

# ANALYSIS METHODOLOGY FOR HYDROGEN BEHAVIOUR IN ACCIDENT SCENARIOS

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## ABSTRACT

Hydrogen is not more dangerous than current fossil energy carriers, but it behaves differently. Therefore hydrogen specific analyses and countermeasures will be needed to support the development of safe hydrogen technologies. A systematic step-by-step procedure for the mechanistic analysis of hydrogen behaviour and mitigation in accidents is presented. The procedure can be subdivided into four main parts: 1.) 3D modelling of the H<sub>2</sub>-air mixture generation, 2.) hazard evaluation for this mixture based on specifically developed criteria for flammability, flame acceleration and detonation on-set, 3.) numerical simulation of the appropriate combustion regime using verified 3D-CFD codes, and 4.) consequence analysis based on the calculated pressure and temperature loads.

## 1.0 INTRODUCTION

Hydrogen and fuel cells are seen as a sustainable energy system that could meet the demands for energy supply security, cost-competitiveness and CO<sub>2</sub>-reduction in a post-fossil era [1]. Such a future hydrogen based economy will bring many new hydrogen-fueled applications into the now existing work and living environment and will lead to widely decentralized use of hydrogen by a large population. For the acceptance of hydrogen as an energy carrier its safety level must be comparable to that of current fossil fuels, for which safe procedures have been developed. The question therefore arises: are there differences in the safety of hydrogen and hydrocarbons?

Fig.1 compares safety relevant properties of hydrogen with those of methane (the major component of natural gas), propane and gasoline vapor. The properties are grouped in six blocks. Each of these blocks corresponds to an accident phase which potentially can be encountered in a hydrogen accident scenario: (1) hydrogen release, (2) distribution and mixing with air, (3) ignition, (4) initial slow laminar deflagration, (5) fast turbulent deflagration, and (6) detonation. All hydrocarbon properties in Fig.1 are normalized to the corresponding hydrogen value. The resulting property profiles of the three hydrocarbons are quite similar, especially in the reactive part of the accident. However, the property differences to hydrogen reach almost a factor of 10 in each of the six accident phases. Since the outcome of a gas release depends on many parameters and complex physics, hydrogen specific safety investigations will be needed for the development of safe hydrogen technologies.

## 2.0 ANALYSIS METHODOLOGY

The Research Center Karlsruhe (FZK) is developing numerical codes and methods aiming at the consistent analysis of hydrogen behaviour in accident scenarios and at the scientific foundation of suitable countermeasures. The present paper outlines a general analysis procedure and gives some examples from recent investigations for safe use of hydrogen. The emphasis is put on a step-by-step description of the deterministic methodology. The general approach is based on 3D computational fluid dynamics (CFD) simulations. References covering the important issue of code validation are given throughout the text. The complete and self-consistent modeling of hydrogen behavior in accidents requires information for four main steps which are outlined in Fig.2. For each of these steps specific input information is needed.

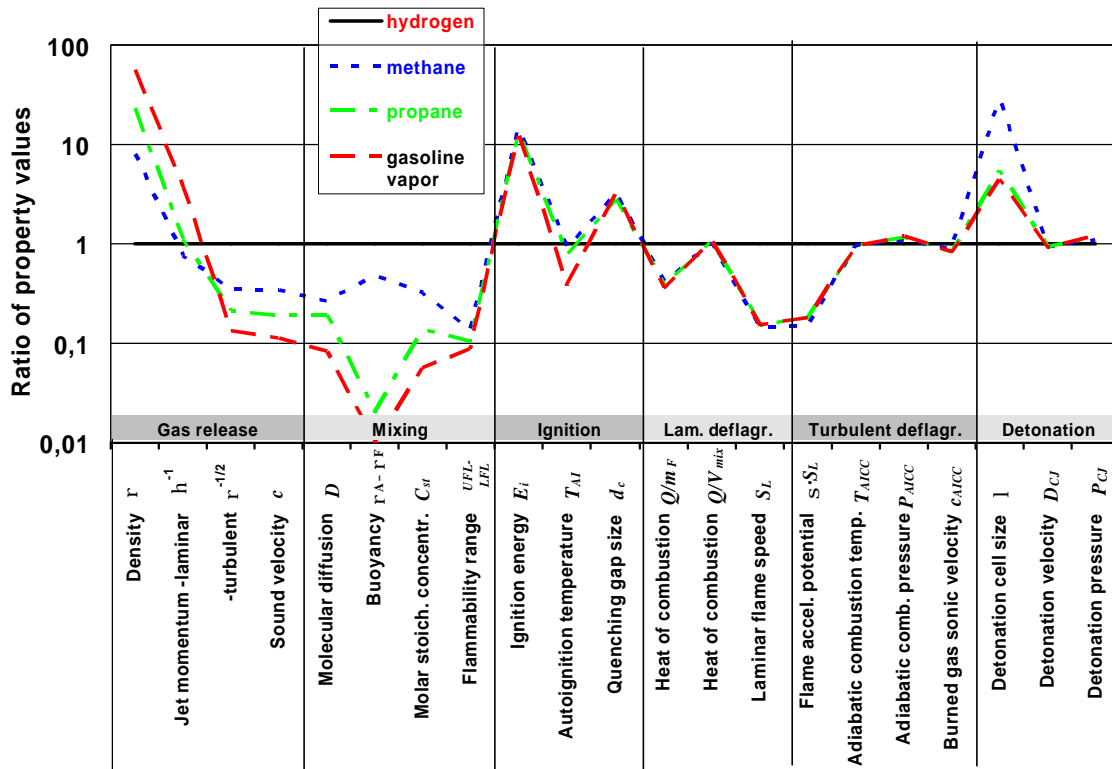


Figure 1. Comparison of safety relevant hydrogen properties with those of current hydrocarbon fuels. Due to the large differences, hydrogen specific safety analyses will be needed for the development of safe hydrogen technologies.

