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# On Detonation Dynamics in Hydrogen-Air-Steam Mixtures: Theory and Application to Olkiluoto Reactor Building

A. Silde, I. Lindholm

VTT Energy, Finland

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## ON DETONATION DYNAMICS IN HYDROGEN-AIR-STEAM MIXTURES: THEORY AND APPLICATION TO OLKILUOTO REACTOR BUILDING

A. Silde I. Lindholm

VTT Energy Nuclear Energy Espoo, Finland

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## ABSTRACT

This report consists of the literature study of detonation dynamics in hydrogen-air-steam mixtures, and the assessment of shock pressure loads in Olkiluoto 1 and 2 reactor building under detonation conditions using the computer program DETO developed during this work at VTT. The program uses a simple 1-D approach based on the strong explosion theory, and accounts for the effects of both the primary or incident shock and the first (oblique or normal) reflected shock from a wall structure. The code results are also assessed against a Balloon experiment performed at Germany, and the classical Chapman-Jouguet detonation theory. The whole work was carried out as a part of Nordic SOS-2.3 project, dealing with severe accident analysis.

The initial conditions and gas distribution of the detonation calculations are based on previous severe accident analyses made by MELCOR and FLUENT codes.

According to DETO calculations, the maximum peak pressure in a structure of Olkiluoto reactor building room B60-80 after normal shock reflection was about 38.7 MPa, if a total of 3.15 kg hydrogen was assumed to burned in a distance of 2.0 m from the wall structure. The corresponding pressure impulse was about 9.4 kPa-s. The results were sensitive to the distance used. Comparison of the results to classical C-J theory and the Balloon experiments suggested that DETO code represented a conservative estimation for the first pressure spike under the shock reflection from a wall in Olkiluoto reactor building.

Complicated 3-D phenomena of shock wave reflections and focusing, nor the propagation of combustion front behind the shock wave under detonation conditions are not modeled in the DETO code. More detailed 3-D analyses with a specific detonation code are, therefore, recommended. In spite of the code simplifications, DETO was found to be a beneficial tool for simple first-order assessments of the structure pressure loads under the first reflection of detonation shock waves.

The work on assessment of detonation loads will continue in the future with full 3dimensional simulations with detailed DET3D computer program.

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## **EXECUTIVE SUMMARY**

Combustion of hydrogen (deflagration or detonation) evolved during severe accidents can significantly increase the pressure and temperature in a confined volume. Especially, the dynamic loads associated with local or global detonations may induce a potential threat to containment integrity.

A special motivation for studying detonation phenomenology derives from the recent studies of hydrogen leakage from overpressurised BWR containment and consequent accumulation of hydrogen into the surrounding reactor building rooms during severe reactor accidents. The atmosphere in the reactor building is normal air, making the hydrogen combustion possible. Recent studies by Manninen and Huhtanen (1998) on hydrogen distribution in the selected reactor building rooms in Olkiluoto 1 and 2 BWR suggest that hydrogen accumulates closer to the ceilings of rooms. Furthermore, the stratification tends to be rather stable and yield very high hydrogen concentrations. The safety concern is if a hydrogen detonation in the reactor building can damage the containment or the containment penetrations from outside. This technical problem has not been widely studied to date.

The purpose of this report is to give an overview of physical mechanisms under detonation conditions in premixed hydrogen-air-steam mixtures, and introduce basic laws and relationship applicable to first-order estimates of pressure loads connected to detonations and eventually apply the developed method to Olkiluoto 1 and 2 reactor building. The computer DETO, which has been developed during this work at VTT, is used for estimations of the detonation pressure loads. The code is based on the strong explosion theory, and accounts for the effects of both the primary or incident shock and the first (oblique or normal) reflected shock from a wall structure. This work was carried out as a part of the Nordic SOS-2.3 project, dealing with severe accident analysis.

The detonation shock pressure loads were analysed in three different base cases. In two of them, the leak area from containment to reactor building was 20 mm<sup>2</sup>, and detonations were assumed to start in two different instants of time 13 000 s and 7500 s, corresponding the detonable hydrogen mass of 1.428 kg and 3.15 kg in the reactor building, respectively. The third case considered 2 mm<sup>2</sup> leak area (containment design leakage), in which the detonable hydrogen mass was 1.4 kg. It was assumed conservatively that the hydrogen leak from the containment occurs to one reactor building room. More realistic assumption would be that the leak is diffused to all parts of the reactor building. The distance from the explosion origin to wall was assumed to be 2.0 m in all base cases.

The peak pressure maximum after normal shock reflection ranged from about 12.6 MPa to 38.7 MPa. The corresponding maximum pressure impulses to the concrete wall ranges from about 2.3 kPa-s to 9.4 kPa-s. The duration of overpressure phase ranged from about 3.6 ms to 7 ms. The shock pressure spikes and corresponding impulses decreased as the angle between the incident shock wave and the wall surface increased. Furthermore, the results were sensitive to the distance. For example, the decrease of initial distance from 2.0 m to 1.5 m leads to increase of peak maximum pressure from 38.7 MPa to 106 MPa. Predicted shock pressure is also dependent on the total amount of hydrogen which is assumed to burn during explosion, and the properties of undisturbed

gas medium just before the shock wave. Comparison of the results to classical C-J theory and the Balloon experiments performed at Fraunhofer-Institut fuer Chemische Technologie in Germany suggested that the DETO code represented a conservative estimation for the maximum pressure spike after the first normal shock reflection from wall of Olkiluoto reactor building room B.60-80.

Uncertainties of the results are primary caused by the fact that only the first reflection of 1-D shock wave is considered, and due to lack of modeling of propagating combustion front behind the shock wave. Also multiple shock wave reflections, collisions and possible focusing in three-dimensional geometry may results in local pressure in the detonation front higher than predicted by approximate 1-D theories such as used in the DETO code. More detailed three-dimensional analyses with a specific detonation code is therefore recommended in order to assess these complicated interactions and their influences on pressure loads under detonation conditions.

The basic simplification of the DETO code is that the all energy is instantly released in the explosion origin inducing a "freely" propagating spherical shock wave without modeling of propagation of combustion front. Estimated velocity and pressure of the shock wave are, therefore, very sensitive to the distance from the explosion centre, and may significantly exceed the theoretical C-J values if the distance is very small. In spite of the limitations and simplifications, the computer program DETO is found to be a beneficial tool for simple first-order assessments of the structure pressure loads under the first reflection of detonation shock waves.

The work on assessment of detonation loads will continue in the future with full 3dimensional simulations with detailed DET3D computer code. Development of interface between the DETO code and ABAQUS structural analysis code is also under way.

## 1. INTRODUCTION

Combustion of hydrogen (deflagration or detonation) evolved during severe accidents can significantly increase the pressure and temperature in a confined volume. Especially, the dynamic loads associated with local or global detonations may induce a potential threat to containment integrity.

A special motivation for studying detonation phenomenology derives from the recent studies of hydrogen leakage from overpressurised BWR containment and consequent accumulation of hydrogen into surrounding reactor building rooms during severe reactor accidents. The atmosphere in the reactor building is normal air, making the hydrogen combustion possible. Recent studies by Manninen and Huhtanen (1998) on hydrogen distribution in the selected reactor building rooms in Olkiluoto 1 and 2 BWR suggest that hydrogen accumulates closer to the ceilings of rooms. Furthermore, the stratification tends to be rather stable and yield very high hydrogen concentrations. The safety concern is if a hydrogen detonation in the reactor building can damage the containment from outside. This technical problem has not been widely studied to date.

The purpose of this report is to give an overview of physical mechanisms under detonation conditions in premixed hydrogen-air-steam mixtures, and introduce basic laws and relationship applicable to first-order estimates of pressure loads connected to detonations, and eventually apply the developed method to Olkiluoto 1 and 2 reactor building. Computer code DETO, which has been developed during this work at VTT, is used for estimations of the detonation pressure loads. The code is based on the strong explosion theory, and accounts for the effects of both the primary or incident shock and the first (oblique or normal) reflected shock from a wall structure. The results of the DETO code are compared to classical C-J theory and a Balloon experiment performed at Fraunhofer-Institut fuer Chemische Technologie in Germany.

This work was carried out as a part of the Nordic SOS-2.3 project, dealing with severe accident analysis.

Chapters 2, 3, 4, and 5 of this report consist of a short overview (literature review) of the detonation dynamics and related research efforts performed worldwide. In chapter 5, some important aspects in respect to assessment of flame acceleration and detonations in real containment conditions are discussed. Generally, these aspects are not valid only for containment compartments, but also for other confined volumes such as reactor building rooms, as well. In chapter 6, detonation shock pressure loads are assessed to Olkiluoto reactor building room B.60-80 using the DETO. The initial conditions of the detonation calculations are based on previous severe accident analyses made by the MELCOR code, and the hydrogen distribution calculations in Olkiluoto reactor building performed by the FLUENT code.

# 2. PRINCIPAL DEFINITIONS OF COMBUSTION MODES IN PREMIXED GAS MIXTURES

In hydrogen-air-steam mixtures, different modes of combustion are possible depending on the initial and boundary conditions such as pressure, temperature, gas composition, degree of homogeneity, turbulence, scale, geometry, and ignition characteristics.

The chemical reaction zone where very rapid burning reaction takes place is often called the "flame zone", " flame front", or "reaction wave". Generally, the flame types can be divided into two categories (Kuo, 1986):

- a) premixed flame where the reactants are perfectly mixed before the chemical reaction, and,
- b) diffusion flame where the reactants diffuse into each other during the chemical reaction.

In this report, we concentrate on the premixed flames only.

Depending upon the speed of wave propagation through a reacting mixture, the reactions of premixed gases can be further divided into two categories:

a) deflagration, andb) detonation.

These two combustion modes have totally different properties, which can be easily distinguished. A schematic of a one-dimensional planar combustion wave (deflagration or detonation) is shown in Figure 2-1 (Kuo, 1986). The wave is moving to the left at a constant velocity  $u_1$ . The unburned gases ahead of the wave can be thus considered to move at velocity  $u_1$  toward the wave front. The subscript 1 indicates conditions of the unburned gases ahead of the wave, and subscript 2 indicates conditions of the burned gases behind the wave.



Figure 2-1. Schematics of a stationary one-dimensional combustion wave (Kuo, 1986).

A <u>deflagration</u> propagates at subsonic speed relative to the unreacted gas ahead of the wave having the typical velocities of the order of some meters per second. A deflagration is an expansion wave, with pressure and density both decreasing across the wave. Deflagrations heat the unburned gas by heat transfer from the hot burned gases. Deflagration mechanism depends very much on external conditions, such as ambient pressure.

