DET3D - A CFD TOOL FOR SIMULATING HYDROGEN COMBUSTION IN NUCLEAR REACTOR SAFETY

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Abstract

In this paper, the CFD code DET3D is described which has been used for simulating assumed accident scenarios in nuclear reactors (fission and fusion, see e.g. [4, 5, 11]) involving hydrogen detonations in complex 3-dimensional geometries.
Two validation calculations against experiments are discussed in detail: (i) a hydrogen-air detonation in a 12 m long straight tube with a truely 3-dimensional inner obstacle, and (ii) a pure radiolytic gas detonation in a 5 m long U-shaped tube at 44 bar initial pressure.

Introduction

During the last years, after the accidents at Hamaoka (Japan) and Brunsbüttel (Germany), the possibility of pipe ruptures from radiolytic gas explosions in Boiling Water Reactors (BWR) has been recognized [1, 2]. To study the danger potential of such explosions (and other hydrogen-related safety issues), a research program was initiated by the Institute of Nuclear and Energy Technology (IKET) at the Karlsruhe Research Center (FZK) consisting of various series of experiments and the concurrent development of predictive numerical tools [3]. One of these numerical tools, the 3-dimensional CFD code DET3D with two exemplary validation calculations will be presented in this paper. For further validations, the reader is referred to [4] and [7].

Originally, in the general context of the FZK-IKET safety analysis approach, DET3D had been developed to simulate hydrogen-air-steam detonations arising in possible severe accident scenarios for large Pressurized Water Reactors (PWR), see e.g. [4, 5]. This approach might shortly be summarized as follows: For a given accident scenario, production and dispersion of the various gas components involved is simulated by appropriate codes. As the composition and state of the (computed) gas mixture evolves over time, its potential for flame acceleration, for deflagration-to detonation transition and, finally, for detonability is checked continuously using the so-called σ and λ criteria involving the expansion ratio σ and the detonation cell size λ of the mixture. If all these criteria indicate that, for the given geometry, the gas mixture is detonable at a certain point in time and in a certain spatial region, then DET3D takes this calculated gas state as initial data, assumes that the gas will actually detonate ("worst case" assumption), and calculates the consequences of such a detonation. See [4, 7] for a more detailed description of this approach, and [11] for an application to a ITER accident scenario. Further information about the $\sigma-$ and $\lambda-$ criteria and their experimental validation over a wide range of initial pressures and temperatures and for various gas mixtures can be found in [8] and the literature cited there.

The main purpose of the DET3D calculations consists in providing pressure-time curves at various locations in the containment during the assumed accident. These pressure histories can then be used in an ensuing structure mechanical analysis to assess the controllability of the accident and/or find possible counter measures. In the validation calculations, the main criterion is therefore a comparison between the experimental and the numerical pressure data.

The paper is organized as follows: In §2, a validation calculation at an initial pressure of about 1 bar and involving a hydrogen-air detonation experiment in a 12 m long tube with an inner obstacle will be described, while §3 deals with a radiolytic gas detonation in a U-shaped, 5 m long tube at an initial pressure of 44 bar. A short description of DET3D is given in §4, and §5 contains some concluding remarks.

Hydrogen-air detonations

The theoretical analysis of hypothetical unmitigated severe accident scenarios in large PWRs with dry containments in combination with related large distribution tests led to the conclusion that, in principle, all combustion regimes are possible, from a slow deflagration up to a stable detonation [6]. The largest pressure loads and thus the highest danger to the integrity of the containment will, however, usually be produced by a detonation. To get upper estimates for the danger potential of an accident scenario it is therefore necessary to have a numerical tool that can simulate hydrogen-air-steam detonations in complex 3d containment geometries.

One of the codes developed for this purpose by FZK is DET3D. The code solves the reactive Euler equations of gas dynamics admitting an arbitrary number of components and reactions. It also has modules for modelling heat transfer between gas and structures, for heat conduction inside structures, and for steam condensation. These latter modules are important for simulating the gas movement behind the detonation wave. A more detailed description of DET3D is given in §4 below.

The codes must be validated against experimental data, and various test series on different geometrical scales were thus conducted by FZK, many of them in close cooperation with the Kurchatov Institute (KI) in Moscow. To name some of the hydrogen-air detonation experiments [7]:

- Hemispherical balloon tests (6 m diameter) with free outow into air, in collaboration with the Fraunhofer ICT (Berghausen),
- Tests in a 12 m long FZK-tube with and without interior obstacles,
- Tests in the 30 m long "TORPEDO"-tube (KI) with interior blockage ratios varying from 10 to 90%,
- Tests in the RUT-facility (KI), having a quite complex 3d geometry with a total length of about 60 m and a total volume of more than 200 m^3.

Fig. 1: The "inclined plane" target (with central pressure gauge) in the 12 m long FZK tube. Other pressure gauges are placed along the tube wall and in the end plate.

The 12 m long FZK-tube has a circular cross section of 350 mm inner diameter. In one of the experiments, an "inclined plane" cylindrical target (see Fig. 1) was installed at one end of the tube and the gas mixture was centrally ignited at the other end. The diameter of the cylinder target is 200 mm,

its (average) length is 600 mm, and the plane is inclined at 45 degrees. This is a truely 3-dimensional geometry which will produce an oblique reflection of a plane detonation wave front.

Since the objective of this experiment was to measure combustion generated loads to structures, fast pressure transducers were selected as the main type of instrumentation and placed along the length of the tube. Furthermore, one transducer was installed in the centre of the inclined plane, and another one in the reflecting end plate of the tube. Thus, basically 3 different pressure-time curves can be expected: side-on, obliquely reflected, and normally reflected. Experimental pressure recording was over a period of 60 ms after ignition.

The tube was filled with a mixture of 30% hydrogen and 70% air at a pressure of 0.965 bar and a temperature of 285 K. According to the STANJAN code [9], this results in a Chapman-Jouguet pressure of 15.8 bar, a von-Neumann pressure of 28.1 bar, and a detonation velocity of 1980 m/s.

