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ITER-FEAT Accident Analysis on Hydrogen Detonation Using DET3D and GASFLOW

W. Baumann, W. Breitung, B. Kaup, R. Redlinger, J. R. Travis

Institut für Kern- und Energietechnik
Programm Kernfusion

Forschungszentrum Karlsruhe GmbH, Karlsruhe
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Abstract

Computer analyses have been performed to assess the dynamic pressure loads to the ITER-FEAT vessel during a conservative accident scenario assuming air ingress, production of 5 kg hydrogen, formation of a local stoichiometric hydrogen-air mixture, and ignition of a local detonation. The mechanical loads from the detonation to the vessel and the ports were investigated with two different 3D-codes, DET3D and GASFLOW, to study the effects from the grid geometry, the spatial resolution, the type and order of the numerical solver. Both codes were validated against experimental data. A geometry model of the ITER-FEAT vessel was developed for each code and used for numerical simulation of the generated pressure loads. The peak pressure values resulting from the calculations depend mainly on the angle of incidence of the detonation wave with respect to the confining surface. Pressures of about 10 bar were predicted for side-on orientation (wave surface perpendicular to the structure), and 25 bar for normal reflection. The best results were obtained with an explicit, second-order solver, Cartesian grid, and high spatial resolution (DET3D, 2.2 million cells). The reflected impulses calculated for the 5kg-H_2-detonation (5 kPa s) correspond roughly to the collision of a passenger car at medium traffic velocity, a value which compares well with results obtained from 1D-calculations. As for the gas temperatures, values up to 3500 K have been calculated.

ITER-FEAT Unfall-Analyse zur Wasserstoff-Detonation mit DET3D und GASFLOW

W. Baumann, W. Breitung, B. Kaup, R. Redlinger, J. R. Travis

Zusammenfassung

Im Rahmen von ITER-FEAT wurden Computeranalysen durchgeführt, um die dynamischen Druckbelastungen des ITER-FEAT-Behälters für ein konservativ angenommenes Unfallszenario mit Lufteintritt abzuschätzen, bei dem gleichzeitig freigesetzte 5 kg Wasserstoff in einem lokal gebildeten stöchiometrischen Luft-Wasserstoffgemisch zünden. Die durch die Detonation entstehende Druckbelastung von Vakuumbehälter und Ports wurde mit den beiden unterschiedlichen 3D-Codes DET3D und GASFLOW untersucht, um die Auswirkungen von Netzgeometrie, räumlicher Auflösung sowie Art und Ordnung der numerischen Löser zu studieren. Beide Codes wurden mit experimentellen Daten validiert. Zur numerischen Simulation der erzeugten Drucklasten wurde für jeden Code ein Geometriemodell von ITER-FEAT entwickelt. Die berechneten Druckspitzen hängen hauptsächlich vom Auftreffwinkel der Druckwellen auf die begrenzenden Oberflächen ab. Für seitliches Auftreffen (Wellenfront senkrecht zur Struktur) wurden 10 bar, für senkrecht reflektierte Druckwellen 25 bar ermittelt. Die besten Ergebnisse erzielte ein expliziter Löser zweiter Ordnung mit kartesischem Netz und hoher räumlicher Auflösung (DET3D, 2.2 Millionen Zellen). Für die Detonation von 5 kg H_2 wurden reflektierte Impulse berechnet, die etwa dem Aufprall eines Pkw bei mittlerer Fahrgeschwindigkeit entsprechen (5 kPa s), ein Wert, der mit den Ergebnissen von 1D-Rechnungen gut übereinstimmt. Als Gastemperaturen ergaben sich Werte bis zu 3500 K.

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Executive Summary

Computer analyses have been performed to assess the ITER-FEAT vessel safety during a conservative accident scenario assuming air ingress, production of 5 kg hydrogen, formation of a local stoichiometric hydrogen-air mixture and ignition of a local detonation. The mechanical loads from the detonation to the vessel and the ports were investigated with the 3D-codes DET3D and GASFLOW to investigate effects from the grid geometry, the spatial resolution, type and order of the numerical solver. Both codes were validated against experimental data. A geometry model of the ITER-FEAT vessel was developed for each code and used for numerical simulation of the generated pressure loads.

The loading in the complex ITER-FEAT geometry consists of three different contributions:
- the initial detonation wave in the region of the reactive H_2-air mixture,
- pressure waves in the burnt gas and in the air volume, which are due to the gas flows created by the chemical energy release, and
- the quasistatic long-term combustion pressure, which remains after dampening of the gas flows in the complex enclosure.

The highest pressures are generated by the initial detonation wave. The peak pressure value reached depends on the angle of incidence of the detonation wave with respect to the confining surface. For side-on orientation (wave surface perpendicular to the structure), peak pressures of about 10 bar were predicted. For normal reflection of the detonation wave, peak pressures around 25 bar were calculated for the assumed scenario. Focussing of the detonation wave in multi-dimensional reflectors can create even higher local pressures.

Typical results on impulse data have been obtained. The detonation impulses are due to the directional gas velocities in reactive flow. In fully developed H_2-air detonations, the velocity attains about 1000 m/s. The reflected impulses calculated for the 5kg-H_2-detonation (5 kPa s) correspond roughly to the collision of a passenger car at medium traffic velocity, a value which compares well with results obtained from 1D-calculations. As for the gas temperatures, values up to 3500 K have been calculated.

The best results were obtained with an explicit, second-order solver, Cartesian grid, and high spatial resolution (DET3D, 2.2 million cells). Small computational cells are important to resolve high local pressures from focussing of the detonation wave in edges and corners of the 3D-geometry. The obtained results represent an adequate data base for future investigations of the structural behavior and integrity of the vacuum vessel.

1 Objectives and introduction

Within the ITER project, a maximum permissible amount of 5 kg hydrogen has been defined as a safety criterion, and this for two reasons. First, the 5 kg amount is based on the flammability limit of H_2-air mixtures (≈ 4 vol.% H_2) and the total vessel volume, assuming a homogeneous hydrogen distribution. Second, in case of a possible combustion during air ingress into a hydrogen containing vessel, the occurring long-term quasi-static pressure would not exceed the design limit of 2 bar [1]. However, since inhomogeneous hydrogen distributions could lead to highly dynamic local loads, bounding detonation calculations in 3D-geometry were performed to identify maximum possible mechanical loads to the vessel. Compared to the 1D-investigations done earlier [1], the refined and more realistic 3D-analysis will allow to better define and justify in-vessel hydrogen limits for ITER-FEAT, avoiding unnecessary over-conservatism.

The flow of gas behind a detonation front was studied by Taylor in [2]. Assuming that the motion of the gas is confined to one spatial dimension (plane Cartesian geometry), Taylor shows that Riemann's method of analysis is applicable, which means that, if the pressure p is assumed to be a function of the density ρ, then the gas flow behind the front (rarefaction wave) can be described in explicit analytic form. In particular, formulas for the isentropic case where $p \cdot \rho^{-\gamma}$ is a (known) constant, are given in [2], coinciding of course with the formulas in [1, §3.2].

Taylor then proceeds to study spherical detonation waves from a formal standpoint, i.e. the gas flow is now 3-dimensional but spherically symmetric. The resulting equations, although quite similar to the ones in the plane case, admit no longer a simple analytic solution, but must be solved numerically. Some solution profiles can be found in [2], but the question whether spherical detonations can be reproduced experimentally is left open to discussion.

The 1D-detonation theory provides reasonable estimates for pressures, densities, temperatures and velocities of gas detonations in semi-infinite, unconfined geometry (provided the length scale of interest is much larger than the detonation cell width of the mixture) [3]. The main point of interest of the current studies are, however, the dynamic loads which can be created by a gas detonation to a confining wall. The magnitude of these loads depends sensitively on the shape and orientation of the wall with respect to the incident detonation front. For instance, the peak detonation pressure exerted to the wall increases in the following order: diverging wall shape, side-on position, oblique reflection, normal reflection, 2D-focussing in edge, 3D-focussing in corner.

Aside from the wall/wave front orientation, additional effects can significantly influence detonation loads in 3D-geometries:

- diffraction of a detonation front at a corner, and
- superposition of different detonation fronts, e.g. behind an obstacle, or due to symmetry conditions.

In the very complex geometry of the ITER vacuum vessel, all these effects can influence the magnitude of local detonation pressures and impulses. For a given initial condition in the vessel, realistic and not too conservative dynamic loads can only be determined with a full 3D-simulation of the detonation front progression.

In the present analysis, the two different codes DET3D and GASFLOW are applied and compared. DET3D has been extensively verified for H_2-air detonations, and serves as benchmark code for GASFLOW detonation calculations [4, 5, 6]. The two existing codes were applied to investigate the sensivity of the results to variation of the grid geometry (Cartesian, cylindrical), the spatial resolution (factor 5 in cell numbers), the type of the numerical solver (explicit, semi-implicit), and the order of the solution scheme (first and second order).

2 Short description of computer codes

2.1 DET3D

DET3D is a finite difference code for the numerical simulation of multicomponent gaseous detonations describing the chemical reactions between H_2 and O_2 [7]. Since gaseous detonations are very fast processes - the usual velocity of a hydrogen-air detonation wave is 1500 m/s and more - it is not necessary to include in the physical modeling effects like molecular diffusion, turbulence, radiation or heat conduction. It suffices to numerically solve the Euler equations of compressible gas dynamics for a mixture consisting of N chemically reacting gaseous components with the addition of a source term in the component mass equations that models changes in the component densities due to the chemical reactions. In DET3D, these source terms are sums of elementary chemical reactions whose reaction rates are governed by an Arrhenius law. Both the number of the gaseous components as well as the number of the chemical reactions (including the Arrhenius constants) can be freely chosen by the user. As for the thermodynamic properties, each component is assumed to be an ideal gas. The specific heats and enthalpies are temperature dependent polynomials, obtained by interpolating the data given in the JANAF tables [8].

As numerical solver, DET3D uses a modern shock capturing scheme [9] which automatically computes such phenomena as the interaction of shock waves or the reflection of a shock wave at a wall. The solution algorithm is explicit, uses finite differences and works on a Cartesian equidistant grid. When doing calculations with DET3D, the user can choose between a first- and a second-order version of this algorithm. The second-order has the advantage of generating 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 often are not so important in large-scale applications, except when local information is needed.

2.2 GASFLOW

The GASFLOW code has been developed in a cooperation between Los Alamos National Laboratory (LANL) and Forschungszentrum Karlsruhe (FZK) [10, 11]. GASFLOW is a 3D-fluid dynamics field code which is used to analyze 3D-flow phenomena such as circulation patterns; flow stratification; hydrogen distribution mixing and stratification; combustion and flame propagation; effects of noncondensable gas distribution on local condensation and evaporation; and aerosol entrainment, transport, and deposition [12, 13, 14, 15, 16, 17, 18].