A <u>detonation</u> propagates at supersonic speed, with typical velocities of the order of few kilometers per second. A detonation is a compression wave with both a pressure and a density increase across the wave. A detonation is therefore characterized by the reaction front in which the combustion is occurring and the strong shock wave ahead of it. This shock front then heats the unburned gases ahead of the combustion wave to temperature high enough for burning. Detonation is relatively independent of ambient conditions, but is quite sensitive to the density of explosive.

Qualitative difference between deflagration and detonation in premixed gases is shown in Table 2-1 (Kuo, 1986). Figure 2-2 shows an idealized representation of variation of properties across a deflagration and detonation waves (NEA, 1992).

	Detonation	Deflagration
$u_1/c_1$	5 - 10	0.0001 - 0.03
$u_2/c_1$	0.4 - 0.7 (deceleration)	4 - 6 (acceleration)
$p_2/p_1$	13 - 55 (compression)	$\approx 0.98$ (slight expansion)
$T_2/T_1$	8 - 21 (heat addition)	4 - 16 (heat addition)
$\rho_2/\rho_1$	1.7 - 2.6	0.06 - 0.25

**Table 2-1.** Qualitative difference between detonation and deflagration (Kuo, 1986).



**Figure 2-2**. Variation of properties across deflagration (above) and detonation (below) waves (NEA, 1992).

In certain turbulent circumstances, the deflagration wave may continuously accelerate leading to sudden change from delfagration mode to detonation mode. This transition process is called **deflagration-to-detonation transition (DDT)**.

An <u>explosion</u> is a general term for all phenomena resulting from a sudden release of energy, but without requirement for propagation of combustion wave through the mixture. There are two mechanisms whereby energy required for activation of the explosion reaction can be transferred from exploded to unexploded material (Kinney & Graham, 1985):

- 1) mechanical in nature where the mechanical energy is transferred through <u>shock</u> <u>pressure forces</u>, which is the basis for the detonation mechanism, and
- 2) thermal in nature where the surrounding material is warmed above its decomposition temperature so that this also explodes.

#### 3. BASIC THEORIES OF DETONATIONS

The following chapter presents a short introduction to classical detonation theories, from which the Chapman-Jouguet (C-J) theory based on the Rayleigh-Hugoniot solution is one of the best known. Due to certain simplifications and limitations of the C-J model, Zel'dovich, von Neuman, and Döring extended the C-J theory to so called ZND theory, which actually was the first theory of one-dimensional detonation structure. Later on, many experiments indicated that the detonations have a three-dimensional cellular structure leading to theories of multidimensional detonation wave structure.

#### 3.1 Rayleigh and Rankine-Hugoniot Solutions

Detonation propagation in a fuel-air mixture can be illustrated most simplistically by considering one-dimensional planar waves (see Figure 2-1 in Chapter 2). The equations of motion for strictly one-dimensional steady flow of an inviscid fluid are

$$\rho_1 u_1 = \rho_2 u_2 \tag{(3-1)}$$

$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2 \text{ (momentum)}$$
 (3-2)

$$h_1 + \frac{1}{2}u_1^2 = h_2 + \frac{1}{2}u_2^2$$
 (energy) (3-3)

If we solve the mass and momentum conservation equations, we obtain the equation

$$(\rho_1 u_1)^2 = (\rho_2 u_2)^2 = \frac{P_2 - P_1}{\frac{1}{\rho_1} - \frac{1}{\rho_2}} = \frac{P_2 - P_1}{V_1 - V_2}$$
(3-4)

where V is the specific volume, P is the pressure, and  $\rho$  is the fluid density. Because the left hand side of Eq. (3-4) is always positive, the end states for a steady one-dimensional inviscid flow are restricted to the regions illustrated in Figure 3-1 (Strehlow, 1991). All thermodynamic states of this system must lie on a single straight line through the point  $(P_1, V_1)$ . This line is called the **Rayleigh line**. We must note that because the energy solution is not included in Eq (3-4), the Reyleigh line does not represent a complete solution to the problem. The equation is also derived without any consideration of the equation of state.



Figure 3-1. The (P, V) plane showing the allowed regions of Eq. (3-4) (Strehlow, 1991).

A solution of all equations of motion (Eqs. 3-1 to 3-3), and eliminating both  $u_1$  and  $u_2$  gives the Hugoniot relationships, which may be written in terms of total enthalpy

$$h_2 - h_1 = \frac{1}{2}(P_2 - P_1)(V_1 + V_2)$$
(3-5)

Enthalpies of reaction will appear in the equation for the Hugoniot when chemical transformations are occurring in a steady, inviscid, one-dimensional flow.

However, the energy that is released in combustion processes is absorbed by the system and causes the temperature of the system to rise. Thus, the enthalpy-temperature relationship for the products does not anymore intersect the enthalpy-temperature relationship for the reactants.

The real enthalpy-temperature relationship can be approximated e.g. by **working fluidheat addition model** (Strehlow, 1991). In this model the chemical energy change is replaced by simple "arbitrary" heat addition to the working fluid using the following relationship

$$h_1 = c_{p1}T$$
 (3-6)

$$h_2 = c_{p2}T - q \tag{3-7}$$

where q represents the heat addition to the flow, and  $c_p$  is the specific heat capacity.

When substituted these relationships into the Hugoniot relationship (3-5), we get the following equation

$$\frac{\gamma}{\gamma - 1}(P_2 V_2 - P_1 V_1) - \frac{1}{2}(P_2 - P_1)(V_1 + V_2) = q$$
(3-8)

where  $\gamma$  is the specific heat ratio, and q is the heat release per unit mass. To express the Hugoniot relationship for the case of a constant heat capacity gas with some heat addition we substitute the variables

$$\eta = \frac{V_2}{V_1} - \frac{\gamma - 1}{\gamma + 1}$$
(3-9)

and

$$\xi = \frac{P_2}{P_1} + \frac{\gamma - 1}{\gamma + 1} \tag{3-10}$$

Changing the coordinate system, and after some algebraic manipulation, the Hugoniot relationship for the case of a constant heat capacity gas with heat addition can be written as

$$\eta \xi = \frac{4\gamma}{(\gamma+1)^2} + \frac{2q}{P_1 V_1} \left(\frac{\gamma-1}{\gamma+1}\right)$$
(3-11)

The plot of  $P_2$  versus  $V_2$  is called the **Rankine-Hugoniot curve** (or Hugoniot) and illustrated in Figure 3-2 (Strehlow, 1991). The Hugoniot is essentially a plot of all possible values of  $(V_2, P_2)$  for a given value of  $(V_1, P_1)$  and q. The point  $(V_1, P_1)$  is usually called the origin of the Hugoniot plot which represents the initial condition of the explosive. Chapman-Jouguet conditions (see next chapter) are satisfied by the points on the Rankine-Hugoniot curve where the tangents from the origin  $(V_1, P_1)$  touch it. Drawing tangents to the curve through the origin, and vertical and horizontal lines from the origin specify regions of all possible solutions. All Hugoniot curves which are displaced to the right and upward represent Hugoniot's for combustion processes. A positive value of q removes, thus, the Hugoniot curve toward the right and upward. In the detonation region, there is a minimum supersonic velocity for steady, one-dimensional inviscid flows called upper **Chapman-Jouguet point (C-J point)**.

Intersections of the Rayleigh line with the Hugoniot curve above the C-J point are called strong (or overdriven) detonations, which are observed experimentally when a shock wave is supported in an exotermic reactive system by a high-velocity piston. The upper C-J point is physically observed as a self-sustaining detonation. The weak detonation is observed physically when the chemistry is triggered at a high-velocity supersonic flow without having a shock wave in the system.



Figure 3-2. Hugoniot curve on p versus V plane for one-dimensional steady process (Strehlow, 1991).

#### 3.2 Chapman-Jouguet Theory

When a detonation is well established in a straight channel of sufficient cross-sectional area, it propagates at a constant supersonic velocity very close to the velocity defined by the upper Chapman-Jouguet point of the Rankine-Hugoniot curve. Jouguet formulated the theory so that it could successfully predict the equilibrium detonation properties such as detonation velocity, pressure, and the equilibrium composition of gases. The C-J Model is derived from conservation of mass, momentum and energy across a one-dimensional flow discontinuity. To complete solution one additional assumption is required: the particle velocity just behind the detonation front is sonic.

The C-J theory does not include knowledge of the wave structure or the chemical kinetics of the reactions. The C-J theory assumes the idealised 1-D reaction zone of zero thickness. Detonations are also assumed to be steady processes. A detonation wave velocity relative to the gas just behind the wave is assumed to be equal or less than the velocity of sound.

In spite of the fact that the real detonations are known to be unsteady processes with a multidimensional complex structure, the C-J theory yields remarkably good results on detonation speed and pressures even near the detonation limits. According to some theoretical considerations, the spontaneous detonation must really correspond to the C-J point i.e. the velocity of detonation wave relative to burned gases behind it is equal to that of sound (Landau and Lifshitz, 1986). A detonation above the C-J points (over-driven detonation) would require an artificial compression of the combustion products.

The C-J theory cannot predict many important dynamic detonation parameters such as detonability limits, critical tube diameter, critical initiation energy etc. These parameters are dependent on the non-equilibrium chemistry and the detailed cellular structure of the detonation front (Berman, 1986).

#### 3.3 ZND Model, One-Dimensional Detonation Wave Structure

As mentioned before, the C-J theory does not allow non-steady flow. More realistic transient analyses can be performed using the ZND detonation theory by Zel'dovich (1940), von Neuman (1942), and Döring (1943). The ZND theory is an extension of the classical C-J theory and it includes a model for the overall reaction kinetics. The ZND modelling is one of the most developed approaches in cell size prediction (Dorofeev et al., 1994).

The ZND model assumes that the detonation wave is composed of a planar shock wave followed by an unstable reaction zone. The thickness of the detonation front was driven by chemical reaction rates Idealised representation of the variation of physical properties through a one-dimensional ZND detonation structure is shown in Figure 3-3 (Kuo, 1986). The ZND model assumes that the propagation of detonation is sustained by ignition via shock-induced adiabatic compression. According to the ZND model, sharp pressure and density gradients exist at the front of the detonation wave. The peak pressure behind the shock wave in the ZND model is called the <u>von Neumann spike</u>. This shock pressure spike is predicted to be much larger than the C-J pressure where all the reactions are assumed to be in equilibrium.



**Figure 3-3.** Variation of physical properties through the ZND detonation wave (Kuo, 1986).

The locus of reacting mixture according to the ZND model on the Hugoniot plot is shown in Figure 3-4. All paths (a, b, c, etc.) can satisfy the conservation equations, by which a reacting mixture may pass through the detonation wave from the inactive state to fully reacted state. For example, path b presents a possible locus for mixtures with fast chemical kinetics, and path c for slow chemical kinetics.



