for assessment of detonation pressure loads in a real 3-D geometry, taking into account the multiple reflections and superposition of shock waves.

Future work will include transfer of DET3D data to the ABAQUS code for structural analyses.

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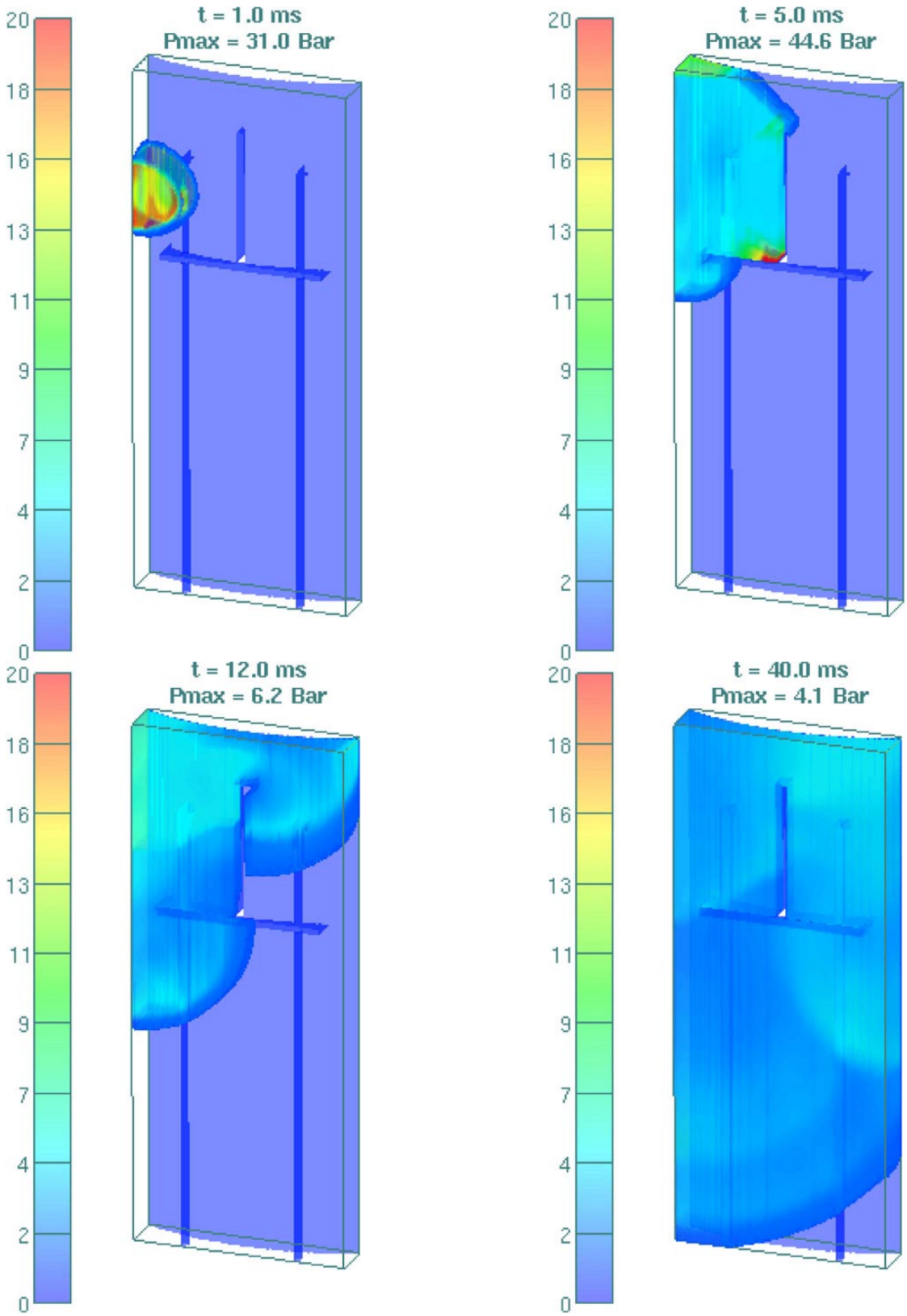
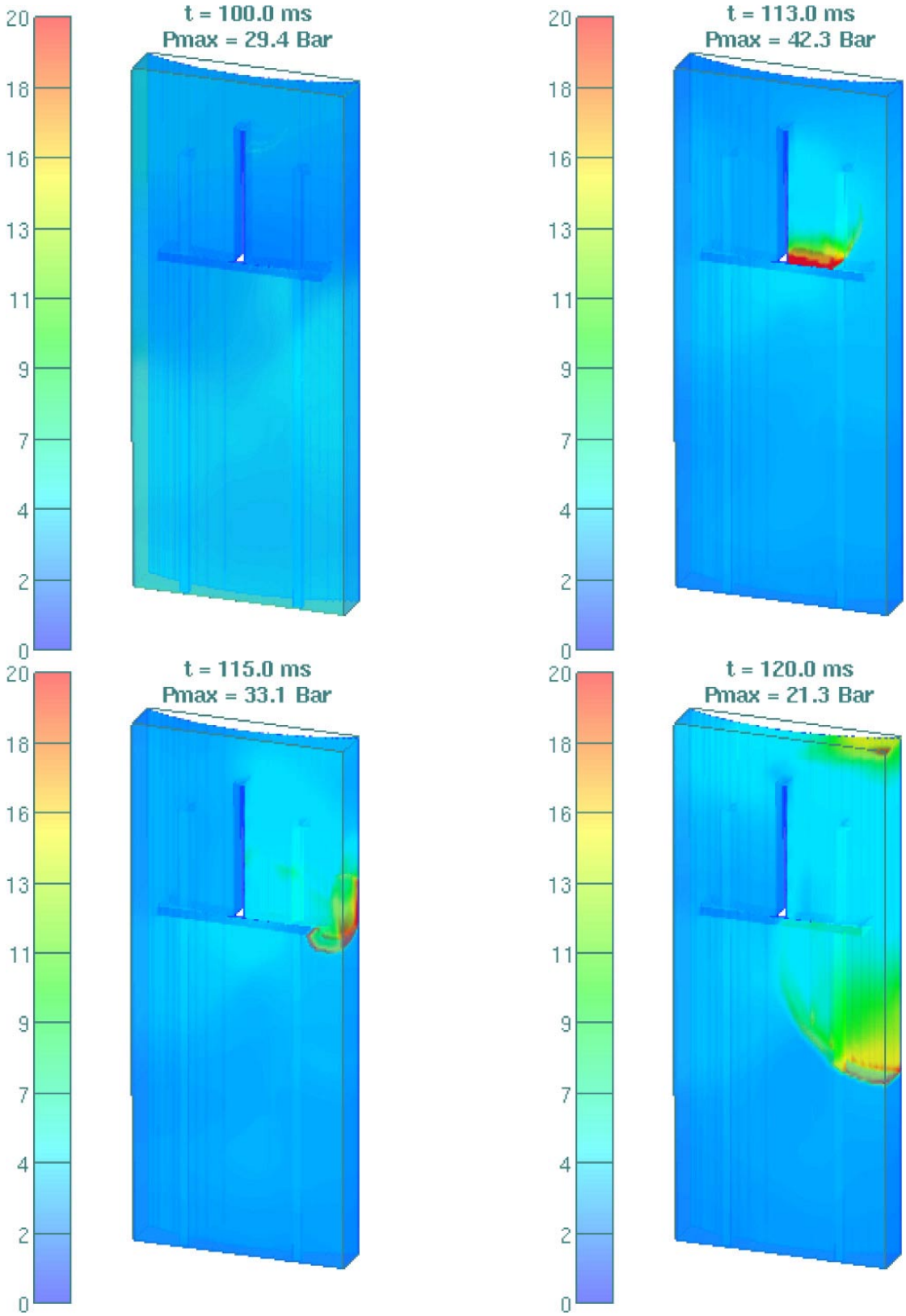
APPENDIX A