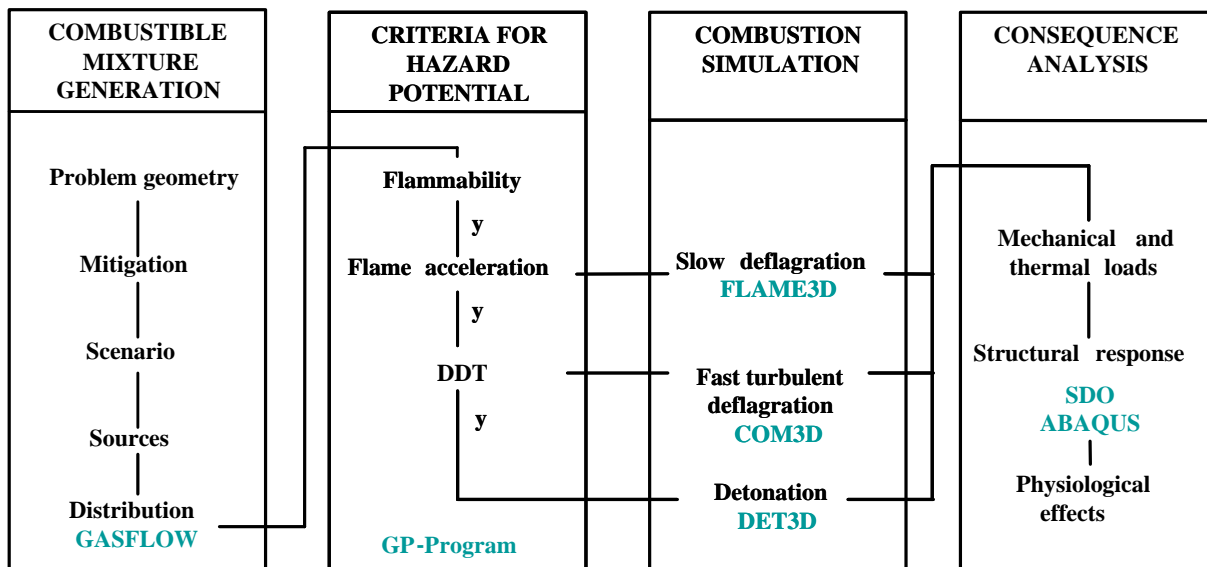


Figure 2. Summary of the FZK methodology for analysis of hydrogen behaviour in accident sequences.

### 3.0 MIXTURE GENERATION

#### 3.1 Problem geometry

Starting point of any analysis is selection of the computational domain and modeling of the problem geometry. The geometry of the installation defines the mathematical boundary conditions for the solution of the 3D fluid-flow equations of the CFD model. The generation of a computational 3D grid for a complex building can be a quite demanding task in terms of balancing the best possible geometry representation and computational effort. Incorrectly modeled flow obstacles or openings can have important implications for natural convection loops and hydrogen distribution dynamics.

#### 3.2 Hydrogen mitigation system

For a given installation, the next important question for the hydrogen analysis concerns the mitigation system under consideration. For this mitigation system, verified CFD-models must exist to predict their efficiency and effects on hydrogen relevant parameters during the further accident progression. The GASFLOW code which is used at FZK for computation of hydrogen distribution [2] has e.g. verified models for blowers, spark igniters, and different catalytic recombiners. If such devices are chosen for hydrogen mitigation, the location of each of these modules must be defined within the grid resolution of the CFD geometry model. If the further analysis of hydrogen behavior (as described below) should lead to unacceptable mechanical or thermal loads, the chosen mitigation concept must be redesigned.

#### 3.3 Accident scenario

For a given plant and mitigation system, the next question is what type of accidents should be covered in the analysis as representative and bounding cases. It is not possible nor necessary to analyze all potential accident sequences with respect to their hydrogen risk.. A number of methods exist to identify the risk dominating scenarios, e.g. FMEA, HAZOP, or "What if". The experience has shown that the inclusion of common mode failures and human behavior can be very important, and difficult at the same time. From a general point of view, the selected scenarios should include the major accident categories of the installation, cover detrimental properties of the H<sub>2</sub> source (e.g. large integral H<sub>2</sub> mass, large release rate) and adverse building conditions (e.g. potential spaces for hydrogen accumulation).

#### 3.4 Hydrogen sources

After definition of the bounding scenarios the next question is what hydrogen sources must be expected for these cases. For consistent CFD calculations, the release location and the time-dependent mass, momentum vector, and energy sources of the released species are needed for the whole duration of the accident. In the case of a gaseous hydrogen source this information must be derived from leak data (location, size, shape, orientation) and the GH<sub>2</sub> pressure reservoir (volume, initial and transient H<sub>2</sub> pressures and temperatures).

In the case of LH<sub>2</sub>-release the source parameters for the gaseous distribution calculation are more complex because spreading and vaporization of LH<sub>2</sub> must be accounted for. These processes have been investigated in detail and can be modeled reliably [see e.g. 3]. Important facts in the present context are: (1) spreading and vaporization of LH<sub>2</sub> from solid surfaces are fast phenomena compared to the subsequent distribution of cold GH<sub>2</sub> in air, (2) the leading front of freely spreading horizontal LH<sub>2</sub>-pools propagates with initial speeds of a few m/s, (3) the maximum pool radius is governed by the LH<sub>2</sub> spill rate, (4) the pool vaporizes completely within few seconds after termination of the spill, (5) the GH<sub>2</sub> density at the boiling temperature (20.3K) is 1.34 kg/m<sup>3</sup>, so that a small amount of mixing with air will make the GH<sub>2</sub>-air mixture buoyant in NPT air.