**Figure 3-4.** *ZND detonation structure on (p, 1/ ) diagram wave (Kuo, 1986).* 

#### 3.4 Multidimensional Detonation Wave Structure

The existence of the von Neumann spike just behind the detonation shock front as predicted by the ZND model led to many experimental investigations of detailed detonation structure. In the 1960s, many experimental studies on detonation structure indicated that all self-sustaining detonations have the three-dimensional frontal structure and non-steady propagation. Denisov and Troshin (1960) first observed transverse waves in detonations with the smoked foil technique. After enormous amount of further experiments a new interpretation of detonation waves was discovered. Detonation waves were observed to be composed of curved triple wave-front intersections shown in Figures 3-5 and 3-6 (Kuo, 1986). Transverse waves of finite amplitude travel across the leading front at the local sound speed and interact with the leading shock to produce Mach stem which propagate across the detonation front (Guirao et al., 1989). A cellular structure is formed by the trajectories of the triple formed by the intersection of the leading shock, the transverse wave and Mach stem. Mach stem is a secondary and approximately vertical shock front formed when a primary shock impinges onto a surface at an angle too great to permit regular reflection.



Figure 3-5. Smoked-foil measurement and schematic diagram of symmetric planar interaction (Kuo, 1986).



Figure 3-6. Schematic diagram of shock-wave pattern and triple point in a twodimensional supersonic flow passing through a convergent ramp section (Kuo, 1986).

Later research has suggested that the detonation cell size (width) is the characteristic length of the cellular structure, and that there is a link between the detonation cell size and many important dynamic detonation parameters. The cell size is also found to have relation to the sensitivity of gaseous mixture to detonation.

#### 3.5 Detonation Pressure Loads in Gaseous Mixtures

The pressure development associates with accelerated flames, DDT, and directly initiated detonations in an enclosed volumes depends e.g. on the combustion mode itself, the volume of enclosure, the fuel concentration, and the size of the combustion region.

In a uniform mixture without heat losses, the loads of relatively slow deflagration are quasi-static approaching the peak pressure that can be determined assuming thermodynamic equilibrium among the combustion products. This final equilibrium pressure is called the AICC (Adiabatic, Isochoric, Complete Combustion) pressure, or the constant volume combustion pressure. On the other hand, DDT-induced pressurisation is dependent on the flame propagation process prior to DDT. The calculations by Craven and Greig (1968) for the worst case scenario, in which DDT was followed by the reflected shock wave indicated that the peak pressure on the wall of an enclosure can be order of magnitude higher than the detonation pressure for given mixture. Generally, initial transient of detonation waves yields very rapid shock pressure loads that are dynamic in nature, and significantly exceed the equilibrium AICC pressure. The duration of detonation peak pressure is very short (few milliseconds), and the pulse-type load as  $\int p \cdot dt$  is the quantity that can be integrated into the structure. In case of a simple, one-dimensional planar detonation, the peak pressure behind the detonation shock wave (blast wave) can be approximated relatively well e.g. with the classical C-J model. In reality, however, the detonation wave has a three-dimensional structure and is not continuously infinitely thin as assumed in C-J model. Due to reflected and transverse wave collisions of shock waves in the three dimensional geometry, the local peak pressure can exceed the C-J values (Boyack et al., 1992). The C-J theory can neither predict many important dynamic detonation parameters which must be must be obtained experimentally if the C-J theory is applied.

From a structural response point of view, not only the peak pressure, but also the pressure history is very important i.e. the time to pressure decay compared to the characteristic response time of the structure.

Boyack et al. (1992) have performed interesting studies on detonations in a onedimensional geometry. These numerical analyses for homogenous hydrogen-air-steam mixtures show that the detonation pressure exceeded the AICC pressure by a little less than a factor of two, and the peak reflected pressures were roughly 2.3 times the C-J pressures. In the same analyses, the ratio of peak reflected shock pressure to AICC pressure was found to be about 4 to 4.7. A stoichiometric hydrogen-air mixture was found to give the highest pressure loads and is considered to be conservative if the exact mixture composition is not known. Theoretical predictions for ratios of AICC pressure, C-J detonation shock pressure, and reflected shock pressure to initial pressure as a function of hydrogen concentration are shown in Figure 3-7 (NEA, 1992). It is worth mentioning that under certain circumstances the pressure loads caused by the shock reflections can still exceed the pressure loads presented in Figure 3-7. More discussion about that will be found in Chapter 6.3.3.



**Figure 3-7.** Pressure ratio of AICC pressure  $(p_{CV})$ , detonation shock pressure  $(p_2)$ , and reflected shock pressure  $(p_3)$  to initial pressure  $(p_1)$  (NEA, 1992).

All the assumptions discussed above apply to a detonation in homogeneous gas mixtures. However, in real accident situations during the hydrogen formation, certain amount of mixture heterogeneity can be anticipated. According to numerical studies by Boyack et al. (1992) the mixture heterogeneity may have important effects on pressure loads. If a thin air layer existed on the wall structure, the peak reflected pressure was found to be 1.4 to 2.6 times higher than if there were no air layer. This is due to different shock impedance of the air compared to the detonation products. Gradients in the detonable mixture were found to produce only minor effect in pressure time histories. Geometry was also found to have an important effect of detonation loads.

Initial pressure and temperature can have a significant influence on the AICC, C-J, and reflected C-J pressures. The simplified proportion can be expressed as  $P_{AICC} \sim P_{initial} / T_{initial}$  i.e. the AICC pressure is proportional to the initial pressure and inversely proportional to the initial temperature i.e. directly proportional to the initial density (Tieszen, 1993). This approximation can be considered to be valid below temperatures of about 500 K (errors less than 10%). The C-J pressure has a similar relation to the initial pressure and temperature. The reflected C-J pressure is also directly proportional to the initial pressure is more complicated, but generally the reflected C-J pressure decreases with increasing initial temperature. The studies e.g. by Tieszen (1993) also show that increasing of hydrogen concentration up to stoichiometric concentration significantly increases the AICC, C-J, and reflected C-J pressures. All these pressures also increase with increasing hydrogen concentration on the rich side of stoichiometric value for the constant volume case. For the constant initial pressure case, the pressures decrease with increasing hydrogen concentration on the rich side of stoichiometric values.

## 4. OVERVIEW OF HYDROGEN DETONATION RESEARCH

The research of detonation propagation was started as early as 1880 leading to observation of propagation of supersonics waves (Dixon, 1903). Chapman and Jouguet stated the wave propagation as the one-dimensional flow requirements, and suggested that the tangency point of the Rayleigh line and Hugoniot curve should represent the general behaviour of detonations (see Chapters 3.1 and 3.2). The formulated theory allowed the calculation of detonation velocity from thermodynamic and hydrodynamic considerations only (Strehlow, 1984). Campbell and Woodhead (1927) first observed the three-dimensional frontal instabilities of detonation near the limit composition (marginal detonation) in a tube. The observation was called the single spin detonation (Strehlow, 1991). The details of the structure could not, however, be identified, and for several decades after the discovery it was thought that the spinning is a specific feature of marginal detonation only. The first theory of self-sustaining detonation structure was formulated by Zeldovich, Von Neuman, and Döring assuming that the detonation wave consists of a shock wave and a chemical reaction zone behind it (see Chapter 3.3).

In the 1960s many experimental studies on detonation structure led to observation that all self-sustaining detonations have a three-dimensional frontal structure and non-steady propagation (Guirao et al., 1989). Transverse waves in detonations were first observed by Denisov and Troshin (1960) using the smoked foil technique. After enormous amount of further experiments new features of detonation waves were discovered. Detonation waves were observed to be composed of curved triple wave front intersections (see Chapter 3.4).

Despite several observations of three-dimensional detonation structure, the basic fundamental processes inside the detonation front were unknown until the late seventies when Lee (1984) recognised that the detonation cell size (width)  $\lambda$  is an important parameter which can be related to the chemical length scale of the detonation processes. He also suggested that  $\lambda$  could be correlated to most important dynamic parameters of detonations (Figure 4-1) (Strehlow, 1979). Further detonation research performed in 1980s e.g. at McGill University and Sandia National Laboratories focused on investigations of the relevant dynamic detonation parameters such as detonation cell size  $\lambda$ , critical initiation energy, detonability limits, critical transmission conditions of detonations, and the processes involved in DDT (Guirao et al., 1989).

Following Berman (1986), the problematic of hydrogen-air detonations can be generally divided into two main issues:

- 1) transition to detonation (direct initiation, DDT)
- 2) propagation of detonation (detonability limits, critical tube diameter)

The first issue is related to question, will a detonation occur if the conditions for propagation (issue 2) are satisfied i.e. the mixture is within the detonability limits. The second issue addresses the conditions under which detonation propagation is possible independent of any ignition mechanism.



**Figure 4-1**. Detonation cells (above) and cell width  $\lambda$  (below) (Strehlow, 1979).

#### 4.1 Detonation Cell Size

Gaseous detonation waves have a three-dimensional, cellular structure with multiple interactions of transverse shock waves with the main shock front. The three-dimensional cellular structure of detonation wave front is consequence of nonlinear coupling between gas dynamics and chemical kinetics. Due to extremely complex processes inside the structure, no comprehensive theory has been developed that could give quantitative estimates of these processes and, thus, detonation dynamic parameters.

As mentioned before, a big step forward in understanding of the fundamental processes of detonation occurred when the detonation cell size  $\lambda$  was discovered to be practical and fundamental (in respect to experimental measurements) parameter for determining the dynamic detonation parameters. It has been later shown that  $\lambda$  can be, therefore, used to represent the detonation sensitivity of the mixture. High values of  $\lambda$  correspond to the low detonation sensitivity.

Cell size  $\lambda$ , even if being probably the most practical characteristic for detonation, is not the only one. Also the critical tube diameter or the chemical induction length could be used as the characteristic length. In any case,  $\lambda$  can be measured experimentally most easily (by e.g. smoked foil technique), but unfortunately, the measurements may include large errors due to possible poor or irregular cell structure. The irregularity observed in some smoked foil records has proved that a detonation wave may have more than one detonation size or modes (Tieszen et al., 1987), and thus, the criticism in use of only one detonation cell size as a fundamental characteristic is justified (Dorofeev et al., 1994).

Several small and large-scale experiments have been performed worldwide in order to measure the detonation cell size. Most of the detonation experiments have been conducted in small-scale cylindrical tubes. The universality of the results is, therefore, difficult. Sandia National Laboratories (Figure 4-2) have conducted some large-scale experiments e.g. in the heated detonation tube (HDT). The diameter of facility was 43 cm and the length 13.1 m. The facility could also operate at elevated temperatures (above 100 °C) (Tieszen et al., 1987, Berman, 1986).



Figure 4-2. Schematic of the HDT facility (Berman, 1986).