Pressure in Case 1



Pressure (Bar) in room B.60.80 at four instants of time, Case 1.

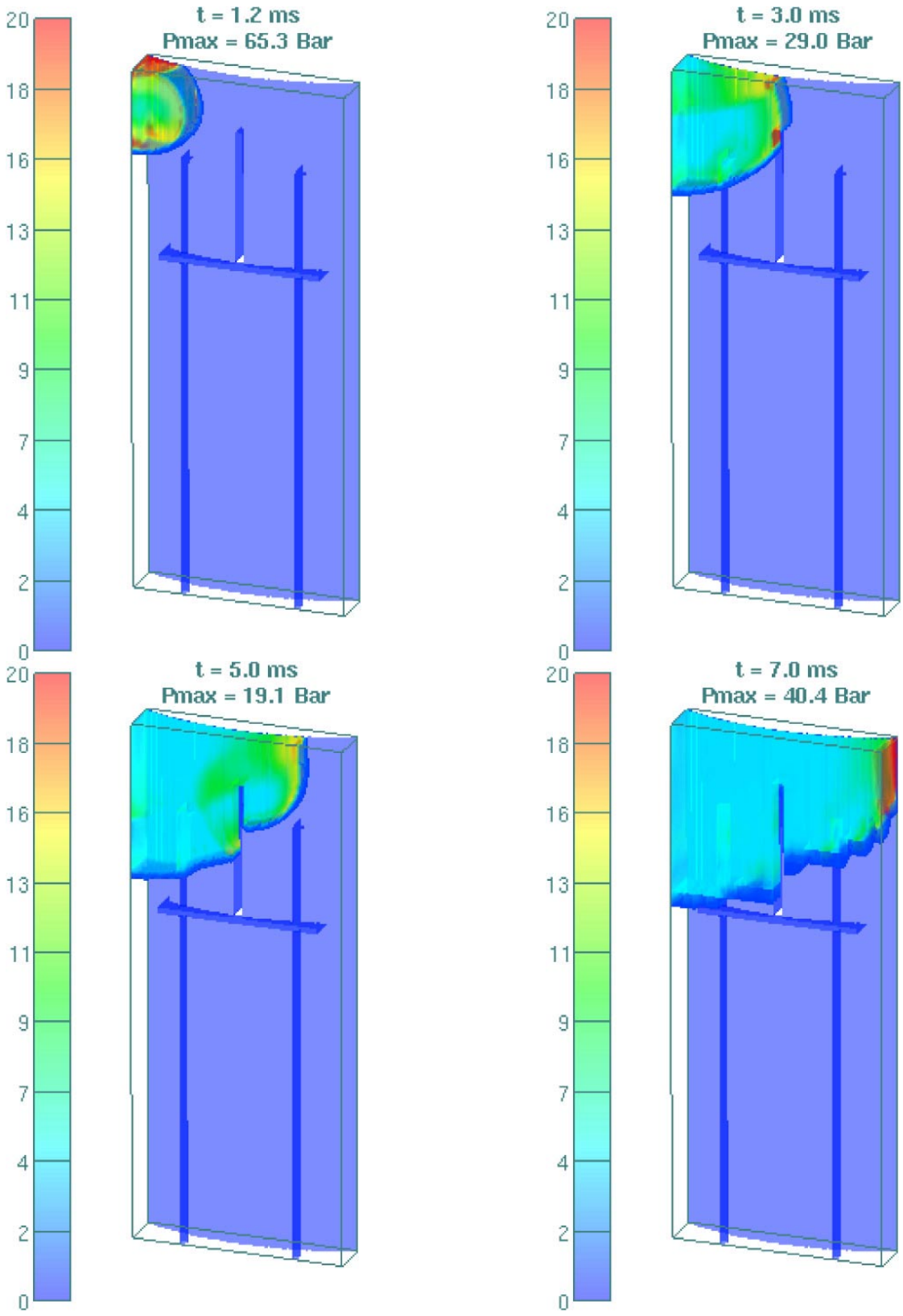
Pressure in Case 1



Pressure (Bar) in room B.60.80 at four different instants of time, Case 1.