Due to these findings it often may be adequate to model a horizontal LH<sub>2</sub> pool as a flat source of GH<sub>2</sub> at 20.3 K with a total release rate equal to the liquid spill rate for the duration of the spill. This approximation avoids a detailed LH<sub>2</sub>-GH<sub>2</sub> two-phase modeling.

### 3.5 Hydrogen distribution

With known hydrogen sources the next task is to calculate, distribution and mixing of the released gaseous hydrogen with the air in the installation. The outcome from this analysis step should be the temperature, pressure and composition of the H<sub>2</sub>-air mixture as function of time and location.

A large number of physical processes must be modeled with high spatial resolution to obtain reliable gas compositions. Reasonable research targets are prediction of hydrogen concentrations within a few absolute percent. The most important modeling subjects are (1) 3D compressible fluid flow, (2) convective heat transfer between gas and structure, (3) radiation heat transfer, (4) condensation of water (fog formation), (5) heat conduction within structures, (6) turbulence modeling, and (7) effect of mitigation devices.

One code which has been developed for 3D modeling of hydrogen distribution is GASFLOW [2], another one is CASTEM developed by CEA and IRSN [4]. The main reason for the use of 3D CFD tools is due to the fact that the combustion regimes of hydrogen-air mixtures can change within a few percent of hydrogen concentration. For instance the transition from slow to fast turbulent deflagration occurs at about  $10 \pm 1$  volume % H<sub>2</sub> at NTP. If the risk for a fast combustion is to be evaluated with confidence, local hydrogen concentrations should be predicted with about the same uncertainty margin. In general such accuracies cannot be obtained with Lumped Parameter models which solve zero-dimensional mass and energy balances in relatively few control volumes with high numerical diffusion.

For a predictive CFD simulation of hydrogen distribution in 3D geometries the compressible Navier-Stokes equations and all sub-models must be evaluated against suitable experiments on different scales. Empirical model parameters must be calibrated and then frozen. Table 1 summarizes the validation work which was performed at FZK for the GASFLOW code [5]. The validation matrix compared GASFLOW predictions to analytical solutions, single effect tests, and integral experiments. The dots in Table 1 indicate which sub-model of GASFLOW was addressed in each validation exercise.

## 4.0 HAZARD POTENTIAL

After calculation of the time and space dependent hydrogen concentration field the question arises what hazard the calculated H<sub>2</sub>-air mixture actually presents. Hydrogen hazard is mainly determined by the maximum possible flame speed which could develop under the given geometrical and mixture conditions. Criteria were therefore developed within the FZK hydrogen research program to estimate the conservative combustion regime for a given H<sub>2</sub>-air distribution.

### 4.1 Ignition

A compilation of 287 accidents with GH<sub>2</sub> or LH<sub>2</sub> has identified numerous ignition sources [6]. Fig.3 depicts the nature and percentage of different ignition mechanisms. The large variety of identified ignition sources and the remaining high percentage of unknown causes has led to regulations which require to operate hydrogen systems as if an unforeseen ignition could occur anytime in case of a release [7]. With a postulated ignition source, ignition is controlled by the gas composition only. Therefore literature data for the ignition limits of H<sub>2</sub>-air mixtures were collected, evaluated and fitted for different inert gas dilutents, initial pressures and temperatures. The multidimensional regression fits were implemented in an interactive program (named GP-code) in tabular form, allowing fast on-line evaluation of flammability limits. A detailed description of the GP software is given in [8]. Fig. 4 shows the GP-code output for H<sub>2</sub>-air-steam mixtures at  $p_0 = 0.1$  MPa and  $T_0 = 300$  K, where the flammability limit is the outermost line.

### 4.2 Flame acceleration

To derive general scaling laws for flame acceleration FZK and Kurchatov Institute Moscow have performed joint test series in obstructed tubes which were geometrically similar on different scales (diameters of 80, 174, 350 and 520 mm, resp.). Experiments in the RUT facility near Moscow provided data for a channel diameter of about 2250 mm. Optimum conditions for flame acceleration were created (strong turbulence, repeated obstacles, no venting) to derive conservative criteria. H<sub>2</sub>-air mixtures with mono-, bi-, and triatomic dilutents were investigated (He, Ar, N<sub>2</sub>, CO<sub>2</sub>) [9].

The systematic analysis of the data showed that the expansion ratio  $\sigma$  (= ratio of specific volumes [ $\text{m}^3/\text{kg}$ ] of burned to unburned gas at constant pressure) is the most important mixture parameter determining the flame propagation regime.  $\sigma$  also represents the ratio of chemical energy in the unburned mixture to the initial thermal energy ( $c_p \cdot T_0$ ). The result is that a borderline exists between tests with accelerating and with non-accelerating mixtures. The border correlates well with  $\sigma \approx 3.75$ , independent of the geometrical scale. This critical expansion ratio is valid for lean and rich hydrogen-air-diluent mixtures at ambient conditions. In  $\text{H}_2$ -air mixtures at NTP this limit corresponds to 10.5 %  $\text{H}_2$  on the lean side and 74 %  $\text{H}_2$  on the rich side. For rich mixtures the flammability and the flame acceleration limits coincide, see Fig. 4.