Some results of detonation cell size measurements for H<sub>2</sub>-air and H<sub>2</sub>-air-steam mixtures at NTP as a function of equivalence ratio (fuel to air molar ratio divided by the same ratio at stoichiometry) are plotted in Figures 4-3 and 4-4, respectively (Tieszen et al., 1987). The minimum cell size was for the stoichiometric composition ( $\phi$ =1). The leanest and richest composition limits 13.6% H<sub>2</sub> ( $\phi$ =0.37) and 70% H<sub>2</sub> ( $\phi$ =5.55) were wider than previous estimates corresponding to the onset of single head spin detonation. The cell size increased faster for lean than rich mixtures indicating a larger detonation sensitivity of fuel-rich mixtures (Tieszen et al, 1987).



Figure 4-3. Experimental detonation cell size with equivalence ratio in hydrogen-air mixtures at NTP (Tieszen et al., 1987).



**Figure 4-4.** Experimental detonation cell size with equivalence ratio in hot hydrogenair-steam mixtures at superatmospheric initial pressures (Tieszen et al., 1987).

Steam concentration has a significant influence on the detonation cell size. As the steam concentration increases also the cell size increases (sensitivity decrease). The studies on the influence of temperature on cell size are conflicting. Generally, an increase in temperature and density at constant pressure, or an increase in pressure at constant temperature tends to decrease the cell size. Some studies, however, indicated that the cell size could increase for near stoichiometric mixtures at constant pressure as the temperature increases (Tieszen et al., 1987).

Typical uncertainty bounds in HDT tests (smoked foil technique) were estimated at +/-25%, for some tests as much as +/- 100%. Development of other techniques are therefore recommended by Guirao et al. (1987) in order to improve the accuracy of measurements of detonation cell sizes.

Conclusively, for hydrogen-air-steam mixtures, the detonation cell size is a function at least of four independent parameters: equivalence ratio, steam concentration, temperature, and air density.

#### 4.2 Transition to Detonation

#### 4.2.1 Onset of Detonation

Principally, the initiation mechanisms of detonation can be divided into two main modes:

- a) direct initiation, and
- b) indirect initiation e.g. by deflagration-to-detonation transition (DDT).

In direct initiation (also called as blast initiation), the detonation is ignited powerfully and very rapidly without any flame acceleration from deflagration regime. In indirect initiation mode induced by DDT, the deflagration flame is firstly accelerated to some critical velocity, after which a sudden transition to detonation occurs.

Lee and Moen (1980) proposed that the essential features of the onset of detonation are similar for different initiation methods. The process starts by the formation of a localised explosions in a turbulent region, which then generate a spherical (or hemispherical) shock wave which amplifies and propagates into the preconditioned (but yet unreacted) mixture behind the shock wave (Utriew & Oppenheim, 1960).

Lee and Moen (1980) have divided the onset of detonation into two phases:

- a) creation of the critical conditions for the onset of detonation (depends on the particular method of initiation), and
- b) the actual formation of detonation wave (is similar to all initiation methods).

In DDT, for example, the critical conditions are reached by the positive feedback mechanism between the turbulent flow field and the flame (see 4.2.3). For the direct initiation, the critical conditions are reached by the non-linear coupling between the decaying shock wave and the chemical reactions. In case of initiation by a hot turbulent jet, the rapid turbulent mixing of the combustion products with the unburned mixture creates the critical states.

Although the occurrence of local auto-explosions is prerequisite for the onset of detonation, it is not sufficient by itself to lead to detonation. The formation of detonation therefore requires the amplification of the shock waves from these localised auto-explosions. This amplification mechanism was first observed by Lee et al. (1978) and is called The Shock Wave Amplification by Coherent Energy Release (SWACER). In SWACER mechanism, the time sequence of chemical energy release in the preconditioned gas region is coherent with the arrival of shock wave adding strength to the shock wave as it propagates (NEA, 1992). In addition to appropriate time sequence, certain minimum coherence or amplification length for the chemical energy release over this distance is needed in order to give enough strength for the shock wave to maintain self-coherence outside of the preconditioned region.

#### 4.2.2 Direct Initiation

The ignition source plays the dominant role in the direct initiation mechanism of detonation. Strong initiation of detonation occurs when the ignition energy generates a sufficiently strong shock with a sufficient duration to heat the reactive gas mixture above its auto ignition temperature, which is kept for a time longer than the induction time. There is a critical energy below which initiation will not occur. The earlier studies have shown that the critical initiation energy with mixture composition forms a U-shape with a minimum around the stoichiometric conditions (Figure 4-5) (Guirao et al., 1987). The critical energy strongly depends on the nature of the ignition source. Some researches have also indicated that the critical energy is related to the characteristic transverse spacing in a well-developed propagating detonation. In any case, the rapid energy release may lead to direct initiation of spherical or cylindrical detonations.



Figure 4-5. Critical energy for direct initiation of spherical detonation as a function of hydrogen concentration in  $H_2$ -air- $CO_2$  mixtures at NTP (heat of detonation = 4.27 KJ/g tetryl) (Guirao et al., 1987).

Direct detonation initiation caused by an energetic impulse source is not believed to be very probable in NPP containments due to high critical energy needed. According to Sandia tests the critical ignition energies for hydrogen-air mixtures with 20%, 18.5%, and 17.4% correspond to about 30g, 150g and 460 g of tetryl high explosive, respectively (Guirao et al., 1987).

Initiation behind the reflected shock is the simplest one-dimensional planar initiation observed experimentally in which the initiation of detonation is primarily caused by the auto ignition due to high temperature behind the shock wave (Sthrehlow, 1991).

Direct initiation of detonation is also observed in conditions where the auto ignition temperature is not exceeded. Auto-ignition can also be obtained by producing free radicals into the mixture (Strehlow, 1991). For example, the irradiation of hydrogen-oxygen mixture may produce radicals that in sufficient high concentration can trigger the chain reaction and cause a local explosion. Contrary to strong shock wave, this mechanism is chemical in nature for generating a detonation shock wave.

Carnasciali et al. (1991) and Knystautas et al. (1978) have investigated the injection of a hot turbulent jet of combustion products into a reactive mixture, which can also lead to direct initiation of detonation. In the jet ignition mechanism, a localised explosion is formed in the turbulent mixing region. Shildknecht, Geiger, and co-workers at Battelle Frankfurt have extended the turbulent jet ignition experiments to large-scale (Berman, 1986). In the jet ignition, the onset of detonation is due to chemical energy release during turbulent mixing alone i.e. there are no external high energy sources to produce

strong shock wave (Lee & Moen, 1980). The results by Carnascialli et al. (1991) also suggested that under optimal conditions of jet initiation there is a minimum value of the ratio D/ $\lambda$  (orifice diameter to cell size of the mixture) to be detonated, which is comparable to that for detonation propagation or the critical tube diameter situation.

Dorofeev et al. (1995) observed in large-scale experiments for high sensitive mixtures performed at KOPER facility that a sudden venting of a hydrogen-air deflagration might lead to transition to detonation. They concluded that the onset of detonation was rather connected to sudden venting than linked to the jet ignition. The mechanism of detonation onset caused by venting might be flame instabilities and a rarefaction wave. A sudden venting can cause flame instabilities which increase mixing of combustion products and reactants. At the same time, the outflow generates a rarefaction wave which can create in partially reacted mixture an induction time gradient leading to conditions for pressure waves amplification due to SWACER mechanism (see chapter 4.2.1). Dorofeev et al. also suspected that the venting-induced detonation observed in sensitive mixtures can also be possible in lean fuel-air mixtures, if the scale is sufficiently large.

#### 4.2.3 Deflagration-to-Detonation Transition (DDT)

It is possible to produce a detonation wave in combustible mixture even though no available ignition source is strong enough to cause direct initiation. The processes involved in continuous flame acceleration and the transition from a subsonic flame to a supersonic detonation wave are called deflagration-to-detonation transition (DDT). Maximum pressure generated by DDT is dependent e.g. on the pre-conditions ahead of the flame front, and can be much higher than the C-J pressure in a case of wave reflections.

Contrary to a stabilised flame, a freely propagating flame has a strong influence on the flow conditions ahead of it, because of the expansion of the burned gas pushes the surrounding gas away. Turbulence of the flow plays a dominant role in these flame acceleration and transition processes. Turbulence can be generated e.g. by flow interaction with obstacles, other boundaries, or reflected waves. When the flame front propagates into the turbulent flow field, its surface area and the burning rate may increase significantly. The increased burning rate may further increase the flow velocity and turbulence leading to positive feedback loop. The positive feedback loop may be repeated several times leading to continuous acceleration of the flame. This interaction (positive feedback) between the fluid dynamics and the combustion process can lead to unstable situation resulting in a flame acceleration to certain limiting velocity, or under appropriate conditions, an abrupt transition to detonation, if a critical velocity is reached. The experiments have also demonstrated that the probability of flame acceleration and DDT increases as the geometry increases.

The processes leading to deflagration-to-detonation transition can be classified into two categories (Breitung et al., 1999):

- 1) detonation auto-ignition caused by the reflection or focusing of shock waves produced by an accelerated flame,
- 2) transition to detonation due to flame instabilities, or due to flame interaction with a shock wave, another flame, structures, or due to the explosion of a previously quenched pocket of combustible gas.

Once the critical conditions are reached for DDT, the essential features of onset of detonation are similar to other methods of detonation initiation (Utriew & Oppenheim, 1960):

- 1) formation of discrete auto-explosion centres leading to localised explosions,
- 2) amplification of the pressure wave from the localised explosion (SWACER mechanism), and
- 3) transition of the detonation wave structure from the preconditioned, reactive mixture to the other part of the gas mixture.

Deflagration-to-detonation transition processes are extensively studied from 1980s e.g. in Kurchatov Institute (Dorofeev et al., 1996), in Sandia National Laboratories (Sherman et al., 1989, and Sherman et al., 1993), at McGill University, at Whiteshell Laboratories Program, at Prints Maurits Laboratory, in Battelle Institute, in FZK, in BNL (Ciccarelli et al., 1996), by Thomas et al. (1997), in Defence Research Establishment, in Defence Construction Service, and in Technical University of Munich (NEA, 1992). Most of these studies are concentrated on the role of turbulence for flame acceleration and DDT, and are performed in confined tubes with wire spirals or repeated obstacles for various fuel concentrations and scales (Guirao et al., 1989). Several experiments concentrated on other combustion regimes such as deflagration and flame acceleration without DDT are not addressed here.

Depending on conditions, three different end states of flame propagation have been observed:

- a) flame quenching,
- b) local speed of sound (choked flow), and
- c) DDT with quasi-, stable, or overdriven detonation.

Flame and detonation propagation modes are described more detailed in chapter 4.3.1.

It appears to be much more difficult to reach DDT conditions for <u>unconfined volumes</u> compared to confined tubes (Khokhlov & Oran, 1997). This is due to geometrical effect of expansion of gases, which may weaken the shock wave and turbulence leading to unfavourable preconditions of the mixture for DDT. The effects of reflected shocks and interaction with walls may also be minimal in unconfined volumes compared to DDT in confined volumes such as the experimental tubes. In large unconfined spaces, turbulence seems to be, therefore, the only mechanism that can form the mixed region thick enough to trigger a detonation. This could explain why DDT in unconfined volumes is relatively rarely observed experimentally.