GASFLOW is a finite-volume code based on robust computational fluid dynamics techniques that solve the compressive Navier-Stokes equations for 3D-volumes in Cartesian and cylindrical coordinates. A semi-implicit solver is used to allow large time steps. The code can model geometrically complex facilities with multiple compartments and internal structures, and has transport equations for multiple gas species, liquid water droplets, and total fluid internal energy. A built-in library contains the properties of 23 gas species and liquid water.

GASFLOW can simulate the effects of two-phase dynamics with the homogeneous equilibrium model, two-phase heat transfer to and from walls and internal structures, catalytic hydrogen recombination and combustion processes, and fluid turbulence. For this particular task a special option of the GASFLOW code was used which only solves the Euler equations (no molecular transport processes).

3 Validation of DET3D and GASFLOW with balloon detonation tests

In order to validate 3D-deflagration/detonation codes available at FZK, several series of experiments were executed at the RUT test facility [19, 20]. Additionally, special H_2-air detonation tests were performed within an earlier FZK project [21, 22]. These experiments were simulated with DET3D and GASFLOW to compare and validate the codes prior to the ITER-FEAT application.

Fig.1 gives a top view of the experimental setup. A hemispherical balloon of 2.95 m radius was filled with stoichiometric H_2-air mixture and centrally ignited with a small high-explosive charge. Pressure gauges were mounted flush with the ground surface at different distances from the central ignition point along two lines of sight.

Fig.2 compares the measured and calculated pressure histories at two different positions, one inside the H_2-air mixture (r = 0.75 m) and one outside of the balloon (r = 6.25 m). The pressure traces are very different at the two positions for certain plausible physical reasons, but both codes are able to reproduce the main features of the measured data, except that the semi-implicit scheme of GASFLOW misses weak shocks, like e.g. the reflection wave from the H_2-air / air interface (Fig.2, top, 3 to 4 ms).

4 ITER-FEAT detonation simulation

4.1 Modeling assumptions

This section describes the modeling assumptions made in the DET3D and GASFLOW calculations (Table 1).

4.1.1 Vessel geometry

Shape and dimensions of the vacuum vessel and the attached upper, middle and lower ports were taken from the CATIA model of the ITER team (version of February 25, 2000).

The DET3D geometry model uses about 2.2 million cubic grid cells of 15 cm length to describe the very complex structure of the torus with attached ports in full 360° symmetry (Fig.3). The DET3D geometry input file contains the vessel dimensions in absolute units (meter), and is written in such a way that finer grids of the ITER-FEAT vessel, e.g. with 10 cm-grid-cells, can be generated automatically. This offers the possibility for easy grid convergence studies.

The geometry model of GASFLOW is based on a non-equidistant cylindrical mesh, using about 430.000 computational nodes (Fig.6a). The cylindrical mesh allows a reasonable approximation of the ITER-FEAT geometry with relatively few mesh cells.

TABLE 1
Modeled volumes of vessel and mixture cloud

	free vessel volume (m^3)	H_2 – air cloud (m^3)
DET3D	2262	290.6
GASFLOW	2048	284

4.1.2 Initial conditions

Contrary to future more mechanistic calculations, the initial conditions of this first analysis were postulated with the aim to generate a combustion event for 5 kg of H_2 which would result in maximum mechanical loads to the torus surface and to the ports. This kind of "first approach" analysis provides data to investigate the limiting hydrogen amount the vessel can withstand.

The following parameters were selected for this purpose:

- stoichiometric mixture of H_2 and air (29.6 % H_2),
- local concentration of the stoichiometric H_2-air mixture in a wedge-shaped region of the vessel, air in the remainder vessel volume (Fig.6b),
- detonation ignition in this mixture at the inner wall of the torus (Fig.6b) ,
- initial gas temperature 140°C (= operating temperature of walls),
- initial gas pressure 1 bar,
- no internal structures in the ports.

When the initial conditions are kept as described, except that the mass of the reacting hydrogen is increased from 5 to 10 kg, the following modification of the dynamic loads to the vacuum vessel can be expected:

- the total area of the vessel experiencing detonation pressures would double (wedge-shaped cloud of stoichiometric H_2-air mixture would cover twice the azimuthal angle as before),
- the local peak detonation pressures and impulses in the vessel region filled by the reacting cloud would remain as before,
- the shock waves traveling from the detonation cloud to the remainder of the (air-filled) vessel would decay more slowly, due to the increased energy release,
- the final pressure increase in the vessel after decay of the shock waves (on the order of 100 ms after ignition) would be twice as high.

Altogether, the increased hydrogen mass and combustion energy release would essentially lead to larger loaded surfaces. The local peak detonation pressures in the reacting cloud remain practically the same. Outside of the cloud, the impulses tend to increase, because larger masses of moving gas are created. The increased hydrogen mass would mainly affect potential global failure modes. Local failure modes would not be challenged to a significantly

larger extent.
In the investigated scenario as defined here, detonation conditions occur only in the reacting wedge-shaped H_2-air cloud of about 284 m^3 volume. The pressure waves created in this part of the vessel volume travel through the remaining other air-filled part without further support by chemical energy release. Gas expansion and momentum loss in the 54 ports extending from the torus rapidly decrease the gas velocities and the peak pressure in the front. About 25 ms after ignition, the two weak pressure wave fronts of about two bar peak pressure interact opposite to the ignition location on the other side of the torus, creating a superposition to only about 4 bar.

If the whole vessel volume would be filled with stoichiometric H_2-air mixture, two fully developed detonation fronts would meet opposite of the ignition location. A corresponding GASFLOW calculation showed the expected front pressures (≈ 24 bar), but also very high local pressures from wave collisions in the burned gas (≈ 50 bar), due to 3D-symmetry conditions of the flow field. This test calculation indicated that, depending on the assumed ignition location and the gas distribution, the symmetric torus geometry of the ITER vacuum vessel can create special 3D-focal points with high local pressures.

4.1.3 Numerical solution schemes

The detailed results of a CFD calculation depend on the applied numerical solution algorithm. Different solvers and time step control mechanisms were used to investigate the sensitivity of DET3D and GASFLOW results (e.g. detonation speed and maximum pressures) on the numerical method. DET3D employs HLL*) solvers of first and second order. GASFLOW offers a choice between a first order "Donor cell" and a "van Leer" solver.

Test calculations have shown that the initial detonation wave can be reasonably well represented by first-order schemes, but that resolution of the reverberations in the burnt gas requires second-order methods. Therefore second-order solvers were used for the ITER-FEAT simulations. A comparison between some selected first- and second-order results is shown in Fig.8.

4.2 DET3D results

The development of the pressure 1 ms after igniting a stoichiometric mixture of 5 kg H_2 and air at the inner torus wall is depicted in Fig.4 which gives a 3D-view of the torus and the pressure field. At this time, the detonation wave has not yet been touching the torus wall, and therefore has kept its spherical shape. Its maximum pressure attains about 10 bar.

An overview of the pressure development between 1 and 6 ms is shown in Fig.5 with a vertical cut through the torus geometry and the pressure field. It is found that, e.g. 2 ms after ignition, the torus wall is loaded with high reflected pressures of about 15 bar. Detailed local pressure histories are presented for 3 positions at mid-plane height: in some distance from the entrance to the central port (3), in some distance after the entrance (2), and at the end wall of this port (1).

At 1 ms, the initial detonation wave has not yet reached position 3 (Fig. 5, top). The area marked in black retains a pressure value of 1 bar until about 1.2 ms as shown in the pressure history plot. Later, two pressure peaks are observed there, the initial one reaching 12 bar at

*) HLL is short for Harten, Lax, van Leer [9].

about 1.25 ms, and the second one, much flatter, reaching 8.5 bar at about 3.4 ms which is caused by wave reflections.

Pressures of about 15 bar occur near the torus wall at 2 ms. This area is marked in white and lies between positions 2 and 3. Therefore, this pressure peak can not been found in the pressure history plot. As the peak related to position 2 does not occur before about 2.4 ms, position 2 is still marked black indicating the initial pressure of 1 bar.

At 3 ms, the detonation wave front has been propagating into the ports. Near-wall areas marked in white between positions 1 and 2, and also in the upper and lower ports indicate side-on reflected pressures of close to 15 bar. At the same time, the contour lines of the area marked in gray along the torus wall suggests a reflected detonation wave front moving back to the ignition point.

At 6 ms, the situation in position 1 has already passed the pressure peak of 24 bar calculated for the time of 3.5 ms, and the pressure level there is back to roughly 7 bar, indicated by gray color (Fig.5, bottom). Wide areas of the torus cross-section are marked in dark gray which points to a pressure level close to 1 bar. The detonation wave reflected at the torus wall has moved back to the area around the ignition point which is marked in white.

4.3 GASFLOW results

A view of the calculated hydrogen concentration contours is shown in an equatorial cut through the torus for the time period between 1.016 and 4.082 ms (Fig.7). As the figure suggests, the H_2-air mixture is being burnt off continuously from the ignition point to the end walls of the ports, without any variation in azimuthal direction. After approx. 5 ms, the chemical reaction is terminated.

The pressure waves initiated by this chemical reaction at first propagate in the mixture area, with peak values occurring when the detonation front is reflected at walls. These reflections, on the other hand, cause a multi-directional spreading of the detonation energy in the torus vessel, gradually leading to reduced pressure levels .

5 Comparison of results

For comparison of DET3D and GASFLOW results, calculated detonation wave parameters and the pressure histories at two locations within the reactive H_2-air cloud were analyzed.

5.1 Detonation wave parameters

Table 2 summarizes the detonation velocity and peak pressures calculated with DET3D and GASFLOW. For the investigated mixture (29.6% H_2, 140°C, 1 bar) the equilibrium thermodynamics code STANJAN predicts a planar wave speed of 1957 m/s and a CJ-pressure*) of 11.4 bar for a planar detonation front. A spherical wave is about 6.8% slower, which gives 1824 m/s as the theoretical reference value for the ITER-FEAT condition.

The detonation speeds calculated with DET3D and GASFLOW using different solvers are within a few percent of the theoretical value. DET3D reproduces also the expected CJ-pressure, whereas GASFLOW shows peak pressures which are about 10 to 20% too low even

*) CJ stands for Chapman-Jouguet [23].

with the nominally second-order "van Leer" solver.

TABLE 2
Comparison of theoretical CJ-detonation speed and pressure based on STANJAN calculation to results of different numerical simulations. Mixture 29.6% H_2 in air (stoichiometric), 140 °C, 1bar.