A first (adiabatic) DET3D simulation calculation of the experiment with a mesh size of 3.5 cm gave the following peak pressure values for the incident detonation wave: about 20 bar side-on, almost 50 bar normally, and about 37 bar obliquely reflected. The calculated detonation wave velocity was 1987 m/s. All these values conform to the theoretical values, and comparison with the experimental data also showed very good agreement for the incident wave. Total calculation time (for 60 ms physical time) on a 2-processor Opteron PC was about 10 minutes.

The adiabatic calculation, of course, overestimates the velocity and the pressure of the ensuing reflected and superimposed shock waves produced by the detonation wave. For an ensuing structural mechanics safety analysis, however, the incident detonation wave is usually the decisive factor, and the obtained pressure data should therefore be sufficient. It should also be remarked here that the duration of the von-Neumann pressure peak is in the range of some micro-seconds, and resolution of this peak is therefore only necessary if the eigen-frequency of the analyzed structure is very high. For containment structures, resolution of this peak is thus normally not necessary.

To confirm the obtained pressure data, two further adiabatic calculations with reduced mesh sizes of 1.75 and 1.167 cm were performed. It turned out that these two calculations led to practically identical results and that, overall, they also agree with the 3.50 cm calculation. Only the pressure peaks are usually a bit better resolved with the smaller mesh sizes; cf. Fig. 2 which shows, by way of example, the calculated pressure histories for these three mesh sizes at the centre of the inclined plane.

Fig. 2 also confirms the qualitatively good agreement between the calculations and the experiment, especially for the incident detonation wave. However, as already noted above, since these calculations didn't allow for any heat losses, the calculated ensuing shock waves are, of course, too fast and too strong.

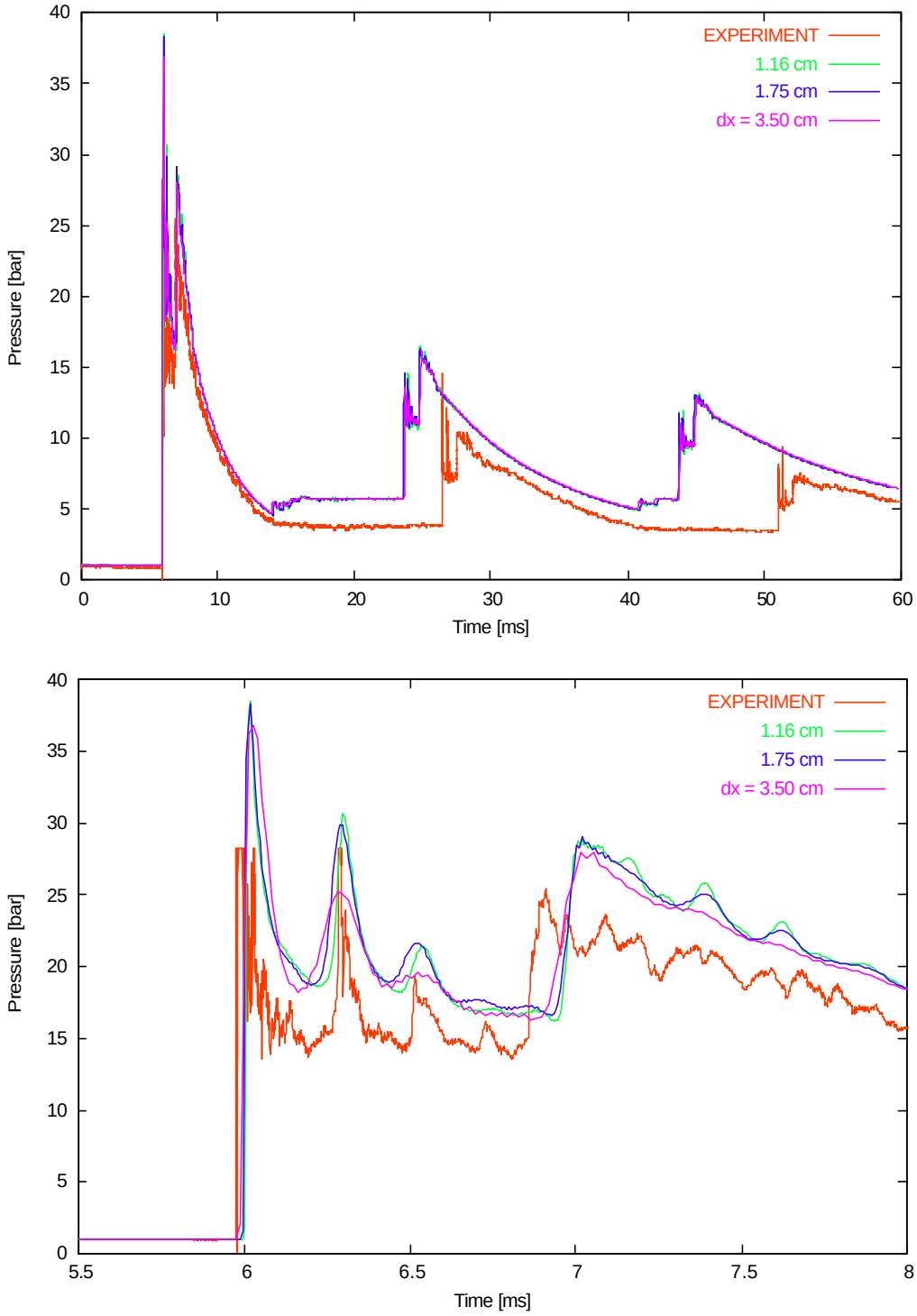


Fig. 2: Comparison of experimental and calculated pressure histories at the centre of the "inclined plane" target. Shown are results of three adiabatic DET3D calculations that differ only by the mesh size used: 3.50, 1.75, and 1.16 cm: (a) full pressure history, (b) close-up view near arrival time of detonation wave.