Dorofeev et al. (1996) have studied <u>flame acceleration and DDT in a large confined</u> <u>volume</u> of 480 m<sup>3</sup>. The geometry of the RUT facility is shown in Figure 4-6. The flame propagation and DDT were studied in hydrogen concentration from 9.8 to 14%. Dorofeev et al. observed that some degree of confinement, partially obstructed flow paths, or a high-speed turbulent jet is required for favourable conditions for the onset of detonation. A certain minimum size of an unobstructed flow channel and a minimum obstacle pacing are required for DDT. As the mixture sensitivity decreases a larger scale is required to produce DDT. They also observed that the reflections of pressure waves from obstacles and surrounding structures (walls) in confined volumes could lead to autoignition of the mixture and formation of localised explosions resulted in DDT. According to RUT experiments, DDT was observed with a minimum hydrogen concentration of 12.5%.



Figure 4-6. Geometry of the RUT facility (Dorofeev et al., 1996).

4.2.4 Mechanisms Affecting the Flame Acceleration and DDT

In spite of large number of studies, a quantitative understanding of all mechanisms involved in DDT has not yet been fully achieved. We know that turbulence induced by obstacles, fans or other boundaries is one but not only mechanism that may cause the acceleration of freely propagation flame. Some mechanisms affected the flame acceleration and DDT are shortly described below. Different propagation modes of accelerated flames and detonations are described more detailed in section 4.3.1.

#### **Turbulence Induced by Obstacles and Boundaries**

As the unburnt gas flow passes over obstacles or other boundaries, the flow field will be distorted. As the flame front propagates into this turbulent flow field, the flame surface will stretch and fold leading to increase in the heat release rate and to higher burning rate and burning velocity. In real containments, the violent turbulence can be also induced by funs (Berman & Cummings, 1984). Lee and Moen (1980) divided the turbulence into two scales.

1) flame folding involves length scales which are larger than the thickness of the flame zone, and

2) small-scale turbulence involves length scales which are smaller than the thickness of the flame zone.

Using this division, the small-scale turbulence enhances the transport rates of heat and mass (local burning rate), and the flame folding increases the burning velocity due to augmentation in the flame surface area. According to some experiments, in the initial stage when the flame speed is low, the dominant flame acceleration mechanism seems to be flame folding. As the flame speed increases the small-scale turbulence also increases, and the burning rate begins to dominate the acceleration processes (Lee & Moen, 1980). The basic mechanisms responsible for the turbulence are the Kelvin-Helmholtz shear instabilities, or the Reyleigh-Taylor instabilities (Breitung et al., 1999).

#### Flame Instability (Taylor Interface Instability)

Another mechanism for generating folded flames is the Taylor's interface instability resulting from the interaction of shock pressure waves with the deflagration front. Any increase in flame speed generates pressure waves. The pressure waves moving away from the flame is reflected from obstacles or other boundaries and interacted with the flame front forming large-scale flame folds. In a closed vessel, new flame folds are periodically generated by the next reflected shock-flame interactions. The continuous generations of the flame folds by the Taylor instability is, therefore, analogous to the role of repeated obstacles for flame acceleration.

#### Interaction Between an Acoustic-Wave and Flame Front

Flame propagation in an enclosure generates acoustic waves that can interact with the flame front leading to flame acceleration through several instability mechanisms (Breitung et al., 1999). These kinds of instabilities are usually related to relatively slow flames in enclosures. The basic mechanism of the flame acoustic instabilities is the flame distortion caused by the interaction between the acoustic wave and flame front, and wave amplification due to the coherence between the acoustic wave and the exothermic energy release (Rayleigh criterion).

#### **Pre-Compression of the Unburnt Gas**

Since the flame velocity also depends on the thermodynamic state (temperature, pressure) of the unburned mixture ahead of the flame, the heating and compression of the unburned mixture by the flame-generated shock waves is also a possible mechanism for flame acceleration. However, investigations have shown that the influence of pressure and temperature on flame acceleration is of minor importance. For example, the higher temperature is compensated by the corresponding increase in sound speed. An increase in the temperature also decreases the density, and hence the volumetric energy release rate in the unburned mixture. Turbulence is, therefore, a much more powerful flame acceleration mechanism than the temperature and pressure increase by compression (Lee & Moen, 1980). For example, the flame acceleration mechanisms in spherical or cylindrical geometry must be sufficiently powerful to provide a critical rate of acceleration to compensate the flow divergence effect with increasing radius. According to Brinkley and Lewis (1959) this relatively weak acceleration mechanism of gas compression plays a role only in the early stages of flame acceleration. Once a turbulent flame is formed, turbulence is much more significant mechanism of flame acceleration.

#### **Collision of a Shock Wave with Obstacles**

The recent experiments by Chan (1995) with stoichiometric hydrogen-air mixtures for highly accelerated supersonic flame have indicated that the collision of leading shock wave with obstacles alone (without requirement for turbulence) can create local hot spots capable of causing a strong ignition and transition to detonation (Figure 4-7).



Figure 4-7. Photographs showing the collision of a shock wave with a pair of baffle obstacles in a stoichiometric hydrogen-air mixture (Chan, 1995).

#### Confinement

The confinement level may also have a significant influence both on flame and detonation propagation.

If the vessel is totally closed and adiabatic, the final equilibrium overpressure increase is equal to the constant-volume combustion pressure. The experiments by Chan et al. (1983) have indicated that the degree and nature (location) of confinement can have a significant influence on turbulence on unburnt gas, and thus on flame acceleration, and pressurisation (Figure 4-8). Only about 10% decrease in the confinement level can significantly reduce the flame speed.

Large-scale experiments by Sherman et al. (1989) have also indicated the strong influence of transverse venting on flame acceleration and DDT. Sherman et al. observed that a small degree of venting could result in a higher flame acceleration rate than when there is significant venting or no venting at all. Insufficient venting may, thus, be worse than no venting under certain conditions. This can be explained by the contradictory effects of enhanced turbulence directly caused by venting, and the decrease in turbulence from a decrease in the unburnt gas flow due to venting (NEA, 1992).



**Figure 4-8.** Flame speed at 1 m from ignition for various degrees of confinement and obstacle configurations (h is the obstacle height and P is the obstacle spacing) (NEA, 1992).

#### **Buoyancy Effect**

Buoyancy has influence on the early stage of flame propagation (Breitung et al., 1999). The gravitational effect tends to lift the flame upwards leading to local cooling in top boundaries. Due to buoyancy the flame propagation may be limited to the upper part of volume. Most likely, this can happen for lean hydrogen-air flames for which the upward and downward propagation limits are different. The upward acceleration strengthened by buoyancy effect can also lead to the Rayleigh-Taylor instabilities, which can further increase the flame acceleration.

4.2.5 Necessary Criteria for Flame Acceleration and DDT

Because of DDT is strongly dependent on complicated interactions between mixture conditions, chemical reactions, gas turbulence, and geometrical scale, no comprehensive tools exist nowadays to predict (or ensure) reliably DDT for given initial and boundary conditions.

In any case, Efimenko and Dorofeev (1999) have performed promising work combining certain criteria of combustion modes (flame acceleration, DDT) into a computer code for **conservative** estimates of possible pressure loads during hydrogen combustion in a containment. All of these criteria are **necessary**, **but not sufficient conditions** i.e. they are supposed to be prerequisite for the flame acceleration and DDT. The proposed three basic criteria for applications to safety analyses are formulated for the flame acceleration, detonation propagation, and DDT (Breitung et al., 1999):

#### 1) necessary conditions for flame acceleration

According this criterion, strong buoyancy effects limit the ability to flame acceleration leading to inhomogeneous conditions and uncompleted combustion. Necessary conditions for mixture composition are:

$\sigma > 3.5 - 4$	for hydrogen-rich mixtures	(4-1)
$\sigma > \sigma^*(\beta)$	for hydrogen-lean mixtures	(4-2)
	- if no additional gas components or dilution than hydrogen,	
	air, and steam exist, $\sigma^*(T_i)$ can be used instead of $\sigma^*(\beta)$	

where  $\sigma$  is the ratio of densities of reactants and products,  $\sigma^*$  is the critical value, and  $\beta$  is the Zeldovich number as

$$\beta = E_a (T_m - T_i) / (RT_m^2)$$
(4-3)

where  $E_a$  is the effective activation energy,  $T_i$  is the initial temperature, and  $T_m$  the maximum flame temperature.

#### 2) necessary conditions for detonation propagation

The basic of the criterion is that DTT can not be possible, if a self sustained detonation propagation is impossible. This implies that detonability limits must apply for detonation propagation too.

#### 3) necessary conditions for DDT

**First sets of requirements** of this criterion are to provide conditions for DDT. Firstly, turbulent flame must be accelerated to nearly choked or sonic combustion regime corresponding flame speed, which is near the isobaric sound speed of about 500 - 1000 m/s in combustion products (see Fig. 4-10). Secondly, the minimum flame Mach number is assumed to be 1.5. Thirdly, the minimum Mach number for the shock wave induced by the flame front is assumed to be 1.2-1.4 (the value decreases as the scale increases) in order to be capable of giving localised explosions and a strong ignition in shock reflections.

<u>The second sets of requirements</u> are to provide the onset of detonations. For very long channels the sufficiently large unobstructed passage is needed to enable the transition to detonation. The minimum tube diameter criterion that is found to be applicable for very long channels can be expressed as

$$d > 1\lambda \tag{4-4}$$

where *d* is the size of unobstructed passage, and  $\lambda$  is the detonation cell size. For different channel types, and obstacle and blockage configurations the ratio of  $d/\lambda$  may range from 0.8 to 5.1.

The effect of scale in different geometries such as in containment compartments is taken into account by the characteristic geometrical size L, which represent the size where detonations might originate and develop. Experimental data show generally good agreement over large range of scale and mixture composition using the following criterion

$$L > 7\lambda \tag{4-5}$$

In a case of a single room, L can be defined as L=(S+H)/2 where H is the room height and S is the length (if both are greater than room width).

An example of the criteria application is shown in Figure 4-7 demonstrating also the recent knowledge of the possible DDT and flammability limits in hydrogen-air-steam mixtures at 1 atm pressure and 375K temperature (Breitung et al., 1999). As can be seen from the Figure 4-9, DDT is possible in hydrogen-air mixtures with a minimum hydrogen concentration of about 10% for rooms with a characteristic dimension about 10 meters.



Figure 4-9. Limits and possible regimes of combustion for hydrogen-air mixtures at 1 atm and 375 K according to Efimenko and Dorofeev (1999).