#### 4.3 Deflagration - to - detonation transition (DDT)

The idea that DDT requires some minimum size of the reactive mixture was first proposed by researchers at Kurchatov Institute and substantiated in 1D numerical simulations [10]. A large number of joint KI-FZK experiments were subsequently performed in various facilities, partly with participation of the US-NRC and the French IRSN to test this hypothesis. In addition, the literature data on detonation on-set conditions were collected and evaluated. The detailed analysis of these test data showed that – in agreement with the scoping numerical simulations – a correlation exists between the occurrence of DDT and the geometrical size of the reacting gas mixture. Furthermore it could be demonstrated with tests in scaled down facilities that the detonation cell width of the mixture allows to scale DDT in different mixtures and facilities in a consistent way. The final result of the analysis is that a minimum scale requirement for onset of DDT exists, which can be expressed by  $D \geq 7\lambda$ , where  $D$  is the characteristic size of the reactive gas cloud and  $\lambda$  is the average detonation cell width of the (generally non-uniform) gas mixture. DDT is only possible if this criterion is met. Further details are given in [11]. It is important to note that contrary to earlier literature data, DDT limits are scale dependent. Fig.4 gives an example for characteristic cloud sizes of  $D = 1 \text{ m}$  and  $5 \text{ m}$ . The larger the reactive cloud, the leaner mixtures can undergo a detonation transition.

#### 4.4 Example for hazard evaluation

The following example for the release of hydrogen in a private garage demonstrates the use of the described criteria for hazard evaluation. Table 2 summarizes the geometrical conditions and the hydrogen source parameters of the investigated scenario [12]. The main difference between cases 1 and 2 is the  $\text{H}_2$ -release rate, the total amount of released hydrogen being 34 g in both cases. Note that the homogeneous distribution of this hydrogen mass in the garage would result in an inert mixture (0.6 volume %  $\text{H}_2$ ).

Fig.5 depicts the  $\text{H}_2$ -cloud 80 seconds after begin of the 0.34 g/s release as calculated with GASFLOW. From the given  $\text{H}_2$ -concentration field, the combustible mixture volume ( $4\% \leq x_{\text{H}_2} \leq 75\%$ ), the mixture volume able to support flame acceleration ( $10.5\% \leq x_{\text{H}_2} \leq 75\%$ ), and the DDT index  $D/7\lambda$  can be calculated. In GASFLOW these evaluations are performed on-line during the distribution calculation. Fig.6 summarizes the results for both release cases.

The small release rate leads only to minor volumes of combustible mixture (equivalent combustible cloud diameter  $d_{\text{CC}} = (6V_{\text{CC}}/\pi)^{1/3} \leq 90 \text{ cm}$ ) which are diluted to inert conditions shortly after termination of the release. The mixture volume with flame acceleration potential is insignificant and DDT is not possible in this case. The natural mixing mechanisms namely turbulent air entrainment and diffusion are sufficient to dilute the weak hydrogen source to widely inert  $\text{H}_2$  concentrations. However, in case 1 with 3.4 g/s  $\text{H}_2$  release rate significant volumes of combustible mixture develop and remain stable over the complete simulation time. Flame acceleration potential exists for about 20 seconds and DDT is possible for about 10 s. To control release rates  $\geq 1 \text{ g H}_2/\text{s}$  additional counter measures, as e.g. active venting, would be needed.

In summary, the use of the described criteria offers two important functions for the analysis of hydrogen behavior: 1) early estimate of the fastest possible combustion regime, and 2) branching from the distribution calculation into the appropriate numerical tool for the 3D combustion simulation, as depicted in Fig.2.

Table 1. Summary of the validation work performed at FZK for the 3D CFD code GASFLOW.

PHYSICAL PROCESS	MODEL	VERIFIATION		
		Analytical solution	Single effect tests	Integral experiment
<b>• Distribution, GASFLOW:</b>				
- geometry	- 3d, cylindrical, cartesian - graphical input		C/B1 BMC DAT/HET AE/CL C/B2 HDR BMC/PASCO BMC	HDR T31.5 HDR E11.2 THAI PHEBUS FFT0
- flow and transport	- Navier-Stokes, 3d, fully compressibel	• laminar channel flow		
- thermophys. properties	- JANAF Tables			
- molecular transport	- CHEMKIN	• diffusion, 1d		
- turbulence	- $k/\epsilon$		Jk7	
- turbulent heat transfer gas/wall	- wall function	• 1d channel, theory		
- heat conduction in struct.	- Fourier equation, 1d	• 1d Problem		
- radiation	- Momentum approximation,	• 1d, 2d		
- vaporation/condensation	- homog.-equil. model			
- critical flow	- orifice solutions	•		
<b>• Mitigation:</b>				
- recombiners a) Siemens b) NIS	- 1-cell model - 1-cell model		E11.8.1 MC-3	Gx1.6
- igniter	- 1-cell model			Gx7
- sump vaporization	- homogeneous sump model		Rx4,5	

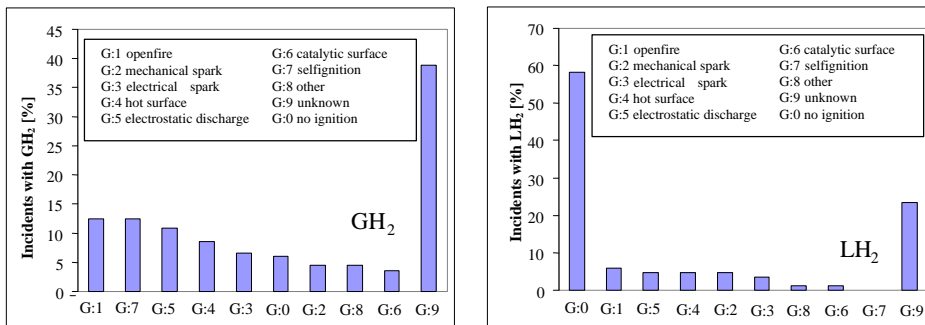


Figure 3. Ignition mechanisms for incidents with GH<sub>2</sub> and LH<sub>2</sub> release [6].