Remark Detonations lead to very high gas velocities and an explicit solver seems therefore to be most appropriate for their simulation. However, studying the influence of the numerical solver on the computed solution is also part of the BPG approach. Thus, as a first result in this direction, Fig. 3 shows a comparison of the computed pressure histories at the centre of the inclined plane between the explicit DET3D solver and a semi-implicit solver that is currently being implemented into an extension of DET3D (see "Concluding remarks" at end of paper) using a mesh size of 1.75 cm. As can be seen, the semi-implicit solver produces somewhat lower pressure peaks for the incident detonation wave, no "under-shooting" at the end of the Taylor wave, and ensuing shock waves that are a bit slower. Overall, however, the pressure histories computed by the two solvers agree quite well.

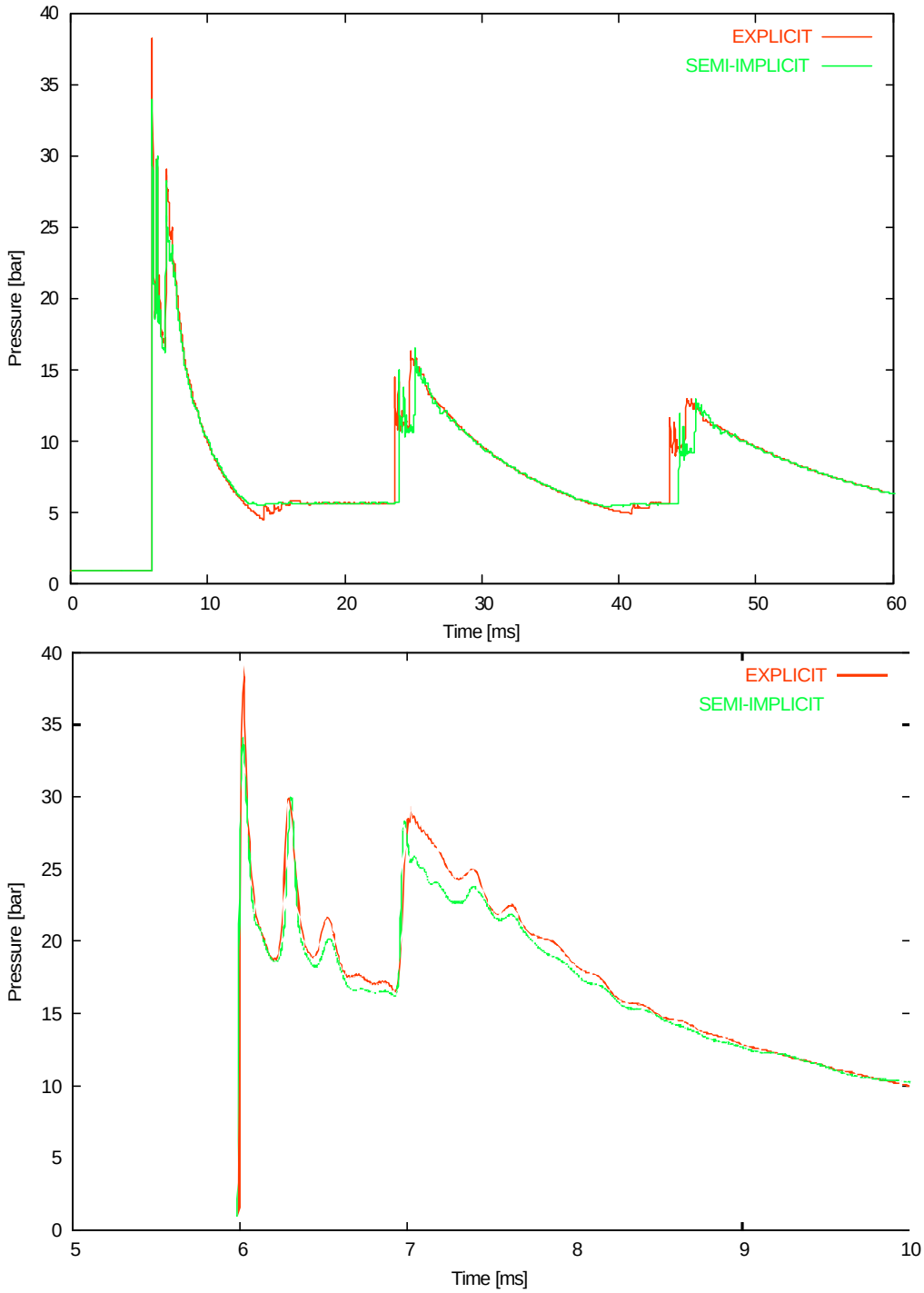
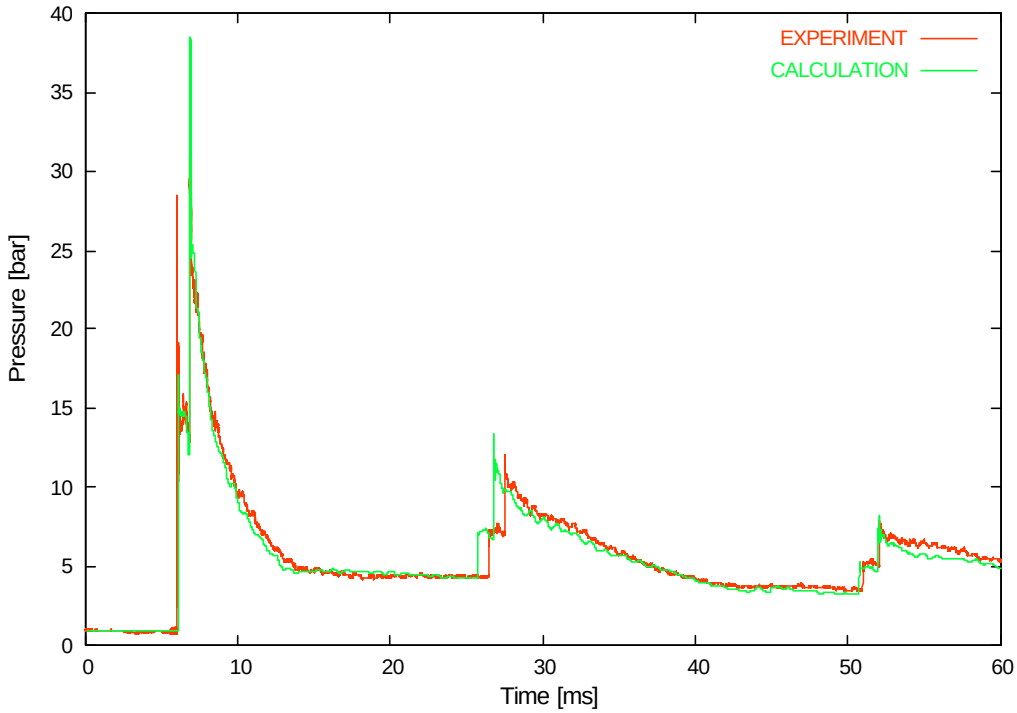