There are several uncertainties taht must be known when applying the above criteria to real reactor conditions. Firstly, the cell size (width) is considered to be only approximate characteristic length of a mixture. However, real cellular structure of detonations may include irregularities e.g. in unhomogeneous mixtures. Average uncertainties in measured cell size can be higher than +/-100% (Breitung et al., 1999). It is therefore possible that a single parameter is insufficient to represent the mixture sensitivity to detonation. Secondly, the clear definition of the characteristic geometrical size *L* may be very difficult in complicated containment geometry. Thirdly, no detonations are observed experimentally with the cell size larger than 2 m, and hence, it is unsure if the cell size data can be extrapolated to values beyond 2 m which corresponds to the volumes with characteristic length of more than 10-15 m.

#### 4.3 Propagation of Detonation

4.3.1 Propagation Modes of Accelerated Flames and Detonation

If the gas compressed by the shock wave is free of disturbances and all the chemical energy released in the reaction zone goes to support the detonation, the process will eventually reach steady state and the shock wave will propagate nearly at the C-J velocity. However, this will not be the case in presence of boundaries or obstacles, since the turbulence behind the shock wave will influence the interaction between the shock wave and the reaction zone. Turbulence will increase losses and quench the flame e.g. by mixing the burned and cold unburned gases decreasing the amount of chemical energy available to support the detonation. Under certain conditions, the propagating flame can also extinguish itself (self-quenching). On the other hand, turbulence can accelerate the flame front and assist the onset of detonation, and may have, therefore, two competing effects on flame propagation. Depending on the geometry and fuel concentration different regimes of flame and detonation propagation are possible.

Figure 4-10 illustrates the maximum flame speeds versus fuel concentration of  $H_2$ -air mixtures measured in three tubes of various diameters (Guirao et al., 1987). These experiments were carried out in long rough-walled tubes (11 - 19 m) of diameter ranging from 5 to 30 cm in McGill University and SNL. Several different regimes of final flame speed were observed depending of the steady-state velocity (Breitung et al., 1999):

- 1) a quenching regime (no propagation),
- 2) a subsonic regime (flame speed is lower than the sound of speed of the combustion products),
- 3) a choked flow regime (flame speed is comparable to the sound of speed of the combustion products),
- 4) a quasi-detonation regime (propagation velocity between the sonic and C-J velocity), and
- 5) C-J detonation regime (propagation velocity comparable to C-J velocity).

Figure 4-10 also shows that not all regimes can be observed for a given tube, thus, the propagation velocity is also dependent on the geometry. In very lean mixtures ( $\leq \sim 12.5\%$  H<sub>2</sub>), a steady-state velocity of turbulent deflagration is of the order of few tens of meters per second. As the fuel concentration increases, the steady flame velocity in the second regime is observed to be of the order of 800 to 1000 m/s. In this regime, the velocity of the combustion products with respect to the flame is sonic, thus flow is choked, and the steady flame speed is close to the isobaric sound speed. In the next regime (increasing the fuel concentration), the steady velocities are more than 1100 m/s, but clearly below the C-J detonation velocity of the mixture. This is called the quasidetonation regime. If the orifice diameter is large enough, a stable detonation wave can be formed. The velocities, however, may be much lower than the C-J velocities due to momentum and heat losses to the walls caused by obstacles. If the fuel concentration is
sufficiently large (near 24%), the transition from quasi-detonation to the C-J detonation regime is observed.



**Figure 4-10.** Thermal flame velocity as a function of hydrogen concentration in hydrogen-air mixtures at NTP (Guirao et al., 1987).

According to McGill and SNL experiments, there are two prerequisites for transition to quasi-detonation in a rough tube. Firstly, the flame must accelerate to supersonic velocity of the order of isobaric sound speed of the burnt mixture. Secondly, the minimum transverse dimension of the tube must fill the criterion  $\lambda/d \leq 1$  where  $\lambda$  is the detonation cell size (width), and *d* is the orifice-opening diameter. For H<sub>2</sub>-air mixtures, DDT was observed in rough tubes (5, 15, and 30 cm) at 22, 18, and 16% H<sub>2</sub>, respectively. The C-J detonation regime is found to be possible, if the unobstructed tube diameter is larger than approximately 13  $\lambda$  corresponding to the critical tube diameter.

4.3.2 Detonability Limits and Critical Tube Diameter

The detonability limits of reactive gas mixture can be defined as the critical conditions for the continuous propagation of self-sustained detonation depending on the initial and boundary conditions (e.g. gas mixture composition, geometry, scale, initial fluid mechanical and thermodynamic state, ignition source strength etc.). At present, there is no quantitative theory to predict the detonation limits which must be, thus, defined empirically. Earlier experiments showed that in a smooth circular tube a self-sustained detonation was replaced by a single-head spinning detonation as the mixture composition became leaner or richer. The single-head spinning detonations were proposed as the detonability limits of confined mixtures. Later on, the propagation of detonations was observed also in mixtures that are less sensitive than the mixture needed for the single-spin detonations. This is explained with possible multiple detonation modes each mode having its own characteristic cell size  $\lambda$  (Berman, 1986).

Little data for  $H_2$ -air-steam mixtures existed prior to the HDT tests and the detonation limits for  $H_2$ -air-steam mixtures were mostly studied theoretically. For example, Shapiro and Moffette (1957) reported a classical triangular diagram for flammability and detonability limits (Figure 4-11).



Figure 4-11. Flammability and detonation limits of the hydrogen-air-steam mixtures according to Shapiro and Moffette (Lee & Fan, 1992).

Shapiro and Moffette examined the detonability limits as a function of mixture coordinates only. However, according to recent studies the detonability limits are also a function of geometric scale, initial pressure and initial temperature. Figure 4-12 shows some HDT data for a mixture temperature of 100 °C and air molar density of 41.6 moles/m<sup>3</sup> plotted in triangular diagram (Tieszen et al., 1987). The lines of constant cell width correspond to detonation sensitivity. As the cell width increases, the smallest room dimension that will allow detonation propagation increases. The area to the left of a given cell width is detonable for the given temperature and air density. A large room will allow detonation propagation in a broader range of mixtures compared to a smaller room.



**Figure 4-12.** Constant detonation cell width and detonation limits for temperature of 100 °C and air molar density of 41.6 moles/m<sup>3</sup> (Tieszen et al., 1987).

According to HDT results, the increase of steam content reduces detonability significantly (Figure 4-4). The addition of 10, 20, and 30% steam increased the cell size by factors 6, 20, and 60 respectively. This result is contrary to predictions by Shapiro and Moffette where the steam content below 25% was assumed to have negligible influence on the detonation limits. Shapiro and Moffette also predicted that 32% steam concentration could completely inert a detonation, but in the HDT tests performed by 30% steam concentration the detonation cell size was still well below the detonation limit (Tieszen et al., 1987).

Stamps and Berman (1991) have reviewed the effect of elevated temperature on ignition limits of different combustion modes such as detonation. They concluded that the detonability limits for hydrogen-air mixtures widen with temperature and scale of the test facility. The detonation limits approach the flammability limits at high temperature.

Historically the detonations were considered to be possible for hydrogen concentration between about 18% to 59%. Recent large-scale experiments e.g. by Dorofeev et al. (1994) have shown that detonation is possible in hydrogen-air mixtures with hydrogen concentration between about 10% and 77%. The increase of diluent (e.g. steam) content reduces significantly the detonability of a mixture.

The detonability limits are observed to be dependent on the apparatus (geometry) and ignition source strength used (Guirao, 1989). Dupre et al. (1985) has suggested that the criterion of  $\lambda = \pi D$  could be the most representative one. The <u>limiting tube diameter</u> D (minimum diameter that permits stable propagation of detonation) for H<sub>2</sub>-air-steam mixtures at 100 °C predicted directly from the detonation cell size data are shown in Figure 4-13 (Guirao, 1989). The minimum of the curve occurs at about the

stoichiometric composition. It should be remembered that the  $\lambda = \pi D$  criterion only applies to ignition by a strong source in a cylindrical, smooth-walled tube. Some studies have proposed a different criterion for a limiting tube diameter as  $\lambda = 1.7D$  or  $\lambda = D$ . In any case, most criteria proposed that the detonability limits in smooth round tubes are exceeded when the tube diameter is of the order of detonation cell size  $\lambda$  (or higher) (Guirao et al., 1989).



Figure 4-13. Limiting tube diameter as a function of hydrogen concentration in hot hydrogen-air-steam mixtures at superatmospheric pressures (Guirao et al., 1989).

Ciccarelli et al. (1996) have studied the influence of initial temperature on flame acceleration and DDT in 27-cm diameter long heated detonation tube. They observed that generally the D/ $\lambda$  =1 criterion for transition to detonation was consistent with their results. However, this criterion is not sufficient for the DDT in ducts with several obstacles. In dry hydrogen-air mixtures at 650 K, the DDT was observed at 11% H<sub>2</sub> corresponding the criterion for detonability limit D/ $\lambda$  =5.5. They warned that one must be careful in applying the DDT limit criterion due to the uncertainty in the experimental measured cell size caused by e.g. the cell non-uniformity.

Ciccarelli et al. (1996) also observed that the distance required for the flame acceleration to detonation was a function of both hydrogen mole fraction and the initial temperature. The transition distance increased as the hydrogen mole fraction was decreased, or the initial temperature was increased. The two important parameters that govern the rate of flame acceleration were observed to be the density ratio of the unburned to the burned gas and the mixture laminar burning velocity. Mixtures with a larger density ratio and laminar burning velocity have higher flame acceleration rates. <u>Critical tube diameter</u> is defines as the minimum diameter of a detonation tube from which a steady planar detonation wave can penetrate into an unconfined volume with same mixture transforming continuously propagating spherical detonation wave. Definition of this dimension must be distinguished from the limiting tube diameter definition described above.

Figure 4-14 shows an overview of recent knowledge of the effect of geometry and scale on detonation propagation based on several small and large-scale experiments (Berman, 1986). Figure 4-15 shows some results of the critical tube diameter for hydrogen-air mixtures at NTP (Guirao et al., 1989).

Unfortunately, we still not have any quantitative theory to predict the critical tube diameter, but Lee (1984) has developed some qualitative criteria for the transmission phenomena. The latest studies by Ciccarelli and Boccio (1998) have demonstrated that the  $d/\lambda = 13$  criterion for the critical tube diameter obtained at room temperature is not applicable at elevated temperatures. They also suggested that a simple  $d/\lambda$  correlations cannot be applied when the re-initiation due to shock reflection is possible.



•Minimum Cloud Thickness for Propagation Confined on One Side:



• Propagation Down a Cylinder (One-Dimensional):



• Propagation Down a Wide Channel (Two-Dimensional):











Figure 4-15. Variation of critical tube diameter with hydrogen concentration in hydrogen-air mixtures at NTP (Guirao et al., 1989).