	D (m/s)	P_{max} (bar)
STANJAN, CJ parameter		
- plane wave	1957	11.4
- spherical wave	1824	≈ 11.3
DET3D		
- HLL, 1st order, automatic time step	1809	11.2
- HLL, 2nd order, automatic time step	1820	12.9
GASFLOW		
- Donor cell, 1st order, automatic time step	1779	9.35
- van Leer, 2nd order, automatic time step	1810	9.9

5.2 Local pressure histories

Two positions within the reactive H_2-air cloud were selected for detailed comparison of local pressure histories. The first one at the entrance to the central port at mid-plane height, the second at the end wall of this port. Fig.8a depicts calculated pressures for the first point. The time of arrival of the detonation front at this point was about 0.5 ms later in the GASFLOW calculation than in the DET3D calculation. This delay is due to dimensional differences in the two geometry models, which could not be avoided completely with the two different computational grids (cylindrical vs. Cartesian).

The first peak in Fig.8a represents the initial detonation wave, the remaining peaks are due to reflected pressure waves in the burnt gas and surrounding air. The predicted shapes of the detonation wave are similar, although the GASFLOW pressures are consistently below the DET3D values. Quite significant pressure differences are observed for the reverberations in the burned gas (e.g. at 3 ms). The DET3D second-order calculation resolves the reverberations much better than the first-order calculation. Both GASFLOW calculations resemble the first-order DET3D result, showing the same peak pattern. The time differences between the peaks of DET3D and GASFLOW are due to the differences in the geometrical dimensions of the used vessel model and the different numerical diffusion effects of the used solvers.

Fig.8b compares the calculated pressure loads at the end wall of the central port in mid-plane. Thermodynamic equilibrium calculations predict that the normal reflection of the incoming detonation wave should increase the peak pressure by about a factor of 2.3. This is well obeyed by the DET3D result, whereas GASFLOW shows a substantial pressure deficit for the initial peak detonation pressure. The second-order DET3D calculation shows two additional weak shock reflections which are not resolved in the other computations. Aside from the semi-implicit solver, another possible reason for the lower detonation peak pressure of the GASFLOW calculation may be the divergence of the port geometry in azimuthal direction, which is an unavoidable geometry effect of the used cylindrical grid.

In summary, Figs.8a and 8b show typical worst-case values for side-on and normally reflected pressures on vessel and port walls from the detonation of 5 kg hydrogen. The discussed differences in peak pressures and timing are mainly due to different numerical solution algorithms and the current geometrical representations of the ITER-FEAT vessel. The uncertainty contribution from the geometry model can be reduced by a further refined future vessel model. The second-order, explicit, high-resolution calculation with DET3D clearly provides the best results of the tested modeling approaches. DET3D should be the preferred tool for numerical solution of detonation generated pressure loads in ITER accident sequences.

5.3 Local impulses*)

Depending on the ratio of loading time T_{load} to natural period of the loaded structure T_{osc}, either the peak pressure ($T_{osc} << T_{load}$) or the impulse ($T_{osc} >> T_{load}$) can determine the dynamic response of the structure [24]. The impulse may therefore be an important quantity, needed to evaluate the maximum elongation of the ITER-FEAT vessel.

The range of impulses computed for the 5-kg-H_2-detonation is shown in Fig.9, using the pressure curves of DET3D from Fig.8. The shown values were calculated from the predicted overpressures according to

$$I(t) = \int_0^t [p(\tau) - p_o] d\tau \qquad (1)$$

where p_0 = initial pressure before arrival of detonation wave.

Although the time-dependent pressure histories show noticeable deviations between the first and second order result (e.g. Fig.8a), the impulses are very similar for both computations (Fig.9, side-on impulse). The first-order calculation tends to broaden and flatten the pressure peaks which are better resolved with higher-order differencing schemes, but it conserves the wave impulse.

5.4 Scaling of 1D-calculations

For hydrogen-air-steam mixtures with up to 30% hydrogen and up to 40% steam, the following approximate relations were derived for the wave parameters in 1D-planar detonations [25]:

The detonation peak pressure p_{det} is proportional to the adiabatic-isochoric-complete-combustion pressure p_{aicc} of the mixture and independent of the scale x of the reacting gas cloud:

$$p_{det} \approx 1.8(\pm 0.1) \cdot p_{aicc} \qquad (2)$$

The detonation impulse i_{det} increases with p_{aicc} and with the scale x. The sound velocity a is approximately constant for the above mentioned mixtures (960 ± 100 m/s):

$$i_{det} \approx 0.24 \cdot p_{aicc} \cdot x / a \qquad (3)$$

*) Impulse means overpressure integrated vs. time (Pa·s) in contrast to momentum which is the time integral of a force (N·s).

The load duration T_{det} from the pressure wave following immediately the detonation front (the so-called Taylor wave) is mainly determined by the scale x and depends only weakly on the mixture composition due to the sound velocity a:

$$T_{det} \approx 0.21 \cdot x / a \quad (4)$$

6 Summary and conclusions

To better define and justify in-vessel hydrogen limits for the ITER-FEAT safety assessment and licensing process, three-dimensional distribution / deflagration / detonation calculations are being performed for various accident sequences.

The first investigated scenario assumed air ingress, production of 5 kg hydrogen, formation of a local stoichiometric hydrogen-air mixture and ignition of a local detonation.

The mechanical loads from the detonation to the vessel and the ports were investigated with the 3D-codes DET3D and GASFLOW. Both codes were validated against experimental data, one example is discussed in Fig.2. A geometry model of the ITER-FEAT vessel was developed for each code and used for numerical simulation of the generated pressure loads. The best results were obtained with the second-order DET3D calculation.
The loading in the complex ITER-FEAT geometry consists of three different contributions:

- the initial detonation wave in the region of the reactive H_2-air mixture,
- pressure waves in the burnt gas and in the air volume, which are due to the gas flows created by the chemical energy release, and
- the quasistatic long-term combustion pressure, which remains after dampening of the gas flows in the enclosure.

The highest pressures are generated by the initial detonation wave. The peak pressure value reached depends on the angle of incidence of the detonation wave with respect to the confining surface. For side-on orientation (wave surface perpendicular to the structure), peak pressures of about 10 bar were predicted (Fig.8a). For normal reflection of the detonation wave, pressures around 25 bar were calculated for the assumed scenario (Fig.8b). Focussing of the detonation wave in multidimensional reflectors should create even higher local transient pressures. It is important to note that the calculated pressures represent only short transient loads, they should not be confused with the static design pressure of the vessel.

It is known that gaseous detonations have a three-dimensional structure due to the collision of transverse waves. High resolution calculations have shown that the wave front possesses a fine structure in terms of local pressures which is of the order of the so-called detonation cell width λ (λ = 1.5 cm in the present case). The grids used in the described calculations are too coarse to resolve this fine structure. Therefore, the calculated front pressures represent average values, which are adequate for the structural response calculations as long as the characteristic dimension of the loaded structure is much larger than λ. This is the case in the present ITER-FEAT analysis (meters vs. centimeters).

Typical results on impulse data have been obtained. The detonation impulses are due to the directed gas flow. In fully developed H_2-air detonations, the particle velocity reaches about 1000 m/s. The reflected impulses calculated for the 5kg-H_2-detonation (Fig.9) correspond roughly to the collision of a passenger car at medium traffic velocity ($I = m \cdot v / A$, e.g.

$I = 1000\ kg \cdot 10\ m/s / 2\ m^2 = 5\ kPa \cdot s$) which compares well with results obtained from 1D-simulations [1]. As for the gas temperatures, values up to 3500 K have been calculated.

The obtained results represent an adequate data base for future investigations of the structural behavior and integrity of the ITER-FEAT vacuum vessel. Future work also will include deterministic analyses of combined hydrogen distribution and combustion sequences. The best approach will be to calculate distribution processes with GASFLOW and combustion events with COM3D.