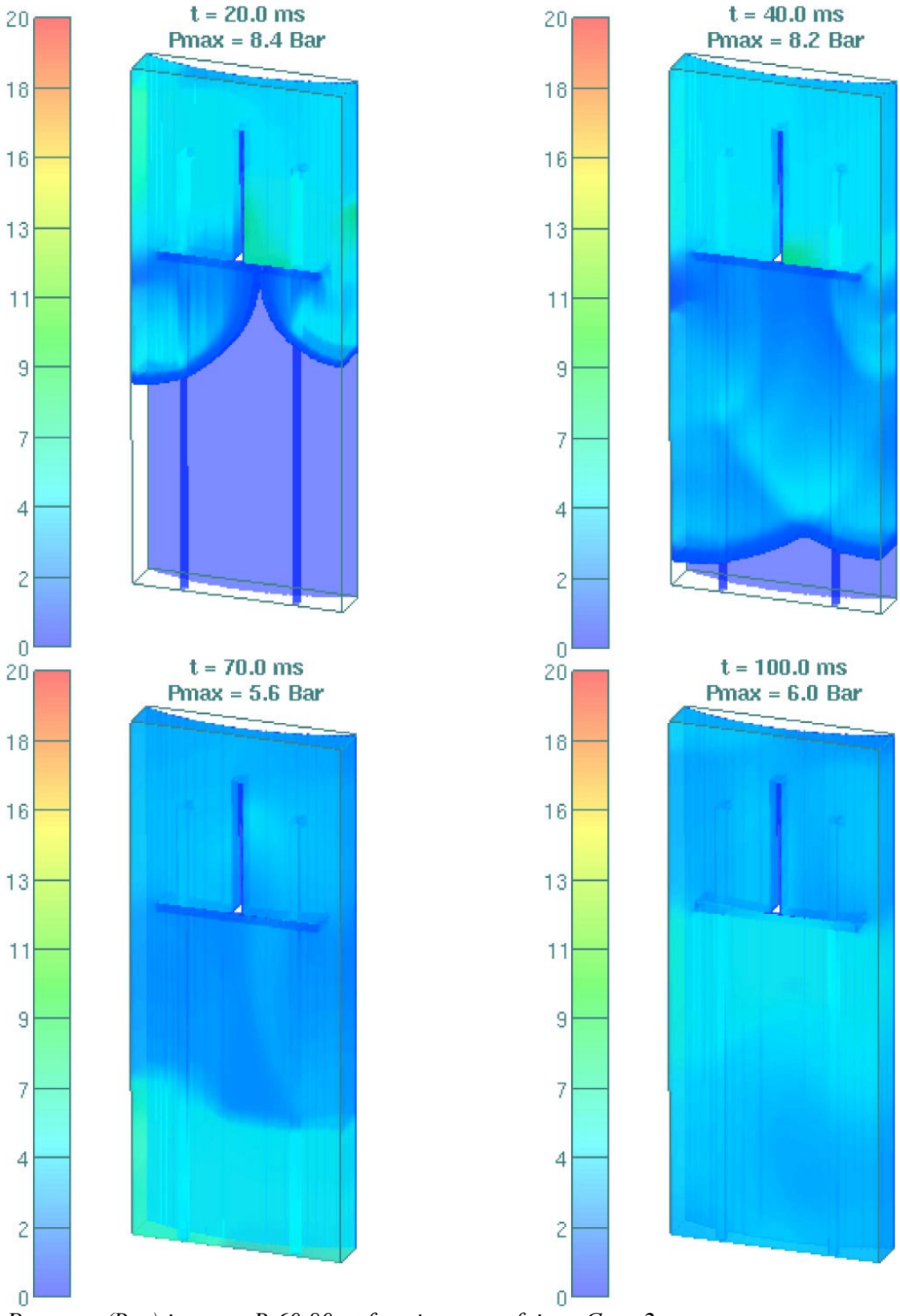
APPENDIX B

Pressure in Case 2



Pressure (Bar) in room B.60.80 at four instants of time, Case 2.