In case of unconfined cylindrical and spherical detonations (absence of boundaries), the detonability limits are more difficult to determine than for confined tubes, because the reaction of unconfined detonations may be quenched due to expansion of gases. Guirao et al. (1989) have pointed out that the average cell size must be constant for the stable propagation and, thus, the number of detonation cells should increase at the same rate as the surface area increase.

#### 4.3.3 Detonation Propagation in Non-Uniform Mixtures

Most studies on the ignition and propagation of detonation waves have been performed in system of uniform (homogeneous) composition. Thomas et al. (1991) and Kuznetsov et al. (1998) have performed experiments on detonation propagation under concentration gradients. They found that the mechanism of detonation initiation in a weaker mixture propagated across a concentration gradient differs from the mechanism in a homogeneous mixture. In conditions with concentration gradients, a secondary shock is observed as the incident shock passes through the interface layer. The reflected shock from the interface can be either a shock or rarefaction depending on the relative acoustic impedances of the reactive and non-reactive gas mixture. Transition to detonation occurred when the reaction wave and the secondary shock coupled depending significantly on the sharpness of the concentration gradients. Smooth concentration gradients tend to assist the transition process, and detonation can propagate though the gradient interface. On the other hand, sharp gradients may separate the shock front and the reaction zone leading to failure of detonation. The possibility of detonation transmission through a gradient interface is also influenced by the property differences of the reactive and less reactive gases.

# 5. FLAME ACCELERATION AND DETONATION IN NUCLEAR REACTOR CONTAINMENTS

Hydrogen behaviour is one of the control issues of severe accidents in light water reactors. Hydrogen can be generated e.g. in core metal-water or metal-concrete interactions. Hydrogen combustion can significantly increase the containment pressure and temperature loads. Depending on combustion time scale the effect of combustion loads may be static or dynamic in nature. Depending on the location of ignition and combustion propagation processes, the effects may be local involving a subcompartment or small part of containment, or can be global involving most parts of containment.

The pressurisation caused by deflagration is relatively slow (several seconds) yielding quasi-static loads normally limited to the adiabatic constant-volume combustion pressure (AICC) with equilibrium thermodynamics (Chapter 3.5). Detonation leads to fast dynamic pressure loads (order of milliseconds) which are well above the AICC pressures. More parameters such as the duration of overpressure phase are, therefore, required to define the load. Maximum pressure generated by DDT is dependent e.g. on the pre-conditions ahead of the flame front and the pressure can be higher than the theoretical C-J value. Although deflagrations are more likely combustion modes than detonation in most reactor accident scenarios, hydrogen detonations have been identified e.g. in the German Risk Study as the significant cause for early containment failure (Breitung, 1993).

Hydrogen combustion has not been considered a major problem in severe accidents for containments that are inerted during normal operation. However, typical BWR containments are surrounded by the reactor building also called the secondary containment. The reactor building usually consists of several rooms where atmosphere is normal air. That makes the hydrogen combustion possible there if hydrogen leaks from overpressurised containment during a severe accident. This technical problem has not been widely studied to date. Also in non-inerted containments, the possibility to hydrogen combustion must be considered.

Theoretically, detonation can be directly initiated by powerful impulse source (strong direct initiation, see Chapter 4.2.2), or in certain circumstances, the initiation may occur indirectly by the flame acceleratation from deflagration to detonation. This abrupt transition regime is called as deflagration-to-detonation transition (DDT, Chapter 4.2.3). Detonation may be initiated also by a hot turbulent jet of combustion products passed into the reactive mixture (Chapter 4.2.2), or by SWACER mechanism (Chapter 4.2.1). Also a focusing of shock waves or very high temperatures above von Neumann values can initiate the detonation. Regardless of the ignition mechanism, the important safety aspect is that the high pressure, temperature and missiles may threaten the containment integrity. Important safety-related equipment may also be damaged.

According to most investigations, direct initiation of detonation by an energetic impulse source such electric sparks is not very probable in NPP containments due to the very high critical energy needed: order of 5 ... 1000 kJ for hydrogen-air mixture with equivalence ratios of 1.0 ( $\sim$ 29.6% H<sub>2</sub>) to 0.5 ( $\sim$ 17.4% H<sub>2</sub>) (Guirao et al., 1987). More probable mechanism is, therefore, an indirect initiation of detonation e.g. by DDT or by

a turbulent jet of combustion products. The flame acceleration is the prerequisite for DDT, but the flame acceleration does not lead inevitably to DDT. Typically the flame acceleration is induced by enhanced turbulence. In real containments, the turbulence can be generated e.g. by obstacles, obstructions, and fans.

Recent experiments have indicated that the detonability limits are much wider than previously believed (Berman, 1986). Scale and geometric effects can significantly influence the probability that a flame propagates or sustains a detonation, or a flame accelerates from deflagration to detonation. In the large-scale experiments for hydrogenair mixtures, DDT has been observed for hydrogen concentrations between about 10% and 77%. In certain experimental conditions in confined tubes, detonations or detonation-like phenomena have been successfully initiated also in mixtures outside the assumed detonability limits, if sufficiently energetic ignition sources are used.

Breitung (1993) has categorised some important parameters affecting the detonations in real containment conditions shown in Figure 5-1.

The initial mixture conditions define the thermodynamic state of the gas mixture prior to combustion. Important parameters are the initial temperature, the gas composition, and the gas mixture homogeneity. Initial pressure has influence on the final pressure after combustion, but not directly affects the combustion flame. Generally, the initial conditions are dependent on the accident sequence and time span considered.

Geometry and boundary are extremely important parameters, especially for the flame acceleration and DDT. Most detonation experiments are performed in relatively simple geometry, such as in cylindrical tubes, whereas realistic conditions can be very complicated 3-dimensional geometries including several rooms with obstacles and obstructions. In 3-D conditions, focusing of reflected shock waves can locally result in very high peak pressures. The scale effect is obvious for many combustion processes. The detonation loads transmitted to a structure will further depend on the energy and momentum transfer at the system boundary.

The location and time of the ignition are very important, because they define the beginning of combustion processes in the containment. The ignition processes may be random or deliberate, and may have influence on the nature of combustion process (e.g. critical energy of direct initiation of detonation). For example, the ignition in confined volumes with several obstacles may favour the creation of flame acceleration and DDT.



Figure 5-1. Parameters affecting the hydrogen-air-steam detonations (Breitung, 1993).

Breitung et al. (1999) have also formulated the procedure (methodology) for assessment of hydrogen behaviour in severe accident conditions. They have also developed certain conservative criteria to assess the probability for flame acceleration and DDT.

First of all, the plant design, possible hydrogen mitigation systems, accident scenario, and possible hydrogen and steam sources to containment must be defined (e.g. by risk assessment methodology). Next task is to calculate hydrogen transport, distribution, mixing and interconnecting physical process such as steam condensation and turbulence in the containment. In order to start the combustion analyses, the ignition type, location, and time must be determined. If the ignition is assumed to occur, the possibility to flame acceleration must be considered. The flame can accelerate forming fast turbulent deflagration or propagate as a slow quasi-laminar deflagration (note that the direct initiation of detonation is considered to be unlike). Breitung et al. (1999) recommend the  $\sigma$ -criterion presented in Chapter 4.2.4 (Eqs. (4-1) to (4-3)) for conservative estimates of the potential for flame acceleration. Depending on the conditions, the accelerated flames may lead to detonation (DDT) or continue to propagate as fast turbulent deflagration. The  $\lambda/L$  and  $\lambda > d$  criteria presented in Chapter 4.2.4 can be used to assess the potential for DDT.) If the all criteria are fulfilled, DDT may be possible (but not necessary). If a potential to flame acceleration or detonations exists, the loads threaten the containment integrity must be considered. All possible combustion regimes (slow deflagration, fast turbulent deflagration, and detonation) have their characteristic influences on surrounding structures. All the combustion regimes may be also possible during the same accident scenario considered.

The methodology for hydrogen analyses in severe accidents as proposed by Breitung et al. (1999) is formulated for use of the numerical models (e.g. lumped parameter and CFD codes) complemented by the certain conservative criteria in order to assess the possibility for flame acceleration and DDT. Once again, it is important to understand that these criteria are **<u>necessary</u>**, **<u>but not sufficient conditions</u>** i.e. they are supposed to be prerequisite for the flame acceleration and DDT. Use of the criteria can be considered as a conservative approach and caution is needed when applying it to decisions concerning the real containment conditions.

The significant advances in the understanding and modelling of flame acceleration and DDT have been obtained in recent years. In spite of these advances, no quantitative and predictive models are available for DDT due to very complicated processes involved in it (Breitung et al., 1999).

The criteria for flame acceleration and DDT presented in chapter 4.2.4 are mostly based on the empirical observations from the flame acceleration and DDT including some uncertainties which must be know when applying the criteria to real containment conditions (Breitung et al., 1999). Firstly, there are some uncertainties in measuring the detonation cell size (width), which is considered as characteristic length of a mixture. Average uncertainties in measured cell size can vary under certain circumstances more than by factor of 2. Secondly, the clear definition of the characteristic geometrical size *L* may be very difficult in a complicated containment geometry containing several compartments and intercell junctions. Thirdly, there are inaccuracies of cell size for volumes with characteristic size exceeding 10 - 15 m. That is partly due to the fact that no detonations are observed in experiments with cell size more than 2 m. The criteria and  $\lambda/L$  correlations for large volumes with L > 10 - 15 m include, therefore, uncertainties, but are not necessarily inapplicable. The definition of representative cell size in non-uniform mixtures is also difficult. We neither have quantitative theory to predict the detonability limits from first principles.

# 6. ASSESSMENT OF HYDROGEN DETONATION LOADS IN THE OLKILUOTO BWR REACTOR BUILDING

### 6.1 Problem Description

The Olkiluoto NPP consists of two ABB Atom 840 MW BWR units. Picture of Olkiluoto containment and surrounding reactor building is shown in Figure 6-1. During a severe accident, a large amount of hydrogen may be released to the relatively small containment. The Olkiluoto containment is inerted during operation and, thus, hydrogen burning there has not been considered a major problem in severe accidents. However, a leakage can not be totally excluded from the overpressurised containment into the surrounding reactor building leading to hydrogen accumulation in air-filled reactor building rooms where flammable conditions may exist. The safety concern is if a hydrogen detonation in the reactor building can challenge the containment integrity from outside.



Figure 6-1. Olkiluoto NPP containment and reactor building.