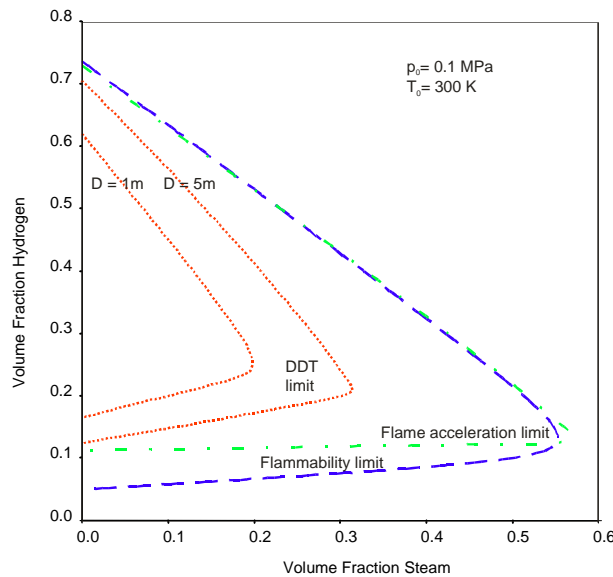


Figure 4. Output of the GP-code for flammability, flame acceleration and DDT limits in H<sub>2</sub>-air-steam mixtures with  $p_0 = 0.1 \text{ MPa}$  and  $T_0 = 300 \text{ K}$ . The scale dependent DDT limit is given for two cloud sizes with characteristic dimensions of 1 m and 5 m, respectively.

## 5.0 COMBUSTION SIMULATION

Because of the different physics involved, three CFD codes are under development and used for hydrogen combustion analysis at FZK: (1) FLAME3D for slow deflagrations, (2) COM3D for fast turbulent deflagrations, and (3) DET3D for stable detonations of (partly) premixed H<sub>2</sub>-air-steam atmospheres. The main characteristics of the codes and the corresponding validation matrices are described in detail in [5]. Additional validation exercises are presented in [13]. All three codes employ cubic grid cells which allow smaller discretization errors, higher computational speed and better anisotropy for flame propagation, compared to irregular grids. A graphical user interface permits easy generation of complex 3D geometry models.

One example of the verification work which is of interest here concerns the detonation of a hemispherical H<sub>2</sub>-air mixture. The balloon of 6 m diameter and 53 m<sup>3</sup> volume was filled with stoichiometric H<sub>2</sub>-air mixture (29.5 vol% H<sub>2</sub>) and detonatively ignited in the center. The experiment was performed for the FZK hydrogen safety program at the Fraunhofer Institute for Chemical Technology in Berghausen, Germany. Fig.7 shows high-speed frames of the propagating detonation wave ( $\Delta t=0.4$  ms). The measured detonation velocity of  $1940 \pm 20$  m/s agrees well with the theoretical CJ-value of 1955 m/s. Fig. 8 shows a comparison of measured and calculated pressure histories for one location inside the reacting H<sub>2</sub>-air mixture and one outside of the balloon in ambient air [5, pp. 8.72-8.74]. DET3D reproduces all important phenomena as e.g. the leading detonation front, the pressure reflection at the balloon boundary from the mixture density jump, and the expansion wave.

An example for a turbulent combustion simulation is given in Fig.9. The depicted test chamber is used at FZK for hydrogen release and local explosion experiments in a confined volume. The inner room dimensions are 5.5 x 8.5 x 3.4 m, the volume is about 160 m<sup>3</sup>, and air flows up to 24.000 m<sup>3</sup>/h can be realized inside the chamber to simulate venting or directed flow effects on H<sub>2</sub> release and mixing. COM3D was used to simulate an experiment in the chamber with fast turbulent combustion of 8 g H<sub>2</sub> concentrated in a 0.5 m<sup>3</sup> volume. Fig.9 shows the chamber geometry and the calculated isobaric surface for 0.11 MPa, about 7.7 ms after ignition of the local H<sub>2</sub>-air charge [14]. At this time the spherically expanding air blast wave has reached floor and ceiling of the test chamber. The computed and measured pressures agree quite well. Fig. 10 compares the data for a location on the floor. This example demonstrates that local pressure loads in complex confined geometries can be well predicted if the flame velocity is modeled correctly.

## 6.0 CONSEQUENCE ANALYSIS

### 6.1 Mechanical and thermal loads

The further flow of the analysis is straightforward. The thermal and mechanical loads of the respective combustion process (slow deflagration, fast deflagration or detonation) are evaluated from the 3D simulation by storing temperature and pressure histories at different building locations. Which of these two load categories prevails, is mainly determined by the time of first ignition. Early ignition generally leads to low pressure amplitudes but high local thermal loads from standing diffusion flames. Late ignition of an accumulated hydrogen mass will generally result in transient high pressure loads but negligible temperature increase in the solid structures. The overpressure generated in a pre-mixed or partly pre-mixed combustion is governed by the flame speed. Fast flames can easily reach overpressures which threaten the integrity of normal buildings, because these are designed for vertical gravitational forces but not for lateral mechanical loads. Few civil constructions will resist a pressure differential across walls of 0.01 MPa. Fundamental data for pressure load generation in H<sub>2</sub>-air-steam detonations have been obtained at Sandia Natl. Laboratory in an earlier contract study for the FZK hydrogen safety research [15].