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8 Appendix

8.1 DET3D input data (DET3D vers. 2)

```
-----------------------------------------------------------------------------------------------------------------------------
25.56  11.771 25.56  0.15035294      # dimensions (x,y,z), mesh size [m]
4   1                                # number of components and reactions

2.0                       component 1:  molar weight (g/mole)
0.0                                     enthalpy of formation (kJ/mole)
-846.56  28.917  .001251                enthalpy coefficients (/mole)
23.314                                  cp-coefficients (/mole)
 3.1871e-02 -7.0165e-05  8.1860e-08          (index 0 -> 9)
-5.2914e-11  2.0487e-14 -4.8821e-18
 7.0237e-22 -5.5985e-26  1.8989e-30

32.0                      component 2:  molar weight (g/mole)
0.0                                     enthalpy of formation (kJ/mole)
-2258.9  33.189  0.0010451              enthalpy coefficients (/mole)
30.000                                  cp-coefficients (/mole)
-1.3554e-02  5.8690e-05 -7.4377e-08          (index 0 -> 9)
 4.9546e-11 -1.9506e-14  4.6982e-18
-6.8066e-22  5.4504e-26 -1.8542e-30

28.0                      component 3:  molar weight (g/mole)
0.0                                     enthalpy of formation (kJ/mole)
-2399.9  32.705  6.04e-4                enthalpy coefficients (/mole)
31.255                                  cp-coefficients (/mole)
-1.9106e-02  5.0961e-05 -5.0938e-08          (index 0 -> 9)
 2.8403e-11 -9.7408e-15  2.1017e-18
-2.7826e-22  2.0662e-26 -6.5892e-31

18.0                      component 4:  molar weight (g/mole)
-239.0                                  enthalpy of formation (kJ/mole)
-5031.2  39.85  2.5366e-3               enthalpy coefficients (/mole)
34.021                                  cp-coefficients (/mole)
-8.9246e-03  3.2019e-05 -2.1678e-08          (index 0 -> 9)
 6.9461e-12 -9.7708e-16 -2.8390e-20
 2.9077e-23 -3.6943e-27  1.5870e-31

-2  -1  0   2             reaction 1: stoech. coeff. + Arrhenius:
10.  1. 73.  1.0                      B, n, E, Tkrit  (in k, except n)

0.9                       sigma    # Courant number

1                         imeth    # 1 = HLL
0                         cshall   # method for sound velocity: 0,1,2
1                         iterm    # 1 = primitive
2                         isteig   # hydrodynamic numerics
1.0                       sk       # factor for minmod, vleer etc (<=1)
1.3                       sk1      # ( only for supbee )
2.0                       sk2      # ( only for supbee )
1.3                       sk3      # ( only for supbee )
10                        qche11   # time step ratio: chemistry / hydrodyn.
1                         irea     # reaction numerics: 0=Euler,  1=Heun
0                         iinduk   # 0= no, 1=model 1, 2= model 2
2                         ichem    # 0=no kin., 1=rho-Arrhenius,
                                   # 2=usual Arrh.,
                                   # 3=Arrh.mod., 4=exo-model g.paczko
0                         ialgo    # 0=hll-che-che-hll..., 1=hll-che...,
                                   # 2=che-hll...
1                         cenerg   # 1=total energy, 0=no
```

```
1                          dimbeh   # 1=dimens. input, 0= no
1                          ceing    # 1=T,u,p, 0=rho,u,p
1                          calpha   # 1=volume, 0=mass (components)

.1    .3                   p0  trho0  # init. press. and density / temp.
0.  0.  0.                 vx0  vy0  vz0   # initial velocities
30.                        alf0 [0]   # initial amount of component 1
14.                        alf0 [1]   # initial amount of component 2
56.                        alf0 [2]   # initial amount of component 3
quit input
R 0.0 26.0 0.0 12.0 0.0 26.0
ITER
1 1 1
0.1 0.413 0. 0. 0.
1  0.
2 21.00841
3 78.99159
quit
0.37       # half angle in radiant
1 1 1
0.1 0.413 0. 0. 0.
1 29.5858
2 14.7929
3 55.6213
quit
r f   11.98 13.58    5.525 7.125   16.285 17.885
1 1 1
4.0 3.0   0. 0. 0.
1 29.5858
2 14.7929
3 55.6213
quit
N  12.78      2.28022   9.225        # gauges
N   9.225     2.28022  12.78
N  16.335     2.28022  12.78
N  12.78      2.28022  16.335
N   5.337     2.28022  12.78
N  20.223     2.28022  12.78

N  12.78      6.325     9.225
N   9.225     6.325    12.78
N  16.335     6.325    12.78
N  12.78      6.325    16.335

N  12.78      9.16797   9.225
N   9.225     9.16797  12.78
N  16.335     9.16797  12.78
N  12.78      9.16797  16.335
N   5.074     9.16797  12.78
N  20.486     9.16797  12.78
N  12.78      9.16797   5.074
N  12.78      9.16797  20.486

N  12.78     11.2      24.50
N  12.78     11.2       1.10
N  12.78      6.325    24.50
N  12.78      6.325     1.10
N  12.78      1.072    25.55
N  12.78      1.072     0.05

N   1.228    11.2      10.745
N   1.228    11.2      14.815
N  24.322    11.2      10.745
```

```
N  24.322    11.2      14.815
N   0.244     1.072    10.5625
N   0.244     1.072    14.9975
N  25.356     1.072    10.5625
N  25.356     1.072    14.9975

N  15.807     6.215    21.196
N  15.807     6.215     4.364
N  14.317     6.215    21.596
N  14.317     6.215     3.964
N  12.78      6.215    21.73
N  12.78      6.215     3.83
N  11.243     6.215    21.596
N  11.243     6.215     3.964
N   9.753     6.215    21.196
N   9.753     6.215     4.364

N  12.78      6.215    24.50
N  12.78      6.215    22.48375
N  12.78      6.215    20.4175
N  12.78      6.215    18.35125
N  12.78      6.215    16.335
N  12.78      6.215    23.115
N  12.78      6.215    19.0325

N   3.83      6.215    12.78
N  21.73      6.215    12.78
N   1.228     6.215    14.815
N  24.322     6.215    14.815
N   1.228     6.215    10.745
N  24.322     6.215    10.745

N  11.88      6.215    23.075
N  13.68      6.215    23.075
N   8.46      6.215    22.145
N  17.10      6.215    22.145
quit
quit
```

8.2 GASFLOW input data (GASFLOW vers. 2.2.3.3)

```
 $innet
 $end
 $xput

    geomodel(1:24,1) =+1.0, 1.0, 0.0, 0.0, 0.0, 000.0,
        1.0, 1.0, 1.0, -21684, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, -808.0,
        -1.0e+50, +1.0e+50, -1.0e+50, +1.0e+50, -1.0e+50, +1.0e+50,  0.0,

   ignitaut = 0,
            iburn = 1,
            ifvl = 0,

      ieopt = 2,
      trange = 'low ',
      icopt = 0,
      itopt = 1,

      tmodel    = 'none',
```

```
    idiffmom  = 0,
    idiffme   = 0,

         nrsdump  = 0,
         autot    = 1.0,
         cyl      = 1.0,
         delt0    = 0.00001,
         deltmin  = 0.100e-06,
         deltmax  = 0.001,
         epsi0    = 1.000e-06,
         epsimax  = 1.000e-06,
         epsimin  = 1.000e-06,
         iobpl    = 1,
         itdowndt = 500,
         itupdt   = 500,
         itmax    = 1000,
         lpr      = 1,
         maxcyc   = 20000,
         ittyfreq = 100,
;        pltdt    =  0.001, 0.0061, 0.002, 0.0101, 0.005, 0.0501,
         pltdt    =  0.001, 0.0065, 0.002, 0.0110, 0.005, 0.0520,
         prtdt    = 9100.,
         twfin    =  0.040,
         tddt     = 0100.0000,
         velmx    = 5.0,
         ibe      = 1,
         ibw      = 1,
         ibn      = 4,
         ibs      = 4,
         ibt      = 1,
         ibb      = 1,

         mat = 'h2', 'h2o', 'n2', 'o2',

  gasdef(1:40,1)=  1,'im1',  1,'jm1',  1,'km1',  1,  1.000e+06, 413.15, 2,
                 0.,  0., 'n2', 0.790, 'o2', 0.210, 'h2', 0.000, 22*0.0,

  gasdef(1:40,2)=  1,'im1', 21,   35,  1,'km1',  1,  1.000e+06, 413.15, 2,
                 0.,  0., 'n2', 0.556, 'o2', 0.148, 'h2', 0.296, 22*0.0,

  gasdef(1:40,3)=  1,'im1', 20,   21, 38, 'km1', 1,  1.000e+06, 413.15, 2,
                 0.,  0., 'n2', 0.556, 'o2', 0.148, 'h2', 0.296, 22*0.0,

  gasdef(1:40,4)=  1,'im1', 35,   36, 38, 'km1', 1,  1.000e+06, 413.15, 2,
                 0.,  0., 'n2', 0.556, 'o2', 0.148, 'h2', 0.296, 22*0.0,

  gasdef(1:40,5)=  1,    2, 27,   29, 30,   31,  1,  1.515e+07,3200.00, 2,
                 0.,  0., 'n2', 0.69, 'o2', 0.00,'h2o', 0.31, 22*0.0,

  holes(1:13,01)=   1, 68,   2,   6, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
  holes(1:13,02)=   1, 61,   2,   6, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
  holes(1:13,03)=  10, 63,   2,   6, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

  holes(1:13,04)=   1, 68,   8,  12, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
  holes(1:13,05)=   1, 61,   8,  12, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
  holes(1:13,06)=  10, 63,   8,  12, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

  holes(1:13,07)=   1, 68,  14,  18, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
  holes(1:13,08)=   1, 61,  14,  18, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
  holes(1:13,09)=  10, 63,  14,  18, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

  holes(1:13,10)=   1, 68,  20,  24, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
  holes(1:13,11)=   1, 61,  20,  24, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
```

```
holes(1:13,12)=  10, 63,  20,  24, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,13)=   1, 68,  26,  30, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,14)=   1, 61,  26,  30, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,15)=  10, 63,  26,  30, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,16)=   1, 68,  32,  36, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,17)=   1, 61,  32,  36, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,18)=  10, 63,  32,  36, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,19)=   1, 68,  38,  42, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,20)=   1, 61,  38,  42, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,21)=  10, 63,  38,  42, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,22)=   1, 68,  44,  48, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,23)=   1, 61,  44,  48, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,24)=  10, 63,  44,  48, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,25)=   1, 68,  50,  54, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,26)=   1, 61,  50,  54, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,27)=  10, 63,  50,  54, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,28)=   1, 68,  56,  60, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,29)=   1, 61,  56,  60, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,30)=  10, 63,  56,  60, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,31)=   1, 68,  62,  66, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,32)=   1, 61,  62,  66, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,33)=  10, 63,  62,  66, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,34)=   1, 68,  68,  72, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,35)=   1, 61,  68,  72, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,36)=  10, 63,  68,  72, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,37)=   1, 68,  74,  78, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,38)=   1, 61,  74,  78, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,39)=  10, 63,  74,  78, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,40)=   1, 68,  80,  84, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,41)=   1, 61,  80,  84, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,42)=  10, 63,  80,  84, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,43)=   1, 68,  86,  90, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,44)=   1, 61,  86,  90, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,45)=  10, 63,  86,  90, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,46)=   1, 68,  92,  96, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,47)=   1, 61,  92,  96, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,48)=  10, 63,  92,  96, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,49)=   1, 68,  98, 102, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,50)=   1, 61,  98, 102, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,51)=  10, 63,  98, 102, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

holes(1:13,52)=   1, 68, 104, 108, 01, 14,   1,  0, 0,   -1, -1,  0, -1,
holes(1:13,53)=   1, 61, 104, 108, 24, 38,   1,  0, 0,   -1, -1, -1, -1,
holes(1:13,54)=  10, 63, 104, 108, 54, 61,   1, -1, 0,   -1, -1, -1,  0,

mobs(1:8,1)=   1,  2,   1, 109,   55, 61,    1, 0,
mobs(1:8,2)=   2,  4,   1, 109,   56, 61,    1, 0,
mobs(1:8,3)=   4,  5,   1, 109,   57, 61,    1, 0,
mobs(1:8,4)=   5,  7,   1, 109,   58, 61,    1, 0,
mobs(1:8,5)=   7,  8,   1, 109,   59, 61,    1, 0,
```

```
  mobs(1:8,6)=   8, 10,   1, 109,   60, 61,    1, 0,

$end
-----------------------------------------------------------------------
              h e a t - t r a n s f e r
-----------------------------------------------------------------------
$rheat

       ihtflag = 0,

$end
-----------------------------------------------------------------------
              m e s h
-----------------------------------------------------------------------
$meshgn

          iblock = 1,

 nkx = 5,
 xl(1) =  404.0, xc(1) =  404.0, nxl(1) = 0, nxr(1) = 40, dxmn(1) = 9999.,
 xl(2) =  834.0, xc(2) =  834.0, nxl(2) = 0, nxr(2) = 10, dxmn(2) =   12.,
 xl(3) = 1006.5, xc(3) = 1179.0, nxl(3) =10, nxr(3) =  0, dxmn(3) =   12.,
 xl(4) = 1179.0, xc(4) = 1179.0, nxl(4) = 0, nxr(4) =  2, dxmn(4) = 9999.,
 xl(5) = 1204.0, xc(5) = 1204.0, nxl(5) = 0, nxr(5) =  5, dxmn(5) = 9999.,
 xl(6) = 1274.0,

 nky = 1,
 yl(1) =   00.0, yc(1) =   00.0, nyl(1) = 0, nyr(1) = 108,dymn(1) = 9999.,
 yl(2) =  360.0,

 nkz = 1,
 zl(1) = -430.0, zc(1) = -430.0, nzl(1) = 0, nzr(1) = 60, dzmn(1) = 9999.,
 zl(2) =  430.0,

$end
-----------------------------------------------------------------------
              g r a p h i c s
-----------------------------------------------------------------------

$grafic

      thdt=0.00001,

  pnt(1:4,1) =      1,   28,     1,  1,   ; rz top
  pnt(1:4,2) =  'im1',   28, 'km1',  1,
  pnt(1:4,3) =      1,   55,     1,  1,   ; rz left, no port
  pnt(1:4,4) =  'im1',   55, 'km1',  1,
  pnt(1:4,5) =      1,   82,     1,  1,   ; rz bottom
  pnt(1:4,6) =  'im1',   82, 'km1',  1,
  pnt(1:4,7) =      1,    1,     8,  1,   ; xy bot
  pnt(1:4,8) =  'im1','jm1',     8,  1,
  pnt(1:4,9) =      1,    1,    31,  1,   ; xy med
  pnt(1:4,10) = 'im1','jm1',    31,  1,
  pnt(1:4,11) =     1,    1,    57,  1,   ; xy top
  pnt(1:4,12) = 'im1','jm1',    57,  1,
  pnt(1:4,13) =     1,   52,     1,  1,   ; rz left, port
  pnt(1:4,14) = 'im1',   52, 'km1',  1,

   c2d(1:4,1)  =  1,  2, 'vf',  'h2',
   c2d(1:4,2)  =  3,  4, 'vf',  'h2',
   c2d(1:4,3)  =  5,  6, 'vf',  'h2',
   c2d(1:4,4)  =  9, 10, 'vf',  'h2',
```

```
   c2d(1:4,5)  =  1,  2, 'pn',   0,
   c2d(1:4,6)  =  3,  4, 'pn',   0,
   c2d(1:4,7)  =  5,  6, 'pn',   0,
   c2d(1:4,8)  =  7,  8, 'pn',   0,
   c2d(1:4,9) =  9, 10, 'pn',   0,
   c2d(1:4,10) = 11, 12, 'pn',   0,
   c2d(1:4,11) = 13, 14, 'pn',   0,
   c2d(1:4,12) =  1,  2, 'tk',   0,

  thp(1:6,01) = 02, 28, 31, 1, 'pn',     0, ;2
  thp(1:6,02) = 20, 28, 31, 1, 'pn',     0, ;3
  thp(1:6,03) = 40, 28, 31, 1, 'pn',     0, ;4
  thp(1:6,04) = 50, 28, 31, 1, 'pn',     0, ;5
  thp(1:6,05) = 60, 28, 31, 1, 'pn',     0, ;6
  thp(1:6,06) = 50, 26, 31, 1, 'pn',     0, ;7
  thp(1:6,07) = 50, 29, 31, 1, 'pn',     0, ;8
  thp(1:6,08) = 67, 28, 07, 1, 'pn',     0, ;9

  thp(1:6,09) = 60, 52, 31, 1, 'pn',     0, ;10
  thp(1:6,10) = 02, 55, 31, 1, 'pn',     0, ;11
  thp(1:6,11) = 40, 55, 31, 1, 'pn',     0, ;12
  thp(1:6,12) = 60, 58, 31, 1, 'pn',     0, ;13
  thp(1:6,13) = 02, 82, 31, 1, 'pn',     0, ;14
  thp(1:6,14) = 60, 82, 31, 1, 'pn',     0, ;15

  thp(1:6,15) = 67, 52, 07, 1, 'pn',     0, ;16
  thp(1:6,16) = 40, 55, 07, 1, 'pn',     0, ;17
  thp(1:6,17) = 67, 58, 07, 1, 'pn',     0, ;18
  thp(1:6,18) = 67, 82, 07, 1, 'pn',     0, ;19

  thp(1:6,19) = 60, 28, 31, 1, 'tk',     0, ;

$end

$special

$end
$parts

$end
; -------------------------  end of data -----------------------------
; -------------------------------------------------------------------
```