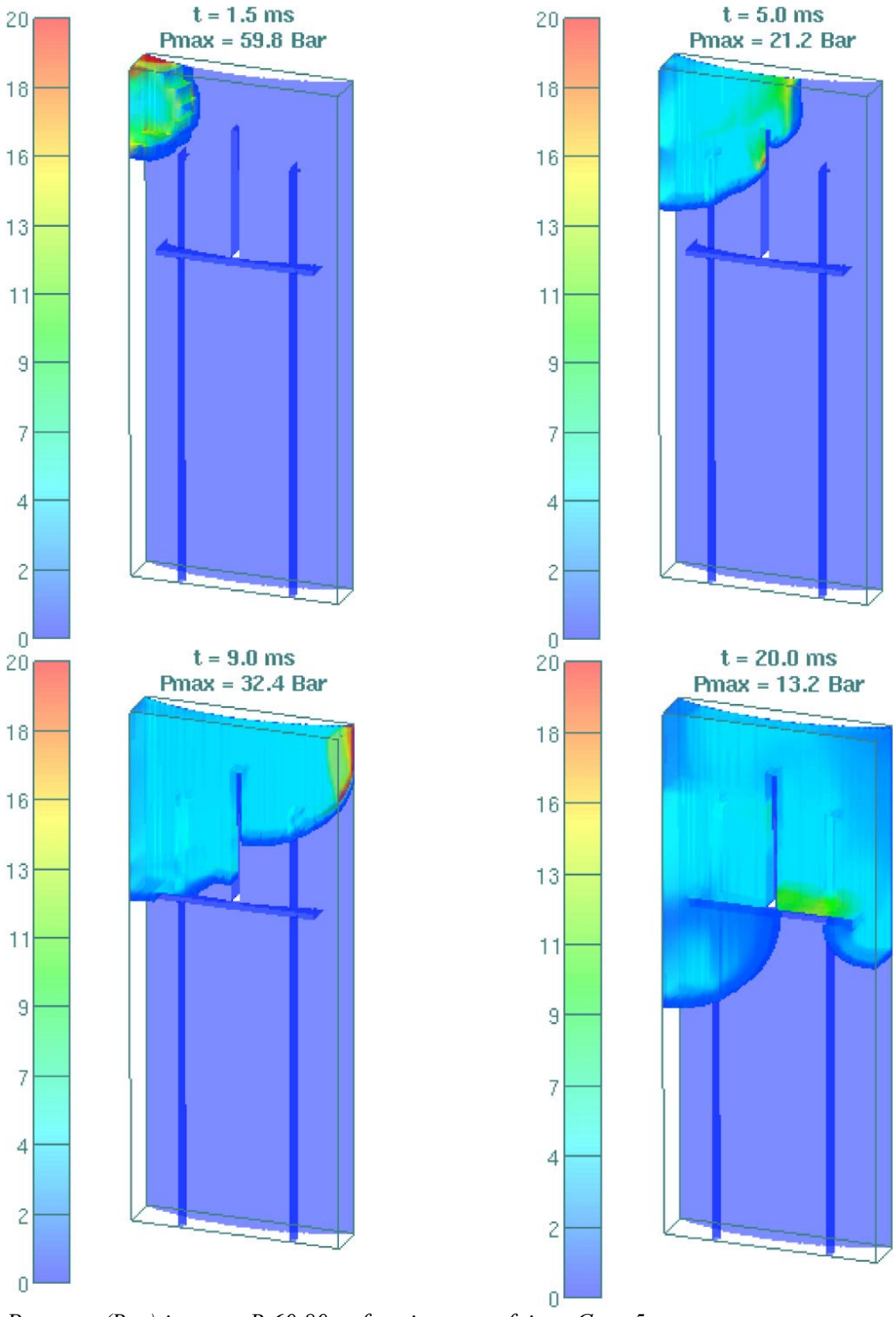
Pressure in Case 2



Pressure (Bar) in room B.60.80 at four instants of time, Case 2.