Fig. 3: Calculated adiabatic pressure histories at the centre of the "inclined plane" target using a mesh size of 1.75 cm. Shown is a comparison between the explicit DET3D solver and a semi implicit solver currently being implemented into an extension of DET3D: (a) full pressure history, (b) close-up view near arrival time of detonation wave.

As a result of these adiabatic calculations, it was decided to do a calculation including models for convective heat transfer from the gas to the tube wall, for heat conduction inside the tube wall, and for steam condensation on the tube wall using a mesh size of 1.75 cm. A comparison of the thus calculated pressure histories with the experimental data is given in Fig. 4. Shown are three typical pressure profiles: (a) "side-on", using a tube wall gauge that lies at a distance of 11.50 m from the ignition point, (b) "normally reflected", using a gauge on the tube end plate opposite ignition, and (c) "obliquely reflected", using the gauge in the centre of the inclined plane. (As with Fig. 2, Fig. 4d) gives a close-up view of Fig. 4c) near the arrival time of the detonation wave.) As can be seen, the agreement is quite satisfactory. Calculation time (on a double processor PC) was about 3 hours.

All these calculations used 4 gas species (H_2, O_2, N_2 and H_2O) and the general overall reaction model $2\ H_2 + O_2 \rightarrow 2\ H_2O$.


EXPERIMENT
CALCULATION
Pressure [bar]
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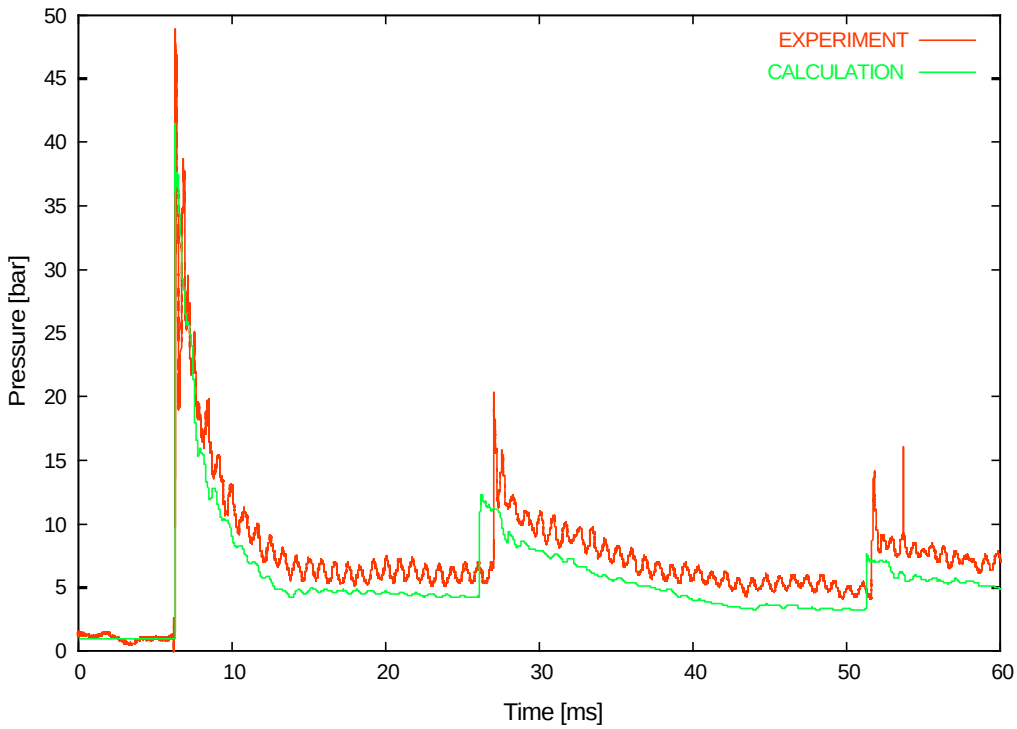
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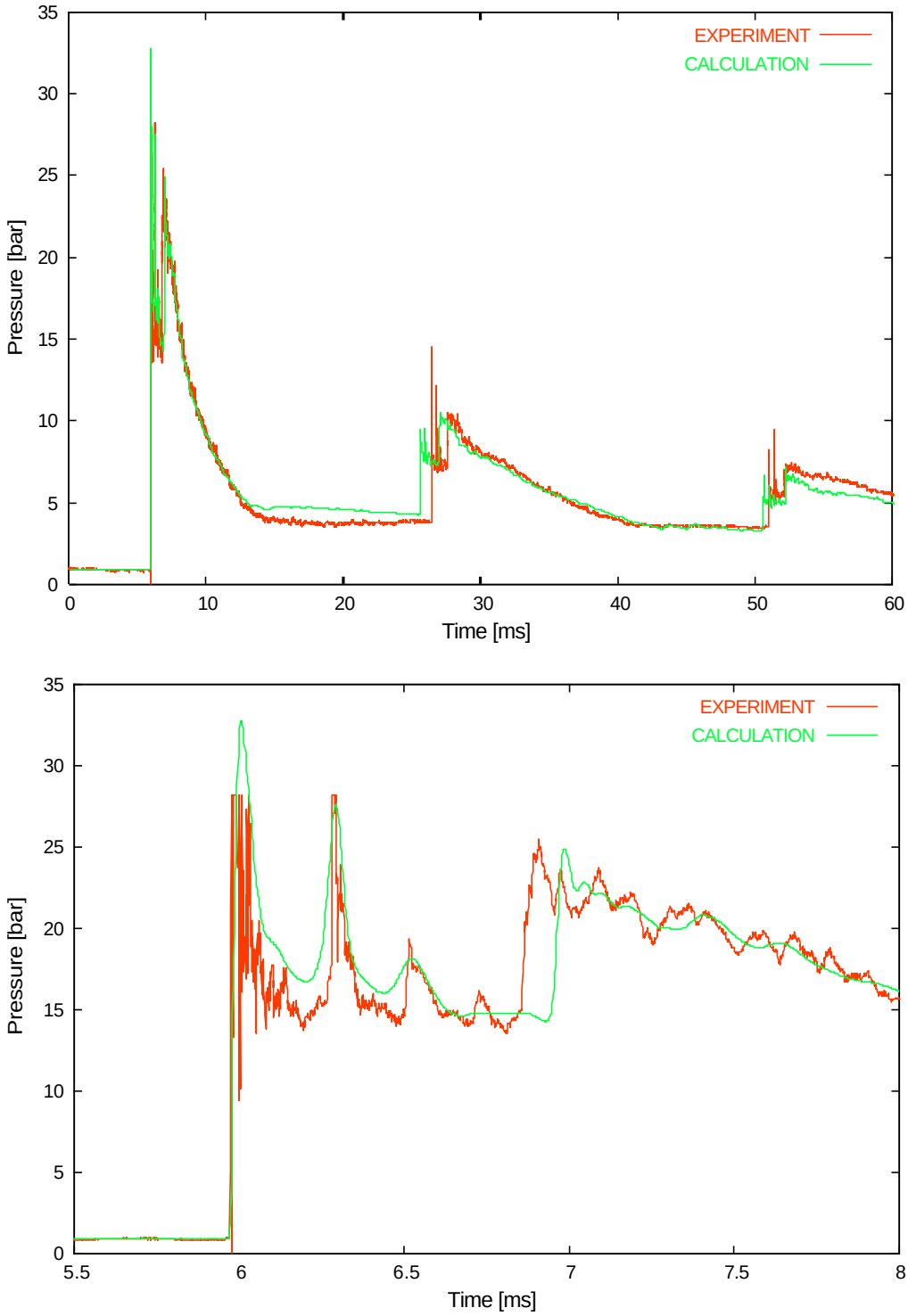