No.	R(m)
1	0.75
2	1.50
3	2.75
4	3.25
5	5.00
6	7.50
7	1.00
8	2.25
9	4.00
10	6.25
11	10.00

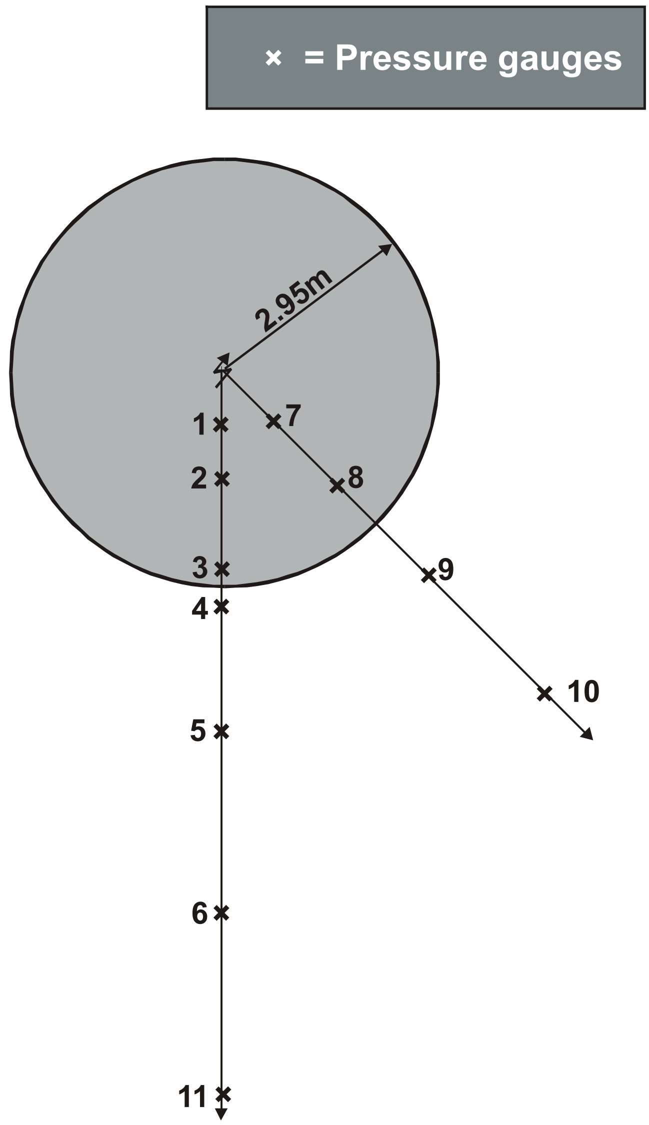

Fig. 1: Positions of the pressure gauges during the hydrogen-air detonation tests with a hemispherical balloon of 53 m^3 volume [FHG91].

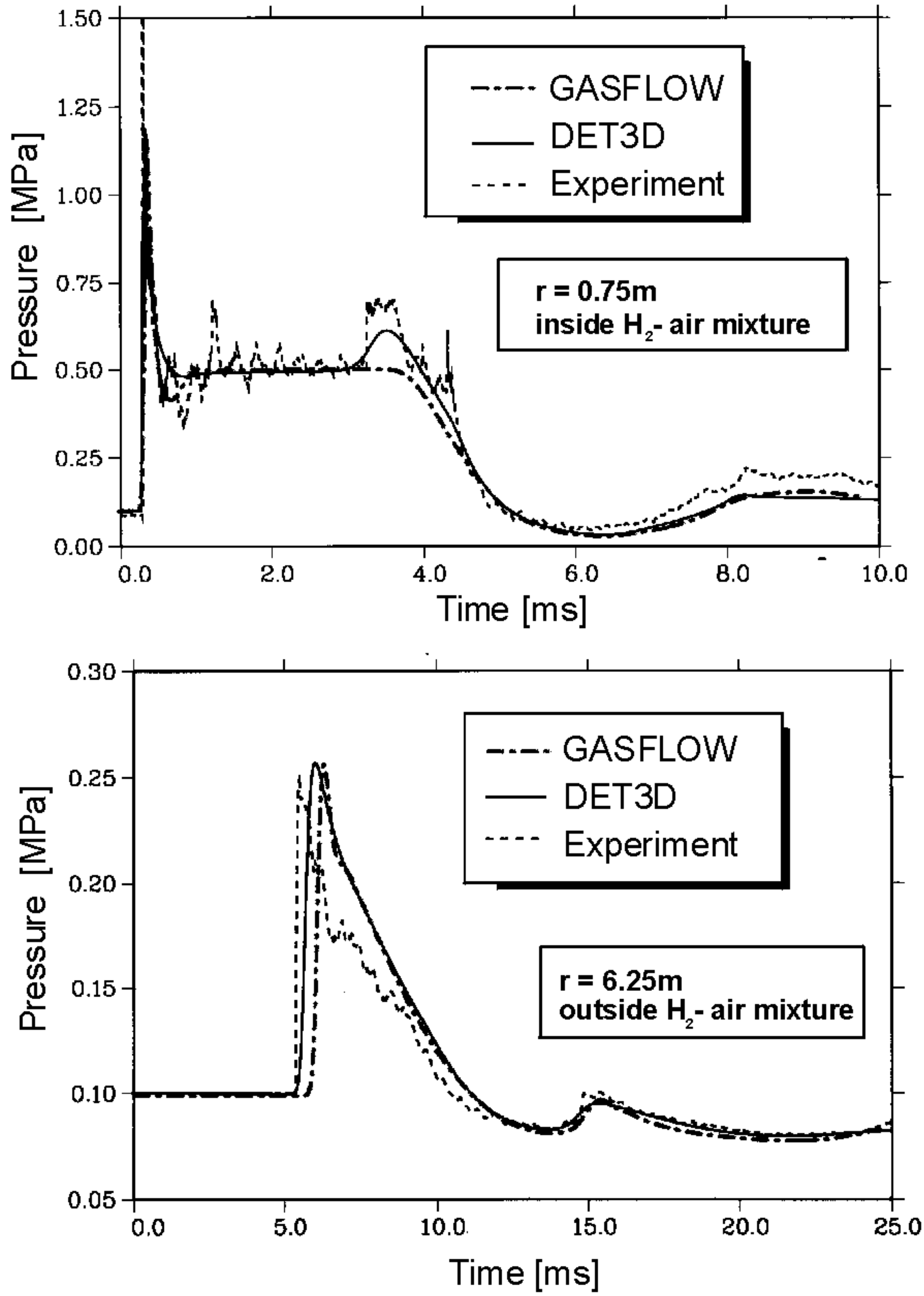

Fig. 2: GASFLOW and DET3D results compared with balloon detonation measurements [CON94].