Table 2. Geometry and investigated hydrogen source parameters for H<sub>2</sub> release in a private garage [12].

GEOMETRY		HYDROGEN SOURCE					CASE
Garage volume (m <sup>3</sup> )	Ventilation openings	H <sub>2</sub> -Rate (g/s)	Release time (s)	Total mass (g)	Release temperature (K)	Release location	Nr.
70.2	two times 10 x 20 cm <sup>2</sup>	3.40	10	34	22.3	below trunk	1
		0.34	100	34	22.3		2

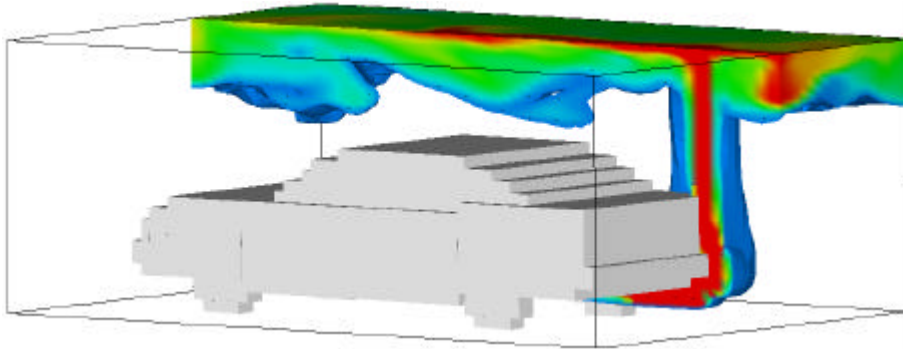


Figure 5. Calculated H<sub>2</sub> distribution with 0.34 g H<sub>2</sub>/s release rate, 80s after begin of release, isosurface for 4% in air [12].

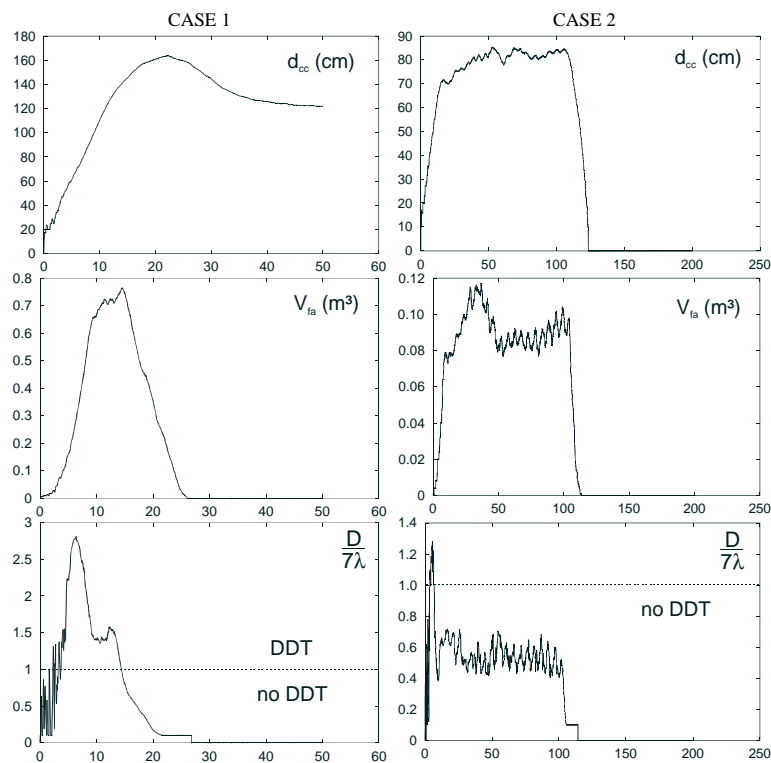


Figure 6. Calculated hazard parameters for two different H<sub>2</sub>-release rates in a private garage [12]. Case 1 (3.4 g H<sub>2</sub>/s) leads to a mixture which could support a fast combustion process. Case 2 (0.34 g H<sub>2</sub>/s) is mitigated naturally by intrinsic mixing processes and results in insignificant hazards.



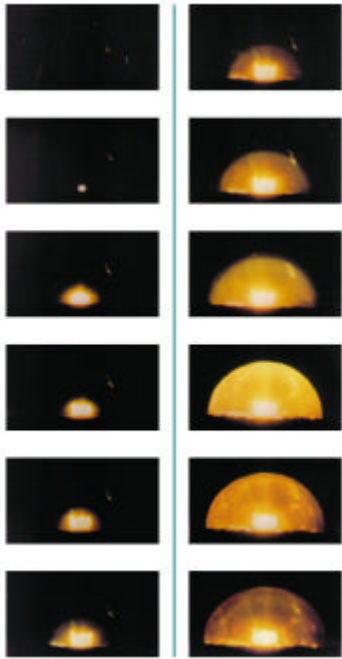


Figure 7. High speed frames of hemispherical H<sub>2</sub>-air detonation, 29.5% H<sub>2</sub> in air, balloon diameter 6 m,  $\Delta t=0.4$  ms, detonation speed  $1940\pm 20$  m/s.