Fig. 4: Comparison of experimental and calculated pressure histories for the "inclined plane target" experiment. DET3D calculation with models for convective heat transfer, heat conduction, and steam condensation included. Mesh size is 1.75 cm. Shown are 3 different types of pressure history: (a) side-on, (b) normally reflected, (c) obliquely reflected with (d) a close-up view near the arrival time of the detonation wave.

Hydrogen-oxygen detonations

After the accidents at Hamaoka and Brunsbüttel, a BWR safety program was started at FZK [3] consisting of various experimental test series and supporting numerical calculations and code developments.

For the experiments, tubes with varying diameter, length and shape were filled with radiolytic gas (either pure or diluted with, so far, nitrogen or steam) and ignited by a spark or glow plug. Initial pressures varied between 0.2 and 70 bar, and initial temperatures between 0° and 150° C, see e.g. [10].

One of these experiment series involved a U-shaped tube of about 5 m length with 29.7 mm inner diameter that was instrumented by 5 pressure gauges, cf. Fig. 5. The tube was filled with pure radiolytic gas at ambient temperature and ignited at one end. Initial pressures varied between 20 and 57 bar.

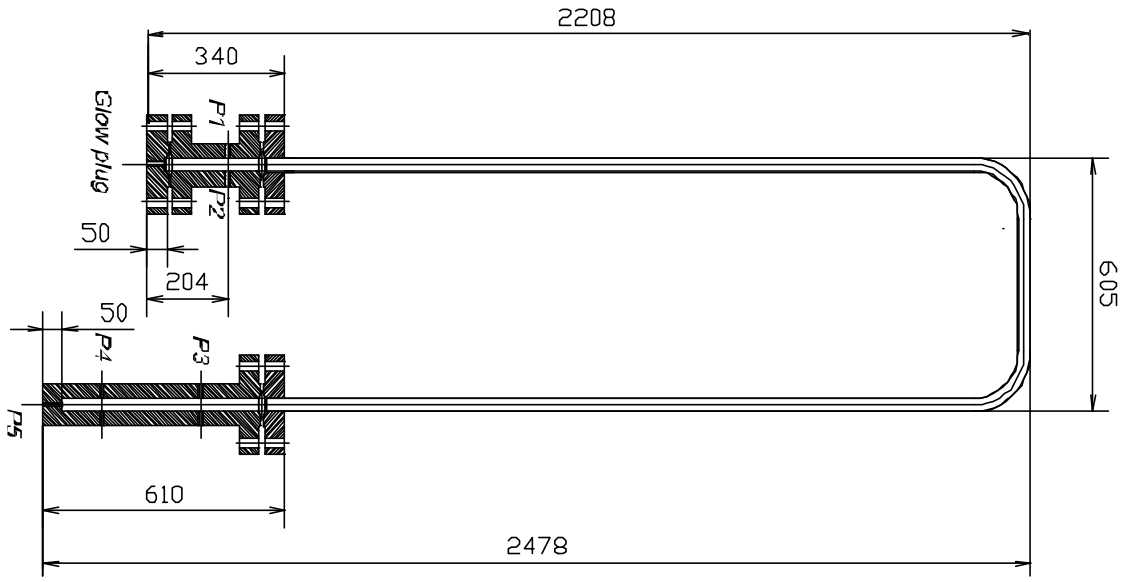
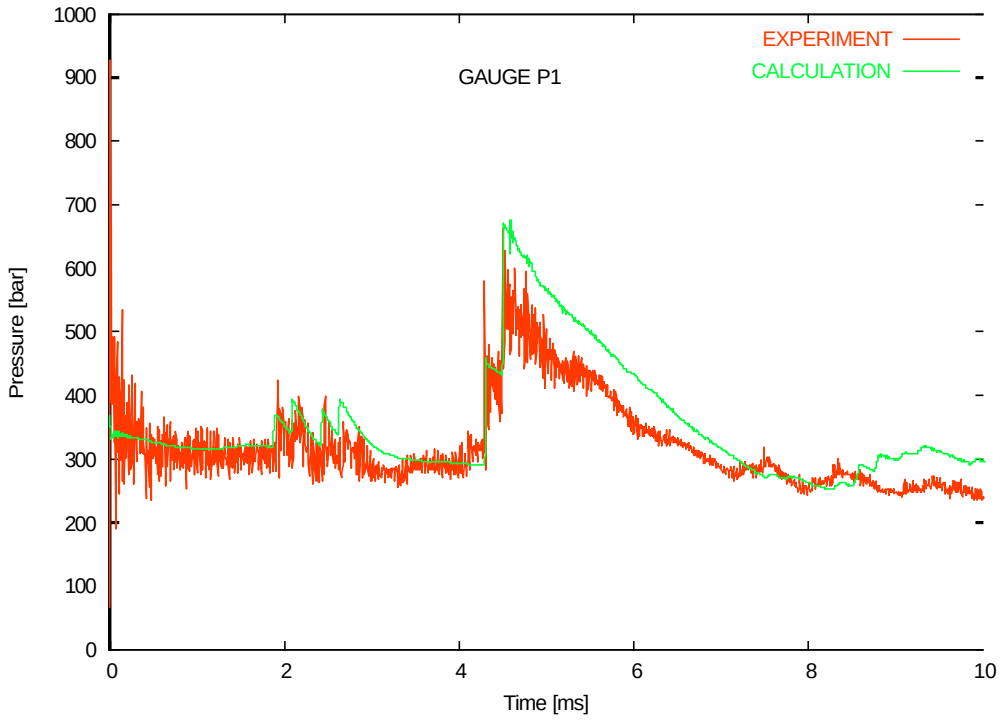


Fig. 5: The U-shaped FZK tube. Total length about 5 m, inner diameter 29.7 mm.

Fig. 6 compares the experimentally obtained pressure data for gauges P1, P3-P5 with a DET3D calculation. The gas mixture had an initial pressure of 44 bar and an initial temperature of 300 K which results in a CJ-pressure of 932 bar and a detonation velocity of 3043 m/s [9].