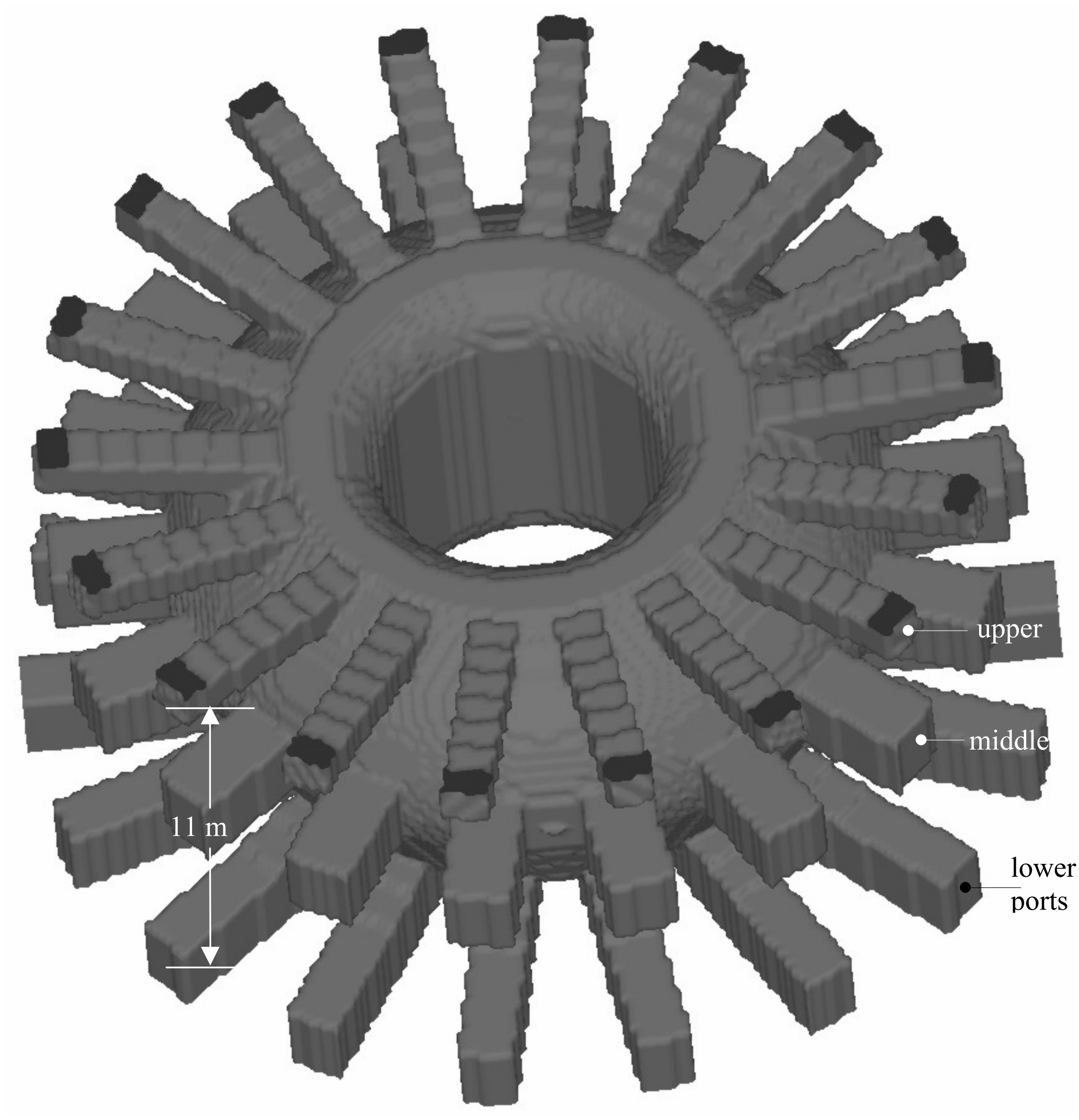

Fig. 3: Geometry model for the DET3D code using 2.2 million grid cells to simulate local detonation in ITER-FEAT.

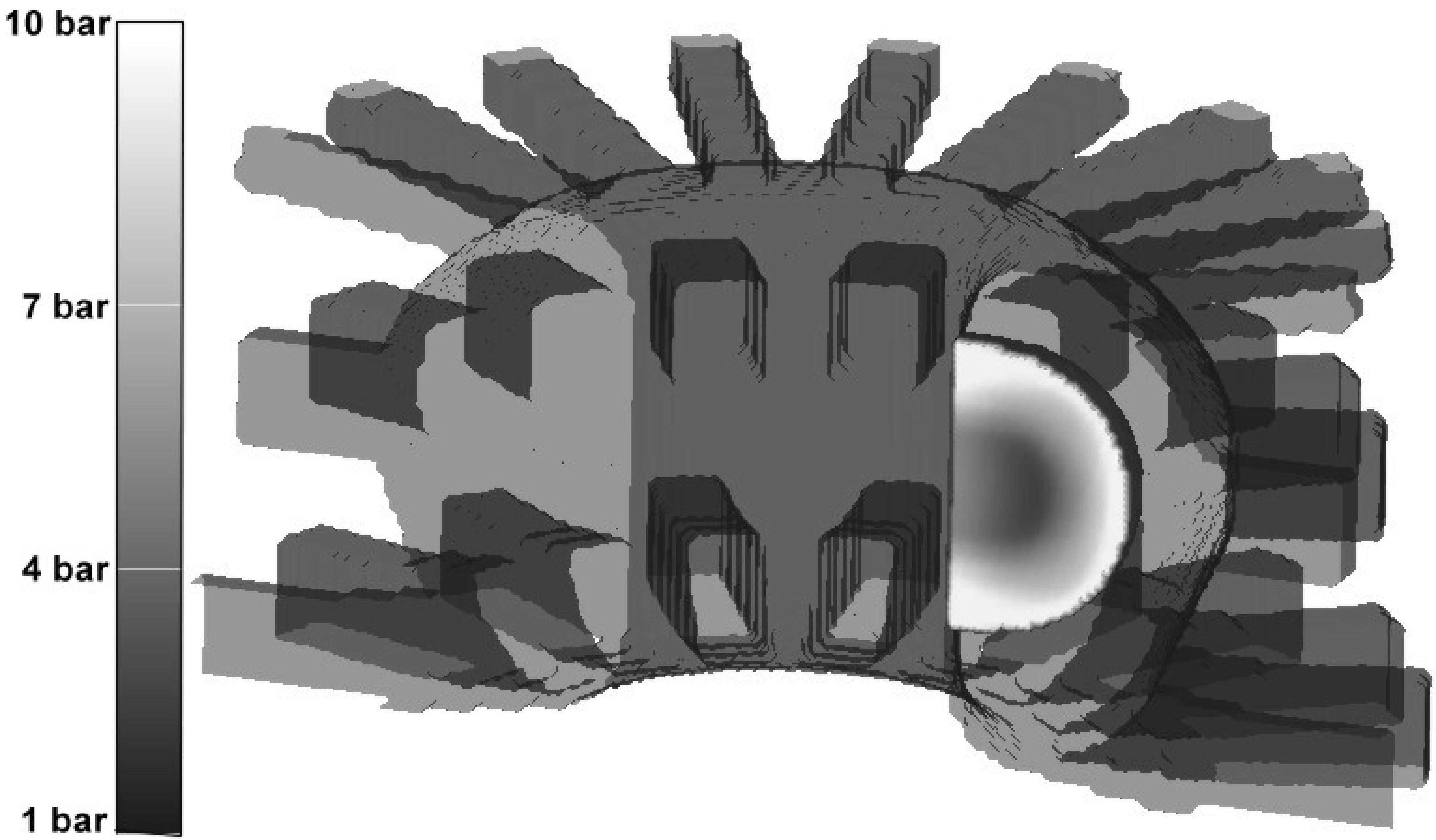

Fig 4: ITER-FEAT detonation simulation with DET3D, 1 ms after igniting a stoichiometric mixture of 5 kg H_2 and air at the inner torus wall, 3D pressure field.

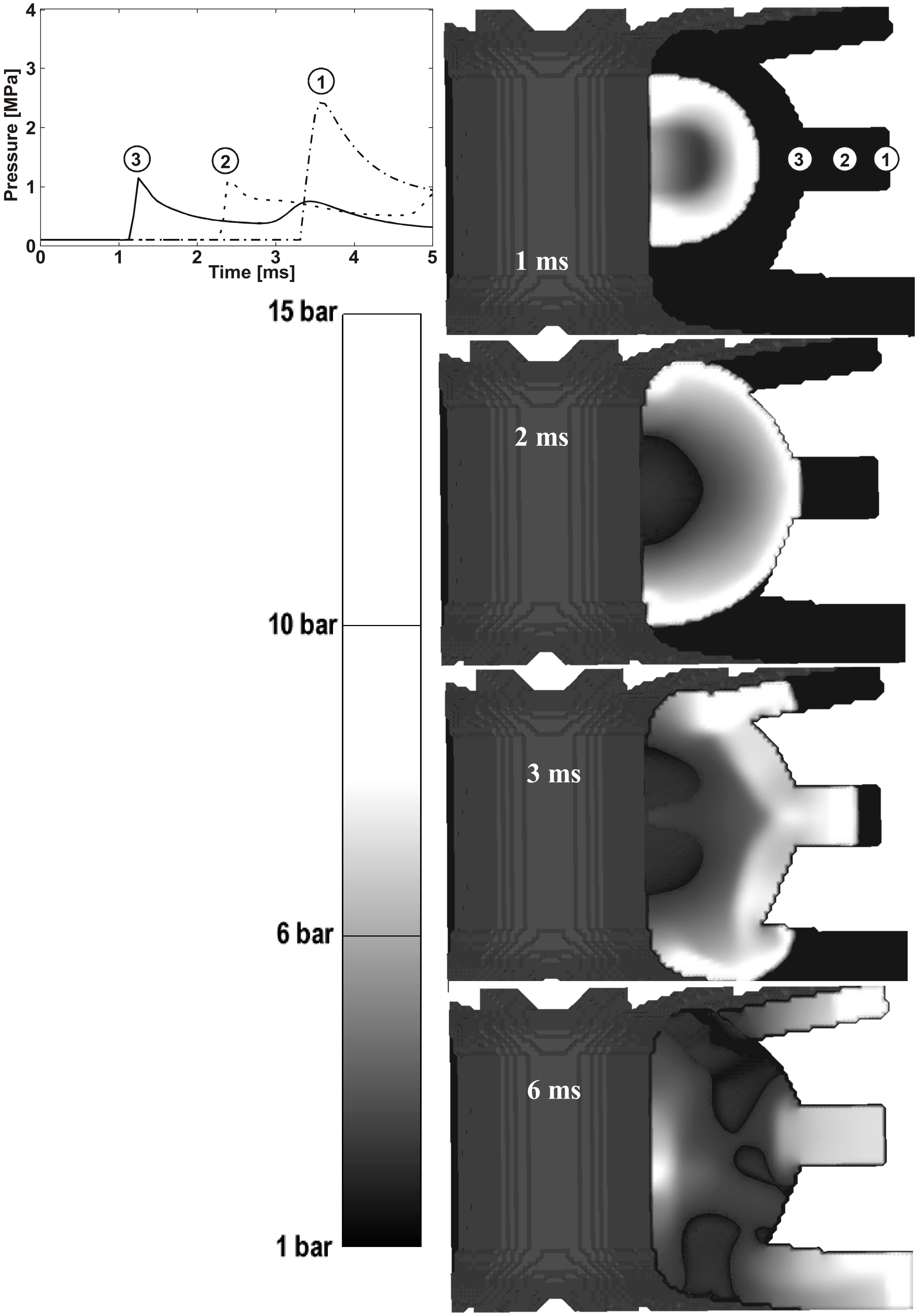

Fig. 5: ITER-FEAT detonation simulation with DET3D, vertical cut through geometry and pressure field