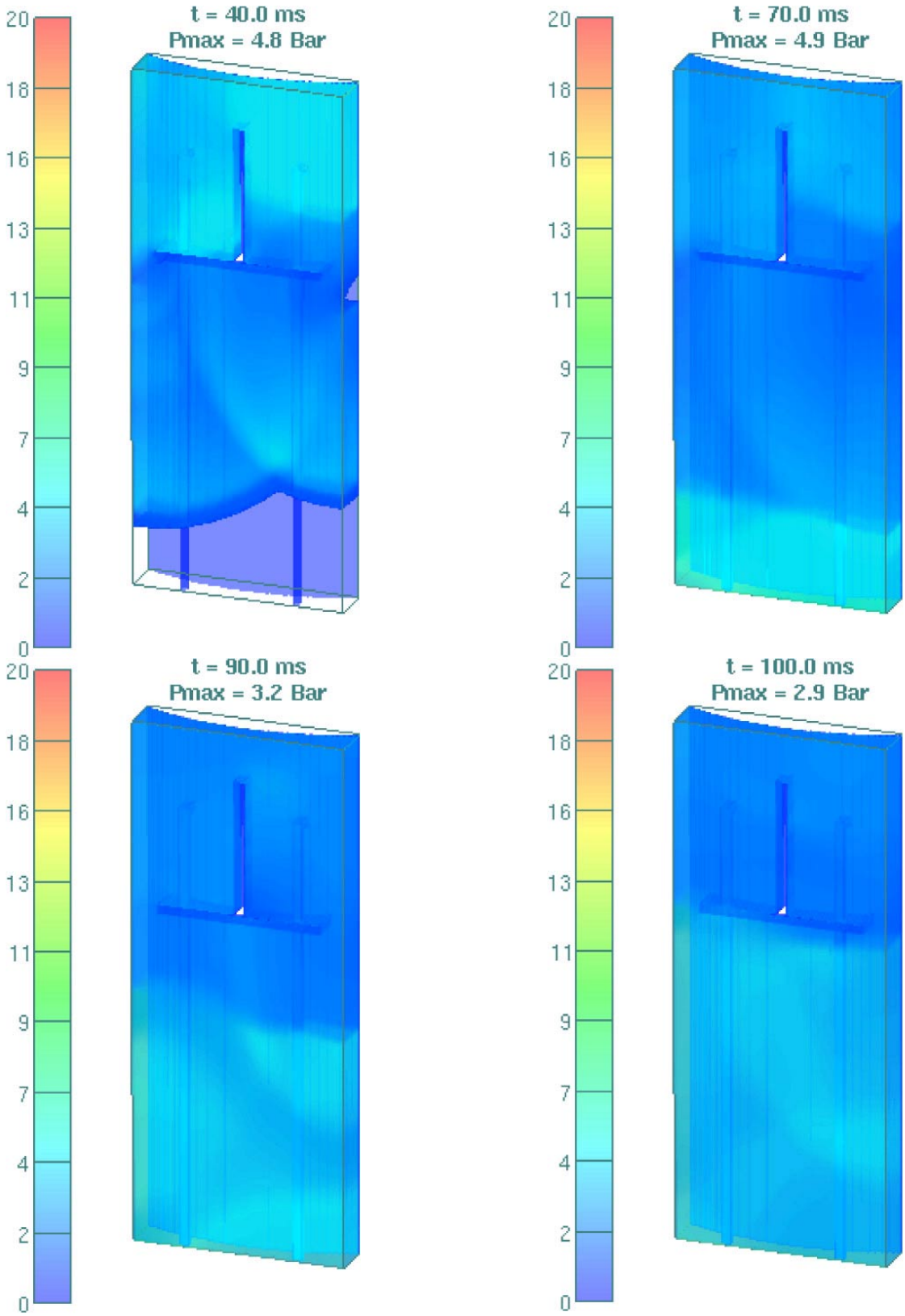
APPENDIX C

Pressure in Case 5



Pressure (Bar) in room B.60.80 at four instants of time, Case 5.

Pressure in Case 5



Pressure (Bar) in room B.60.80 at four instants of time, Case 5.

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Title	Three-dimensional simulation of hydrogen detonations in the Olkiluoto BWR reactor building
Author(s)	Ari Silde, Reinhard Redlinger
Affiliation(s)	VTT Energy, Forschnungszentrum Karlsruhe GmbH
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Abstract	This report describes the numerical simulations of hydrogen detonations in Olkiluoto reactor building room B.60.80 using the DET3D code. The code is developed at Forschungszentrum Karlsruhe (FZK) and uses the finite difference method based on three-dimensional Euler equations for a multicomponent reacting gas. DET3D is mainly developed for modelling of gaseous detonations initiated by a direct ignition. DDT phenomena are not treated. The initial conditions of the detonation simulation were based on previous hydrogen spreading analyses carried out with the FLUENT code. DET3D calculations continued the previous, rough estimates of shock pressure loads performed with a simple DETO code. The DETO analyses were based on the strong ignition theory with oblique and normal reflection relations of the adiabatic shock waves. Shock waves were induced by point-like energy release without modelling of the propagating combustion front. In the DETO modelling, only the first shock reflection was treated. The approach of the DET3D code enables the more detailed assessment of detonation pressure loads in a real 3-D geometry. The objective of the work was to assess the pressure loads on room structures under detonation conditions. The initial conditions of detonation simulation were based on the previous hydrogen spreading analyses performed with the FLUENT code. Two sizes of leakage from the containment to the reactor building were considered: 2 mm^2, which corresponds to the nominal leakage of containment, and a large leak of 20 mm^2. The DET3D simulation indicated that the highest pressure spikes occurred in the room corners due to reflections and superposition of the shock waves. The highest pressure maximum in all simulation cases was about 10.6 MPa. This value was obtained in the upper corner of the room beside the containment wall. The highest pressure impulses to structures during the 150 ms simulation were about 30 - 35 kPa-s.
Key words	severe accident, detonation, hydrogen, reactor building, DET3D, simulation

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