The calculation used a mesh size of 2.5 mm and the same 4 species, overall reaction model as in §2. The models for convective heat transfer to and for heat conduction inside the tube walls were turned on, as was the model for steam condensation on the tube wall. Agreement between experimental and calculated pressure data as well as for the wave velocities is quite satisfactory. It should be remarked that for this short time span (10 ms) the calculated amount of condensed water remains well below 1 g, and inclusion of the condensation module therefore practically makes no difference in the pressure histories. Calculation time (on a single processor PC) was about 10 h.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EXPERIMENT
CALCULATION
Pressure [bar]
Time [ms]
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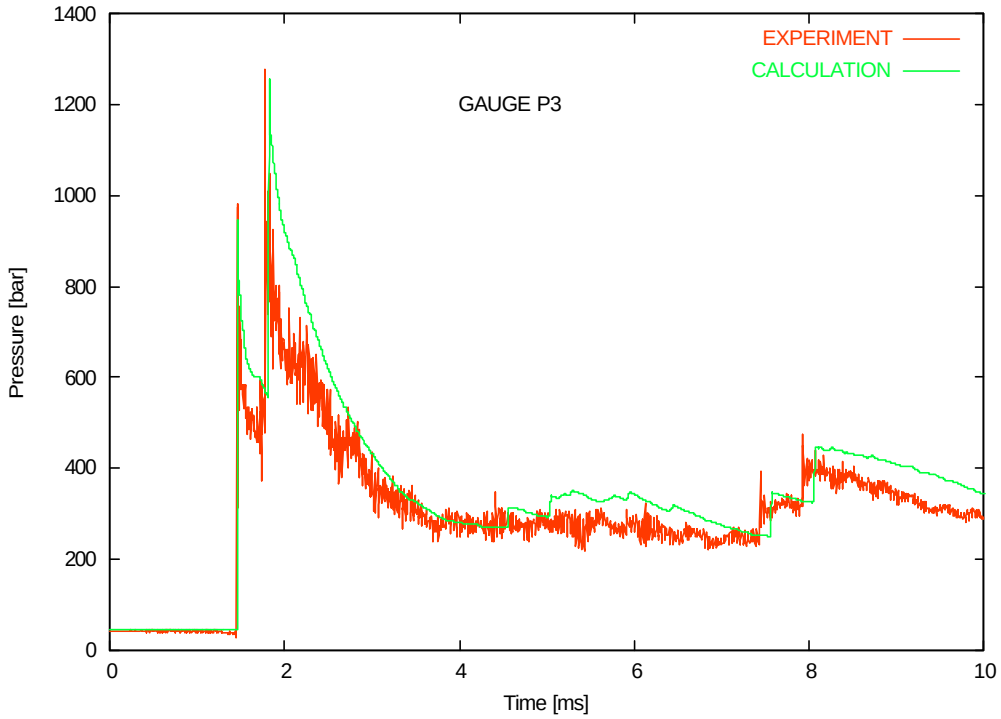
GAUGE P3
EXPERIMENT
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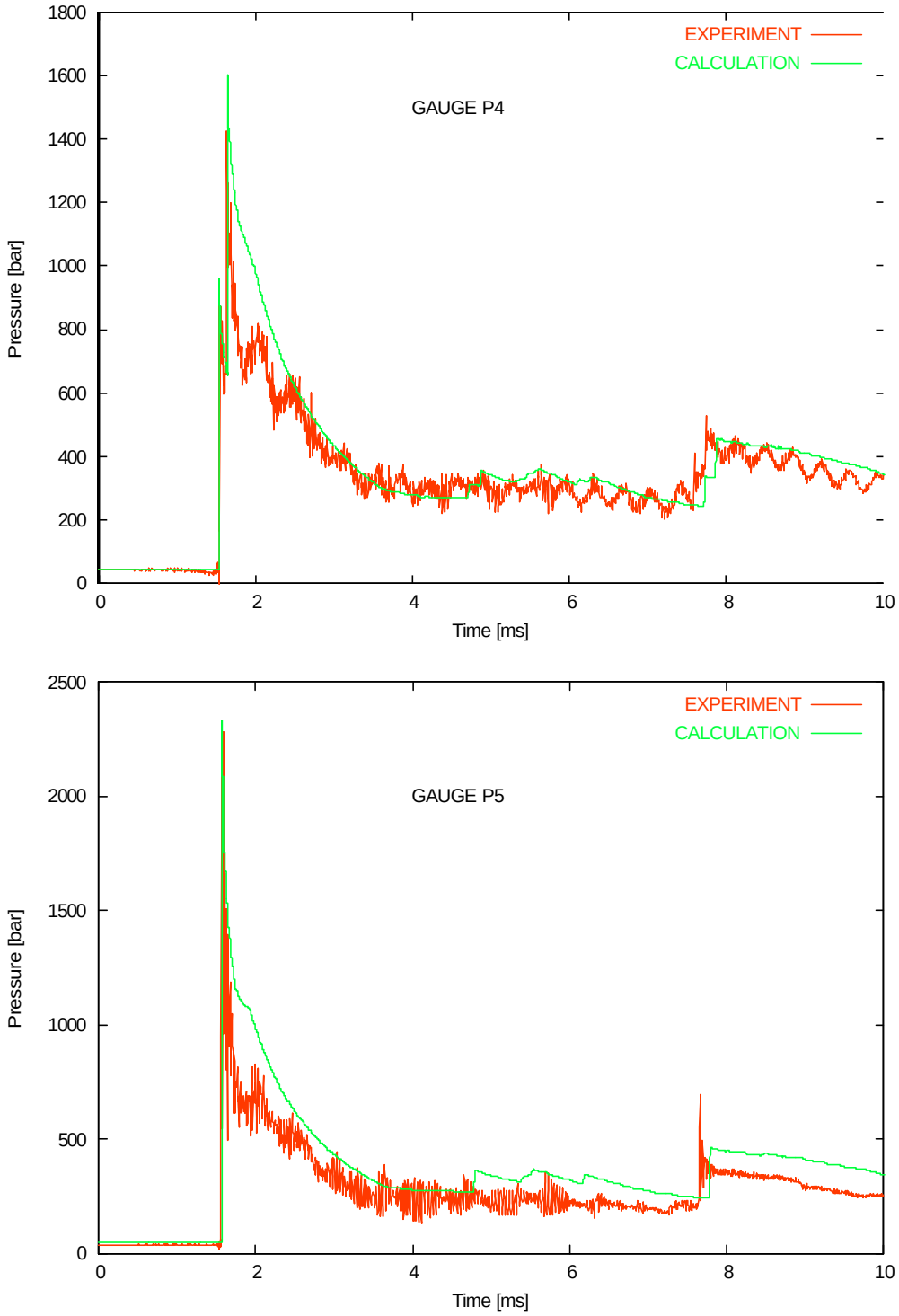

Fig. 6: Comparison of experimental and calculated pressure histories for the U-tube of Fig. 5. Initial pressure is 44 bar. DET3D calculation with models for convective heat transfer, heat conduction and steam condensation turned on. Mesh size is 2.5 mm. Shown are pressure histories at 4 locations (cf. Fig. 5): (a) P1, (b) P3, (c) P4 and (d) P5.

Description of DET3D

DET3D is being developed at the Research Centre Karlsruhe (FZK) as a fast CFD tool for simulating gaseous (especially hydrogen-air-steam and hydrogen-oxygen) detonations in complex 3-dimensional geometries. Main design features of the code are simplicity (modular structure), ease of use, robustness and reliability. The individual code modules (hydrodynamics, chemistry, convective heat transfer etc.) are chosen in accordance with this approach.