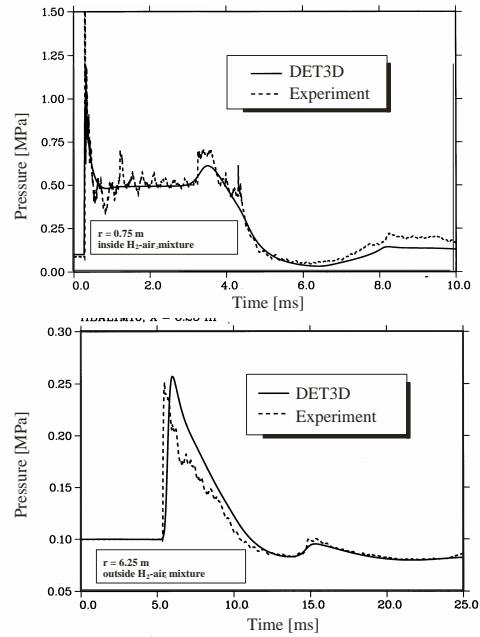


Figure 8. Comparison of measured and calculated pressure histories for the hemispherical detonation. DET3D reproduces all important phenomena with good accuracy.

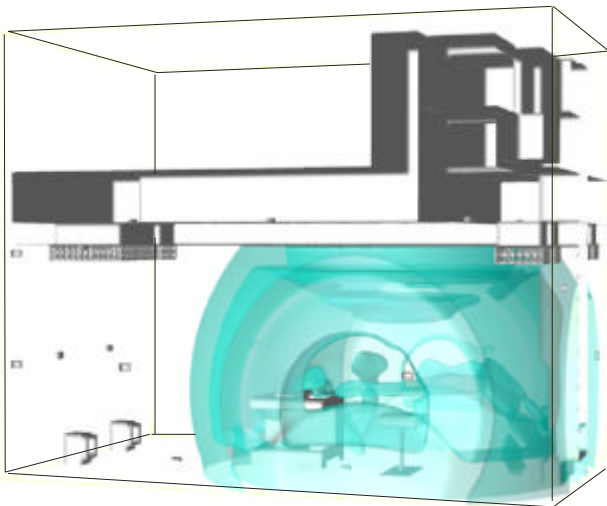


Figure 9. COM3D calculation for local fast deflagration in the FZK hydrogen test chamber, isobaric surface for 0.11 MPa, 7.7 ms after ignition.

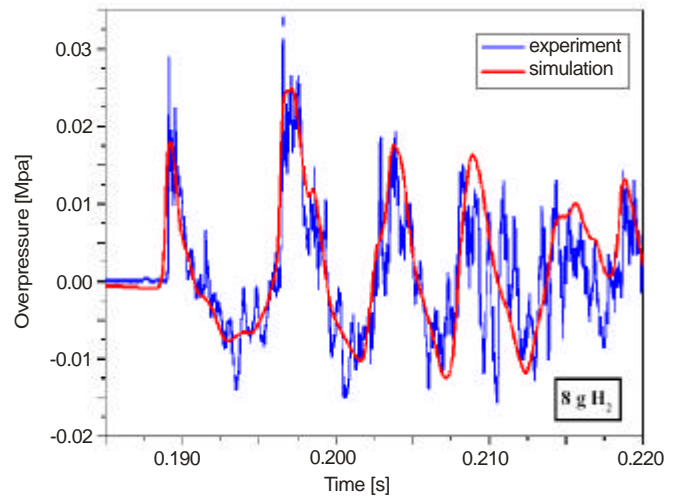


Figure 10. Comparison of measured and calculated pressure histories at a location on the floor of the test chamber.

## 6.2 Structural response

The calculated pressure loads serve as input for the next step in the analysis, which is structural response of the affected building. The investigation of structural integrity under combustion loads is complicated by the fact that confinements for technical installations generally consist of a variety of components which can have largely different mechanical responses. One useful tool which allows fast first estimates about the local response of a given structural element is the Single Degree Oscillator (SDO) model. In this model the structure of interest is described with lumped values for mass  $m$ , force constant  $k$ , and damping  $D$ . The oscillator is subjected to the dynamic pressure load  $p(t)$  and the maximum displacement  $x_{\max}$  is calculated.  $x_{\max}$  can then be related to an effective static pressure  $p_{\text{eff}} = k \cdot x_{\max}$ , causing the same displacement as the dynamic load  $p(t)$ .

Fig.11 shows on left side a local dynamic pressure load which was calculated with COM3D for the deflagration of a homogeneous 12%  $\text{H}_2$ -air mixture in a large complex enclosure. Note that the adiabatic, isochoric, complete combustion (AICC) pressure of this mixture is only 0.54 MPa. The pronounced peaks are caused by reverberations in the burned gas in the respective room of the building. The right hand side of Fig.11 shows the calculated effective static pressures for linear oscillators with natural frequencies up to 500 Hz [5, pp. 9-1 to 9-21]. The effective static pressures can be significantly higher than the applied peak pressures, especially for oscillators which are in resonance with the multiple peak structure of the dynamic load. Only for very massive structures with natural frequencies below 10 Hz, is  $p_{\text{eff}}$  close to  $p_{\text{AICC}}$  of the mixture. In this example  $p_{\text{eff}}/p_{\text{AICC}}$  reaches values of almost up to 6!

If a SDO-model should not be adequate to describe the structural displacement under a dynamic pressure load a three-dimensional code like e.g. ABAQUS can be applied. Fig.12 shows calculated wall displacements and maximum in-plane stresses for the FZK hydrogen test chamber, when subjected to a fast local ( $0,5 \text{ m}^3$ ) internal  $\text{H}_2$ -air deflagration [16]. The calculated time-dependent pressure loads from COM3D were stored at 8000 wall locations and given to the respective wall elements of the 3D ABAQUS model. In this case it could be shown that all strains in the wall construction remained in the elastic regime, that the assumed local  $\text{H}_2$ -detonation can be safely confined, and that no external risk exists. In this way the inherent safety margins of buildings against internal combustion loads can be quantified and used in safety concepts.