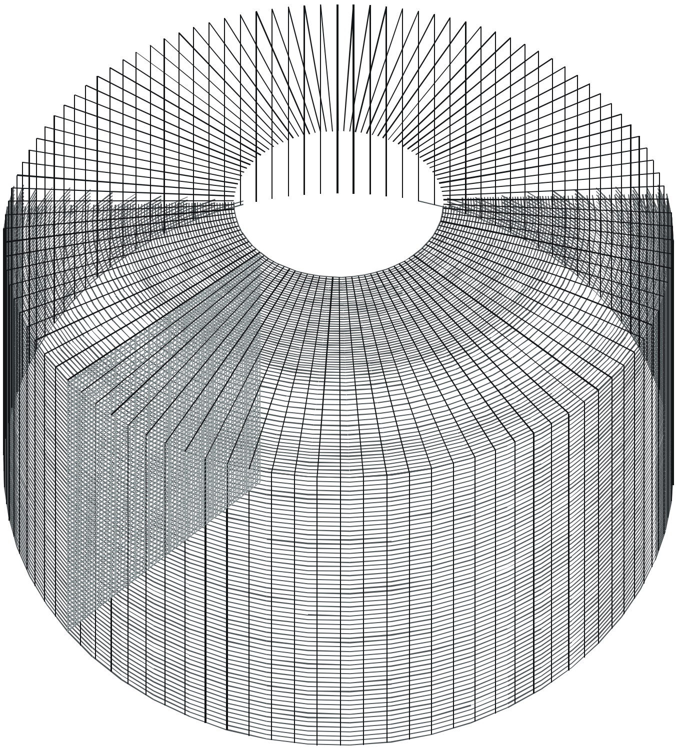

Fig. 6a: **Cylindrical grid of GASFLOW calculation using 67 x 108 x 60 ≈ 430.000 nodes**

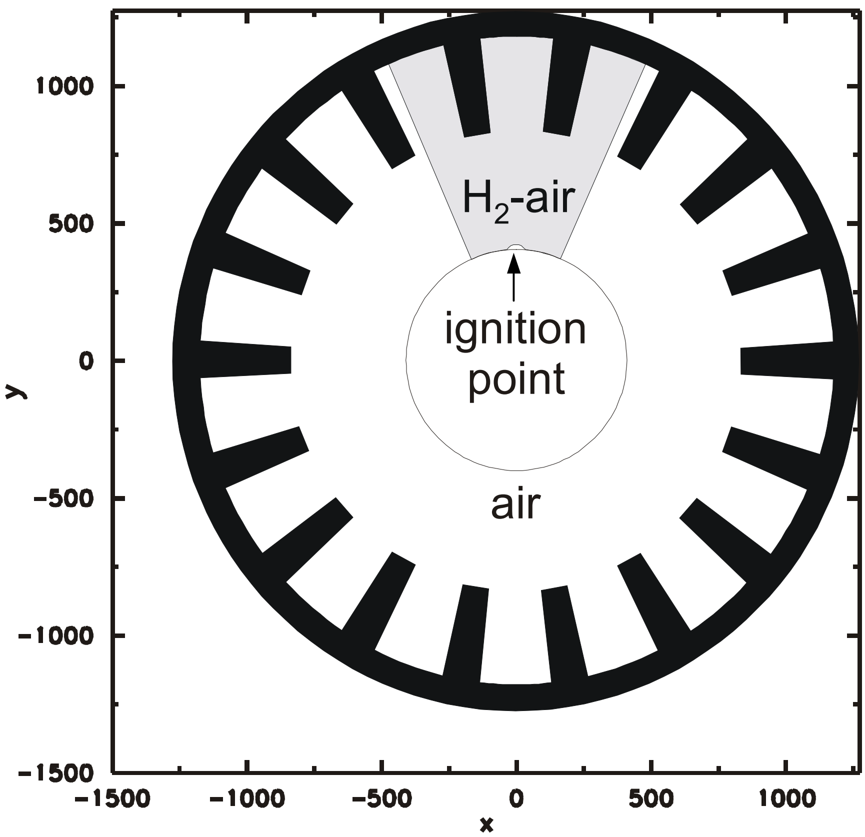

Fig. 6b: **GASFLOW calculation:**
Equatorial cut through the torus with 18 middle ports and initial hydrogen distribution for case 1.

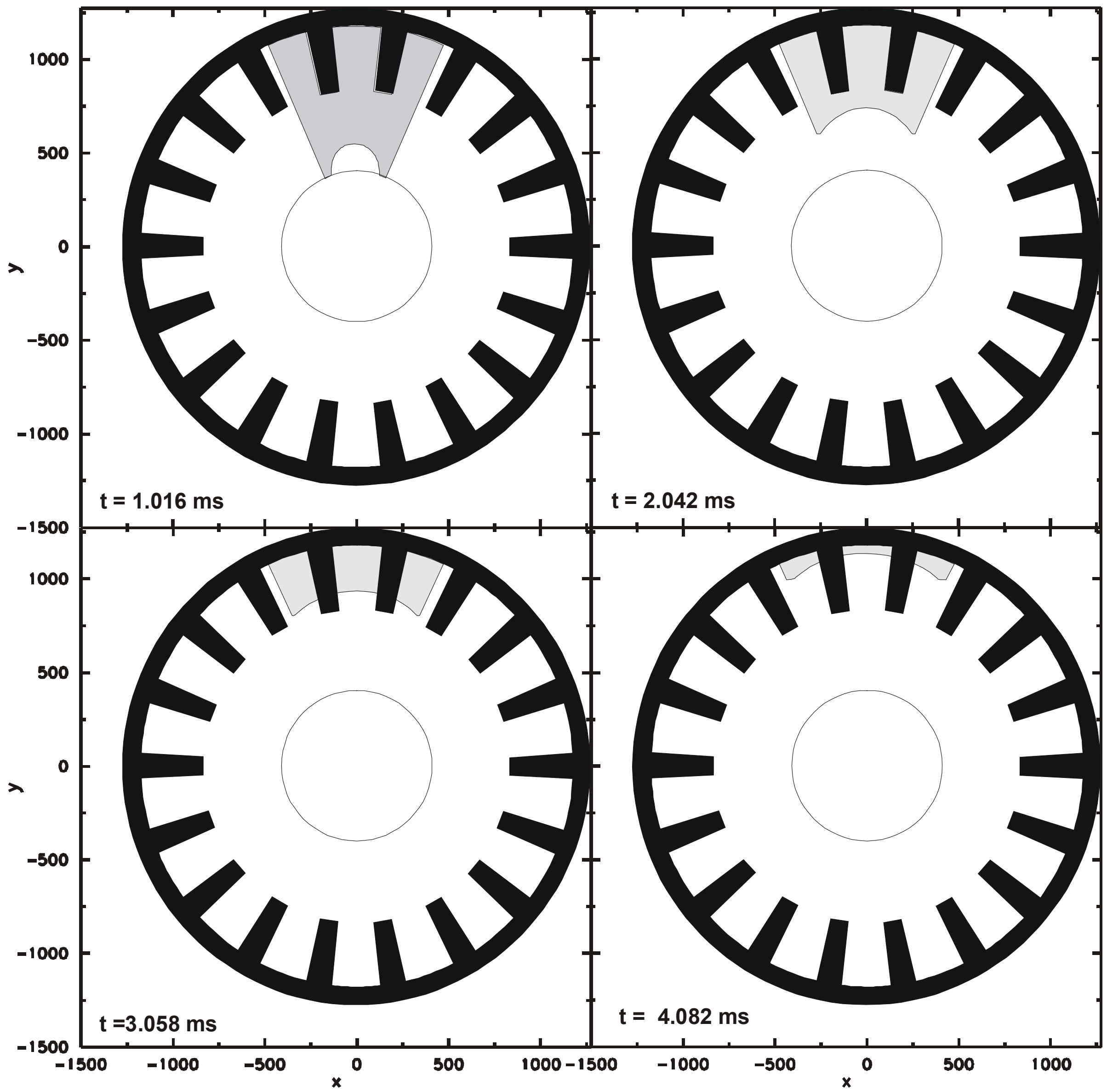

Fig. 7: GASFLOW calculation:
Equatorial cut through the torus showing the hydrogen concentration contours in the time period 1.016 ≤ t ≤ 4.082 ms.