To give an example: DET3D uses an equidistant, cartesian mesh because such a mesh has several advantages: (i) it can be easily generated by the code, (ii) it has a simple, uniform structure which does not lead by itself to numerical instabilities or unnecessarily small time steps, and (iii) changing the mesh size for comparison calculations ("numerical convergence") is straightforward (see below). Furthermore, it should be remarked that all validation calculations so far have shown no loss of accuracy in the DET3D results (e.g. pressure histories, wave velocities), but usually a considerable gain in calculation time, when compared with results from other codes that use unstructured, boundary fitted meshes. Nor have the DET3D calculations shown any noticeable influence of the mesh structure on shock formation, or on the shock reflection at or shock propagation along (curved) boundaries. See e.g. Fig. 4d) where the experimentally obtained multiple reflections of the incident detonation wave at the centre of the smoothly inclined target plane are compared with the calculated pressure history using the discretized staircase-like target, or see the application example "Propagation of detonation wave in a valve geometry" in [12] showing the circular formation and propagation of a detonation wave as well as its reflection at a circular boundary.

Until now, the code has been mainly applied to safety studies in nuclear fission and fusion, with problem geometries ranging from rather small (pipe parts) to very large (full nuclear reactor containment, planned ITER fusion vessel) [4, 5, 11]. Accordingly, the code has also been validated against experiments whose geometric scales range from small over medium to large [7, 12].