## 6.3 Physiological effects

The release and combustion of hydrogen can threaten human health in several ways: (1) asphyxiation due to air replacement, (2) blast wave effects, (3) skin burns from thermal radiation, and (4) cryogenic burns from contact with cold fluids or surfaces. The hazard of asphyxiation is directly related to the oxygen concentration in the  $\text{H}_2$ -air mixture. The severity of physiological effects increases with decreasing oxygen concentration, reaching unconsciousness at 8-10 volume % (for 0.1 MPa total pressure), and death in 8 min at 6-8 volume %  $\text{O}_2$  [7].

The injury from blast waves depends on peak overpressure and specific impulse. At 100 kPa overpressure about 50% eardrum rupture occurs for specific impulses between  $10^2$ - $10^4$  Pa.s [17]. Injury can also be due to whole-body displacement and subsequent impact. The lethality threshold was estimated to 6.4 m/s impact velocity. Damage from thermal radiation depends on a variety of factors, including exposure time, energy flux and exposed surface area. E.g. the threshold for pain from a 2 s thermal radiation on bare skin is reached at a thermal flux of  $2 \cdot 10^4 \text{ W/m}^2$  [17]. Skin burns are reached in 30 s at a flux of  $5 \cdot 10^3 \text{ W/m}^2$  [7]. The analysis procedure described in this paper provides data about oxygen concentrations, temperatures, overpressures and impulses, from which physiological effects can be estimated. Additional data are needed for the radiation fluxes from standing diffusion flames.

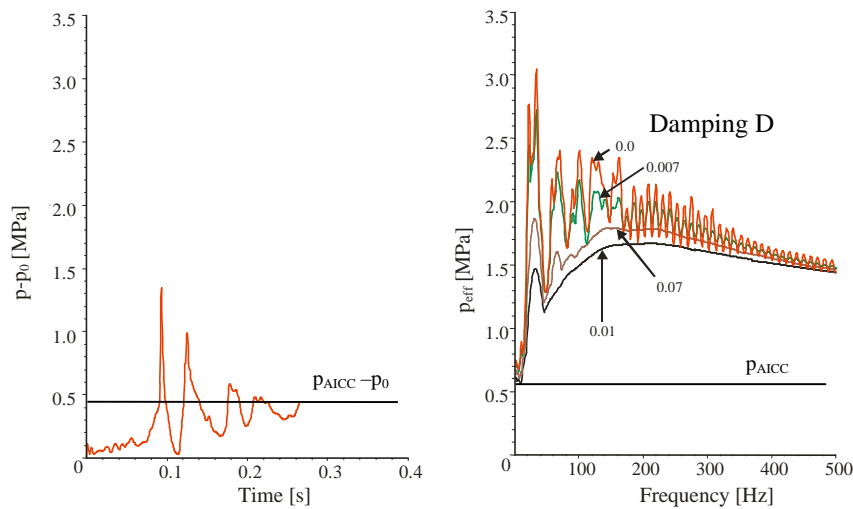


Figure 11. (Left) Calculated local overpressure from a 12% H<sub>2</sub>-air deflagration in a large complex building. Reverberations in the burned gas cause a multi-peak structure with peak pressures well above the adiabatic, isochoric, complete combustion pressure ( $p_{AICC}$ ). (Right) Results of a Single-Degree-Oscillator model for the effective static pressure  $p_{eff}$  from the dynamic load shown on the left.  $p_{eff}$  is significantly above the AICC-pressure of the burning H<sub>2</sub>-air mixture, except for very massive structures with  $f < 10$  Hz.

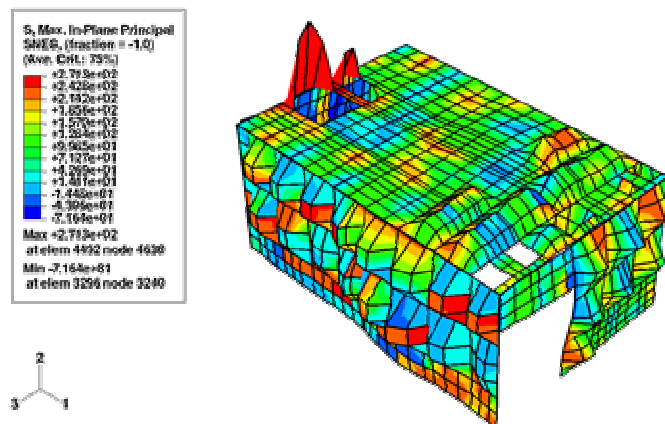


Figure 12. ABAQUS calculation for displacements and in-wall stresses (MPa) in test chamber walls due to a local (0.5 m<sup>3</sup>) fast turbulent H<sub>2</sub>-air deflagration in the chamber [16], time is about 87 ms after begin of combustion. The investigated dynamic pressure load can be safely confined without external consequences.

## 7.0 Summary

This paper describes a step-by-step procedure for the consistent analysis of hydrogen behavior in accident sequences. The methodology attempts to take into account in a systematic way, all parameters in the complex physics which can have important effects on the outcome of a hydrogen release and combustion event. The emphasis of the approach is put on numerical simulation of the unsteady, compressible, turbulent and partly reactive flows with heat transfer in complex three-dimensional domains. A large fraction of the research and development work was devoted to verification of the theoretical models and to generation of an adequate hydrogen combustion data base [5]. The ultimate goal of the analysis is prediction of possible consequences of the accident scenario with respect to personal, buildings and environment. If the potential

damage in a given event should be unacceptable, different hydrogen mitigation schemes can be modeled and their effectiveness on the risk reduction can be quantified.

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