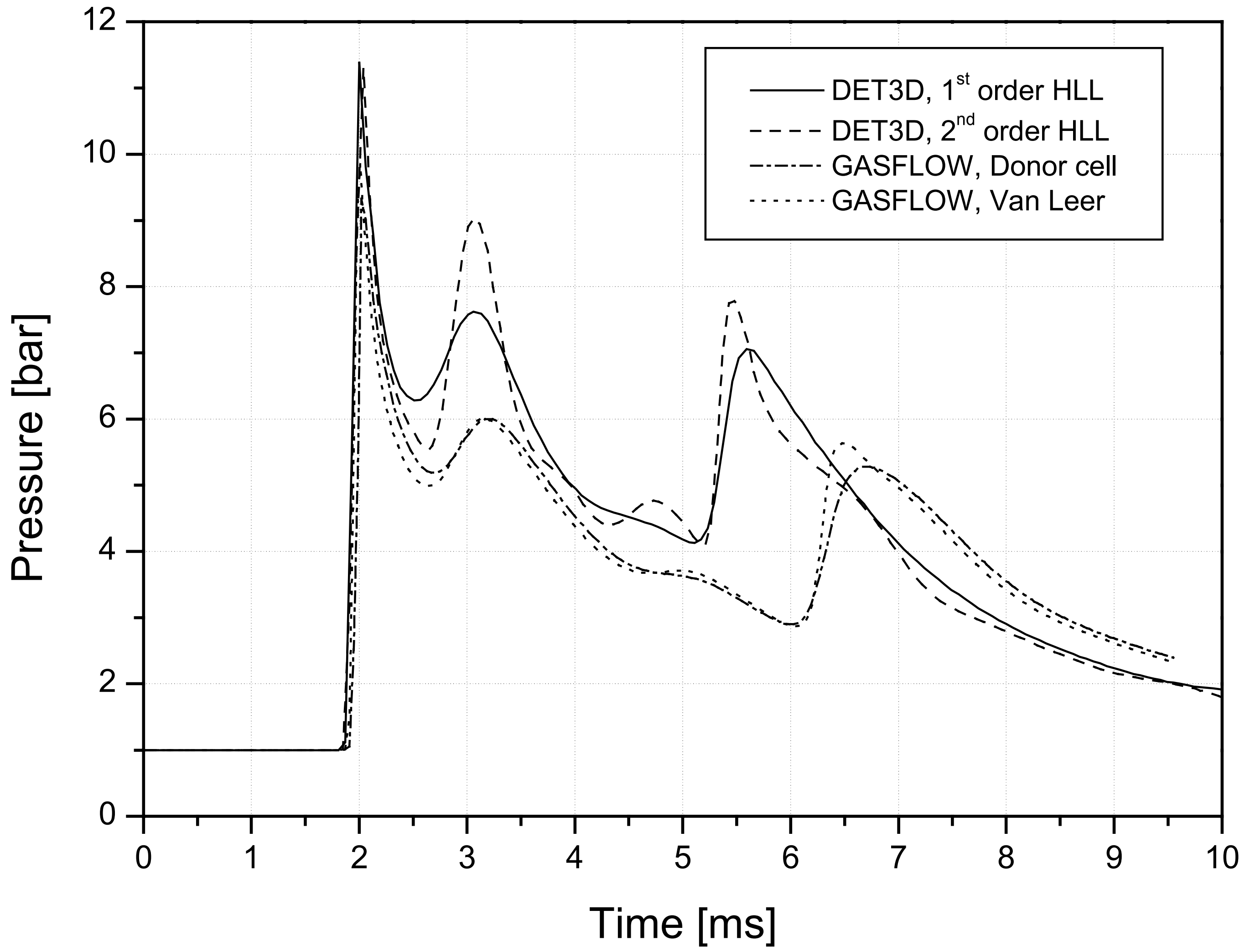

Fig. 8a: **Pressure histories at the port inlet, comparison of DET3D and GASFLOW results obtained from different ITER-FEAT models and numerical differencing schemes.**

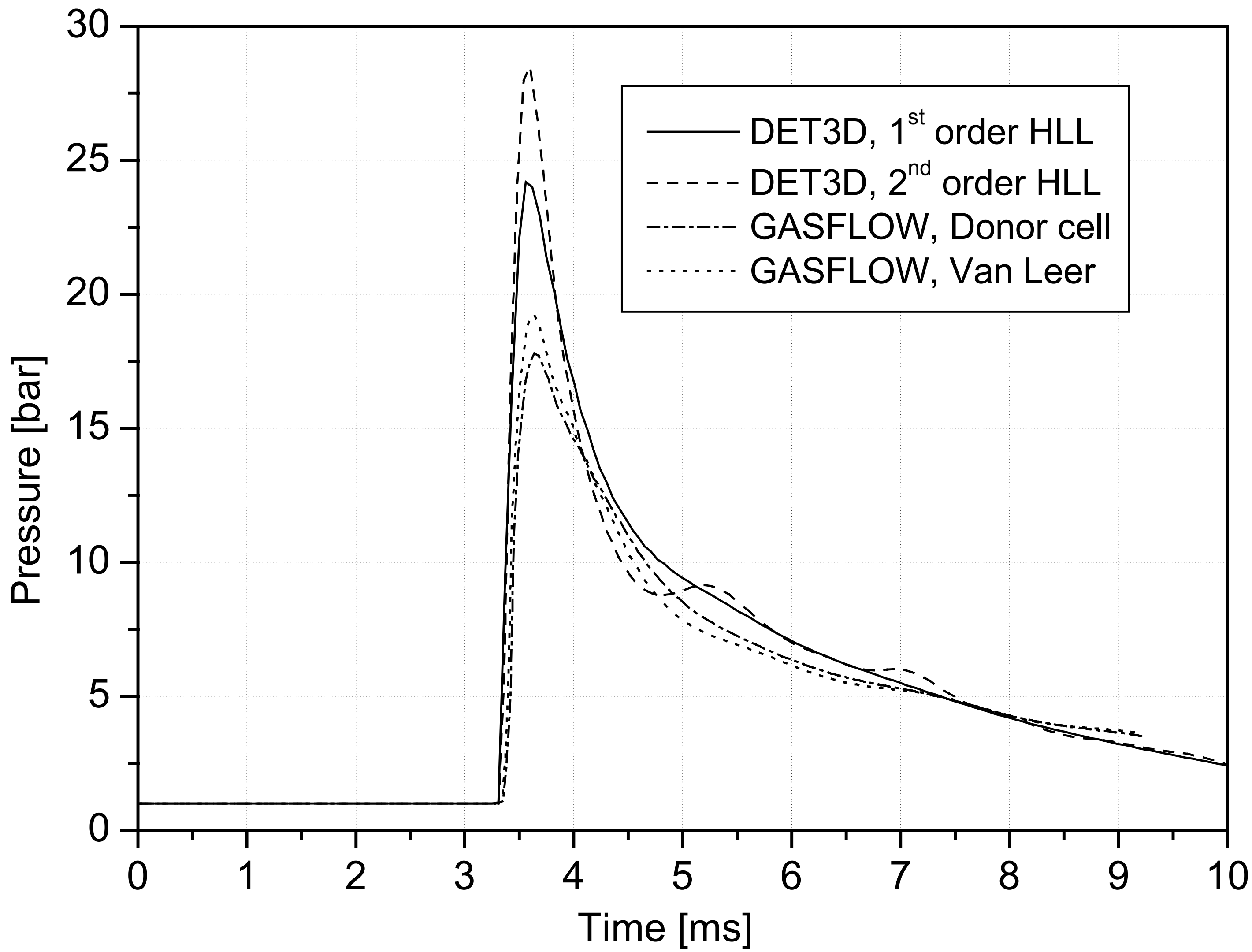

Fig. 8b: **Reflected pressure histories at the port end, comparison of DET3D and GASFLOW results obtained from different ITER-FEAT models and numerical differencing schemes.**

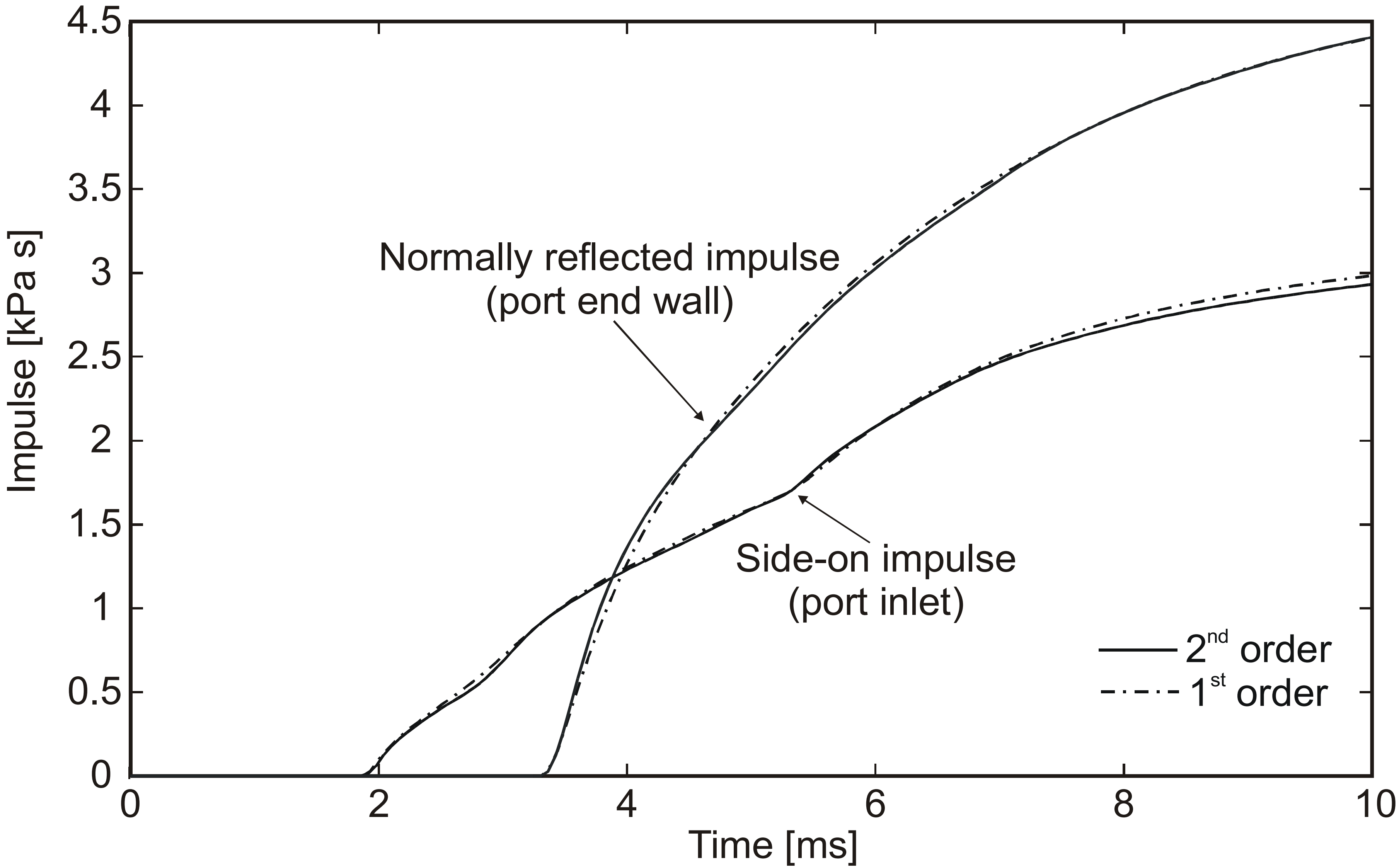

Fig. 9: DET3D results for detonation wave impulse with different orientation between incident wave and vessel wall.