At present, DET3D solves the 3d Euler equations of compressible gas dynamics for a multi-component, chemically reacting gas mixture, i.e. it solves the conservation equations for impulse, energy and the individual gas species with source terms stemming from the chemical reactions. The equation of state is that for a mixture of ideal gases.

The numerical solver for the hydrodynamics part is a 2nd order, explicit TVD scheme (a slight modification of a scheme proposed by Harten, Lax and van Leer [13]), and chemistry and hydrodynamics interact by a splitting algorithm. To evaluate the thermodynamical properties of the individual gas species (enthalpy, specific heat) polynomial interpolations of the JANAF tables are used.

Apart from an arbitrary number of gas species, the code also admits an arbitrary number of chemical reactions (with Arrhenius kinetics) so that simulations with any user defined reaction mechanism can be performed.

The code further has models for convective heat transfer between gas and structures, for heat conduction inside structures, and for steam condensation on structures [14]. Although not necessary for the initial (supersonic) detonation wave, especially the first two of these modules are important for simulating the gas movement behind the detonation wave, i.e. the interaction of shock and expansion waves produced by the detonation.

After defining the (exact) problem geometry in a user-defined subroutine, the code will automatically discretize this geometry by a cubic cell grid using the user-defined mesh size (cell length). Since this cell length can be continuously varied, it is quite easy to run simulations with different mesh sizes and thus to check the influence of the mesh size on the result. In particular, a kind of (automatic) numerical convergence proof can thus be accomplished, cf. §2. It should be emphasized that the actual choice of the mesh size is, in principle, only determined by the wishes and preferences of the user. For example, one criterion could be calculation time, another one resolution of structures. Thus, the initial "rough" mesh size of 3.5 cm in §2 is motivated by the 35 cm tube diameter and the desire to have a small calculation time, while the (exactly) 2.475 mm mesh size in §3 was chosen in order to have a sufficiently good and exact resolution of the tube diameter.

To check the numerically created model, the code has a graphical interface which gives detailed informations for any chosen 2d-cut (orthogonal to the axes) through the problem geometry. This interface can also be used to quickly check the validity of an on-going calculation by visualizing restart files which are produced by the code during a simulation run at user-specified times. Additionally, for fully 3d pictures, an output format is available that can be read by the AVS program.

Finally, it should be remarked that the code is fully parallelized (MPI), so that calculation times on now readily available two-processor PCs are greatly reduced. (The more so, of course, for calculations on PC clusters, see e.g. [15].)

Concluding remarks

During the last years, the code DET3D has been developed at FZK as a fast computational tool for the simulation of hydrogen detonations in complex 3-dimensional geometries. It has been applied to many problems, especially in the field of nuclear reactor safety (fission and fusion). In developing the code, main stress was laid on simplicity and modularity of code structure, robustness and ease of use. The code has been validated against a number of experiments, two of which are presented in this paper.

An extension of DET3D to solve the compressible Navier-Stokes equations, using a semi-implicit hydrodynamics solver [16], the (k; ε)-turbulence, and the CREBCOM [17] chemical reaction model, for applications in gaseous dispersion and deflagration is currently in its testing phase.

References

1. CSNI Technical Opinion Papers No. 3 - Recurring Events (Nuclear Safety), NEA Report No. 4388, OECD 2003, ISBN 9-64-02155-8
2. Hydrogen combustion events in foreign BWR piping, NRC Information Notice 2002-15, April 2005
3. Nuclear Power in Germany - Annual Report 2004, Deutsches Atomforum, pp. 65-69
4. W. Breitung, R. Redlinger, Containment pressure loads from hydrogen combustion in unmitigated severe accidents, Nuclear Technology 111 (1995), 395-419
5. R. Krieg et al., Assessment of the load-carrying capacities of a spherical pressurized water reactor steel containment under a postulated hydrogen detonation, Nuclear Technology 141 (2003), 109-121
6. T. Cron, D. Schrammel (Eds.), Investigation on hydrogen distribution in a reactor containment, Test Group E11, Experiments E11.0-6, Technical Report PHDR 111-92 (1993) (in German)

7. W. Breitung et al., Innovative Methoden zu Analyse und Kontrolle des Wasserstoffverhaltens bei Kernschmelzunfällen, FZK Report FZKA- 7085, Karlsruhe 2005

8. S.B. Dorofeev et al., Evaluation of limits for effective flame acceleration in hydrogen mixtures, J. Loss Prevention Process Industries 14 (2001), 583-589

9. W.C. Reynolds, The element potential method for chemical equilibrium analysis: Implementation in the interactive program STANJAN, vers. 3, Manuscript, Dept. Mech. Engineering, Stanford University, January 1986

10. M. Kuznetsov et al., Structural response of DN-15 tubes under radiolysis gas detonation loads for BWR safety, SMiRT 18, Beijing, August 2005

11. R. Redlinger et al., 3D-Analysis of an ITER accident scenario, Fusion Eng. Design 75-79 (2005), 1233-1236

12. R. Redlinger, DET3D description and validation, see www.iket.fzk.de

13. A. Harten, P.D. Lax, B. van Leer, On upstream differencing and Godunovtype schemes for hyperbolic conservation laws, SIAM Review 25 (1983), 35-61

14. T.L. Wilson, J.R. Travis, Hydrogen mixing studies (HMS): Theory and computational model, Report NUREG/CR-5948, LA-12459-MS, Los Alamos National Laboratory 1992

15. R. Redlinger, L. Obholz, Numerische Simulation von Gasdetonationen im ITER-FEAT-Fusionsreaktor, FZK-Nachrichten 34 (2002), 295-301

16. C.W. Hirt, A.A. Amsden, J.L. Cook, An arbitrary Lagrangian-Eulerian computing method for all flow speeds, J. Comp. Physics 135 (1997), 203-216

17. A.A. Efimenko, S.B. Dorofeev, CREBCOM code system for description of gaseous combustion, J. Loss Prevention Process Industries 14 (2001), 575-581