The following chapters discuss and give rough estimates of detonation shock pressure loads in Olkiluoto reactor building rooms during a severe accident where the ventilation of the reactor building is lost. A simple computer code DETO was developed to assess pressure loads caused by detonation induced shock waves. The code is based on the strong explosion theory, and accounts for the effects of both the primary or incident shock and the first (oblique or normal) reflected shock from a wall structure. The multiple, higher order reflections from the structures, and the superposition of the reflected waves in 3-D-geometry are out of scope of this study. However, the first reflection gives the highest pressure spike and can be used for assessment, if a structure fails from the first impact. The multiple reflections during the whole decay phase may be also damaging, if some the structural resonance effects take place. The results obtained with the shock wave theory are compared to the loads based on the classical Chapman-Jouguet theory. The key difference between the applied shock wave approach and Chapman-Jouguet model is that the total amount of chemical reaction energy is assumed to be released instantaneously, producing a freely propagating shock wave in a chemically inert media, whereas the C-J theory accounts for the continuous, though rapid, release of energy during the propagation of combustion. Therefore, in reality the propagating combustion front also affects the shock front ahead of it. In general, the applied shock wave theory describes a situation of over-driven detonation on normal C-J curve, if the distance from the explosion centre is relatively small, and hence, represents a conservative estimation of the first pressure spike. Sensitivity and uncertainties of the DETO results are also discussed later. The results of DETO calculations are also compared to the Balloon experiments performed at Fraunhofer-Institut fuer Chemische Technologie in Germany (Pförtner, 1991; Breitung & Redlinger, 1994).

#### 6.2 Technical Approach and Applied Models

#### 6.2.1 Strong Explosion Theory with Oblique Reflection Shock Relations

The simple 1-D computer program DETO was developed at VTT for Olkiluoto reactor building pressure load estimates. The formation and velocity of incident shock induced by a detonation is calculated from the strong explosion theory (Landau & Lifshitz, 1986; Zel'dovich & Raizer, 1966). The pressure increase across the incident shock wave and the structure surface pressure after the oblique or normal shock reflections are based on the theory of oblique shock reflection by Kinney & Graham (1985). The reflection phenomena can be normal, oblique or Mach stem formation depending on the angle of incidence between the wave front and the surface of the wall structure. This type of approach has been earlier applied by Saarenheimo and Hyvärinen (1996).

The basic assumption of the strong explosion theory is that a large amount of energy E is instantaneously released in a small volume (explosion origin). The gas around the explosion origin is assumed to be polytropic i.e. perfect gas with constant specific heat and density. A local explosion induces a strong spherical shock wave which propagates freely at velocity  $u_1$  through the gas medium starting from the point where the energy is released (Figure 6-2). Furthermore, it is assumed that the initial pressure is negligibly small compared to the pressure behind the shock wave.



Figure 6-2. Schematic of strong explosion.

<u>The distance R from the explosion center to the wall</u> as a function of incident angle  $\alpha_1$  is

$$R = \frac{R_0}{\cos(\alpha_1)} \tag{6-1}$$

where  $R_0$  is, according to Figure 6-3, the normal distance from explosion origin to the wall. The angle  $\alpha_1$  is also the angle between the shock plane and the wall.



Figure 6-3. Distances from explosion origin to wall.

The time *t<sub>1</sub>* from the start of explosion to the first impact of shock wave to wall is according to Landau and Lifshitz (1986)

$$t_1 = \frac{R^{5/2}}{\beta^{5/2} \sqrt{\frac{E}{\rho_1}}}$$
(6-2)

where  $\beta$  is the numerical constant depending on the specific heat ratio  $\gamma$ , and  $\rho_1$  is the initial gas density. The specific heat ratio  $\gamma$  is strictly not constant, and a function of both temperature and density. It is, however, normally justified to use an approximate, constant value for  $\gamma$ . According to Strehlow (1991), a value about 1.2 for  $\gamma$  can be used for near stoichiometric hydrogen-air mixtures. By assuming  $\gamma=1.2$  yields the value of 0.89 for the numerical parameter  $\beta$ .

Now, the **impact velocity**  $u_1$  of the incident shock wave to the wall can be calculated from the formula

$$u_1 = \frac{2\beta E^{1/5}}{5\rho_1^{1/5} t_1^{3/5}} \tag{6-3}$$

#### The Mach number M<sub>1</sub> for the incident shock is defined as

$$M_1 = \frac{u_1}{a_1}$$
(6-4)

where  $a_1$  is the speed of sound immediately before the incident shock.

According to Rankine-Hugoniot relations for an adiabatic normal shock, <u>the pressure</u> <u>ratio across the incident shock front</u> can be presented in terms of Mach number (velocity) and specific heat ratio according to Kinney and Graham (1985)

$$\frac{p_2}{p_1} = \frac{2\gamma M_1^2 - (\gamma - 1)}{(\gamma + 1)} \tag{6-5}$$

where state 1 is the initial state just before the arrival of the shock wave (ahead of shock) and state 2 corresponds to the conditions immediately behind the shock (Fig. 6-4).

The reflection phenomena of shock wave can be divided into three types:

- 1) normal reflection where the incident shock front is parallel to the reflecting surface  $(\alpha_1 = 0)$ ,
- 2) oblique reflection where a shock impinges with a small angle between the shock front and the reflecting surface, and
- 3) Mach stem formation where the shock front impinges the surface with a large angle and is deflected so that it spurts along over the surface.

# <u>The minimum angle of incidence that results in Mach stem formation</u>, can be obtained approximately from an empirical hyperbolic equation (Kinney & Graham, 1985).

$$\alpha_{\min} = \frac{1.75}{(M_1 - 1)} + 39 \tag{6-6}$$

With Mach numbers larger than 2.75 the Mach stem formation begins at angle about 39  $\dots 40^{\circ}$ .

The oblique reflection of a shock wave can be considered by two different shocks, the incident shock (on the right-hand side in Fig 6-4) and the reflected shock (on the left-hand side in Fig 6-4).



**Figure 6-4.** *Oblique reflected shock with steady flow counterpart of oblique reflection* (Kinney & Graham, 1985).

The stream in region 1 of Fig. 6-4 flows though an oblique shock at angle  $\alpha_1$  into the stream region 2 and is <u>deflected at angle</u>  $\theta_1$ . If  $\alpha_1$  is known, we can solve  $\theta_1$  from equation (Kinney & Graham, 1985)

$$\frac{\tan(\alpha_1 - \theta_1)}{\tan \alpha_1} = \frac{2 + (\gamma - 1)M_0^2}{(\gamma + 1)M_0^2}$$
(6-7)

and we get

$$\theta_1 = \alpha_1 - \arctan\left[\tan \alpha_1 \frac{2 + (\gamma - 1)M_0^2}{(\gamma + 1)M_0^2}\right]$$
(6-8)

where  $M_0 = M_1 \sin \alpha_1$ , and  $M_1$  is the Mach number corresponding the velocity  $u_1$  in Figure 6-4.

<u>The Mach number  $M_2$  in the stream region 2</u> of Figure 6-4 can now be solved from equation (Kinney & Graham, 1985)

$$[M_2 \sin(\alpha_1 - \theta_1)]^2 = \frac{2 + (\gamma - 1)M_0^2}{2\gamma M_0^2 - (\gamma - 1)}$$
(6-9)

and we get

$$M_2 = \frac{1}{\sin(\alpha_1 - \theta_1)} \cdot \sqrt{\frac{2 + (\gamma - 1)M_0^2}{2\gamma M_0^2 - (\gamma - 1)}}$$
(6-10)

<u>The angle  $\theta_2$  for stream entering to the reflected shock in region 2</u> can now be solved iteratively from equation (compare to Eq. (6-7))

$$\frac{\tan(\theta_2 - \theta_1)}{\tan \theta_2} = \frac{2 + (\gamma - 1)M_2^2}{(\gamma + 1)M_2^2}$$
(6-11)

The Mach number M<sub>r</sub> for reflected shock is given as

$$M_r = M_2 \sin \theta_2 \tag{6-12}$$

<u>The final angle of reflection</u>  $\alpha_2$  is given by

$$\alpha_2 = \theta_2 - \theta_1 \tag{6-13}$$

<u>The ratio of pressure across the oblique reflected shock</u> is obtained again according to Eq. (6-5) substituting  $M_1$  by  $M_r$ .

$$\frac{p_3}{p_2} = \frac{2\gamma M_r^2 - (\gamma - 1)}{(\gamma + 1)} \tag{6-14}$$

For normal reflection ( $\alpha_1 = 0$  in Fig 6-4) the corresponding pressure ratio can be expressed as

$$\frac{p_3}{p_2} = \frac{(3\gamma - 1)\frac{p_2}{p_1} - (\gamma - 1)}{(\gamma - 1)\frac{p_2}{p_1} + (\gamma + 1)}$$
(6-15)

#### The total pressure jump across the incident and reflected shocks is now

$$\frac{p_3}{p_1} = \frac{p_2}{p_1} \cdot \frac{p_3}{p_2} \tag{6-16}$$

where  $p_1$  is the initial pressure at the structure surface before the attack of a shock wave and  $p_3$  is the final peak pressure after shock reflection that the structure is exposed to.

If the shock impacts on a surface at very high incident angle i.e. the angle is greater than the limited angle for Mach stem obtained from Eq. (6-6), the shock does not reflect off the surface directly, but rather spurts along over the surface leading to the Mach stem formation. In this case, the <u>Mach number for Mach stem</u> is obtained from the equation

$$M_{ms} = \frac{M_0}{\sin \alpha_1} \tag{6-17}$$

and the overpressure p behind the Mach stem is given by

$$p = p_2 - p_1 = p_1 \frac{2\gamma(M_{ms}^2 - 1)}{\gamma + 1}$$
(6-18)

Next, we estimate the <u>duration of the pressure pulse</u>. This can be obtained according to Kinney and Graham (1985) by using the theory developed for chemical explosions. The pressure pulse after the shock wave has a form where the elevated pressure first decays to the initial pressure and after which a period of underpressure will follow. The duration of positive overpressure phase  $t_{dur,1}$  can be calculated from

$$\frac{t_{dur,1}}{W^{1/3}} = \frac{980 \left[ 1 + \left(\frac{Z}{0.54}\right)^{10} \right]}{\left[ 1 + \left(\frac{Z}{0.03}\right)^3 \right] \left[ 1 + \left(\frac{Z}{0.74}\right)^6 \right] \sqrt{1 + \left(\frac{Z}{6.9}\right)^2}}$$
(6-19)

where Z is the scaled distance based on the principles of geometric similarity and conservation of momentum (Kinney & Graham, 1985). The <u>scaled distance</u> can be calculated from the equation

$$Z = \frac{h(\rho / \rho_0)^{1/3}}{W^{1/3}}$$
(6-20)

where *h* is the actual distance of explosion centre from the location of interest,  $\rho$  is the density of the gas mixture through which the shock wave travels,  $\rho_0$  is the reference density (1.2 kg/m<sup>3</sup> for air), and *W* is the explosive energy release expressed as equivalent mass of TNT. The <u>equivalent energy release</u> is given by

$$W = \frac{E}{4.61 \cdot 10^6 J / kg}$$
(6-21)

where *E* is the actual energy released in explosion and  $4.61 \cdot 10^6 J/kg$  is the explosion energy of standard kilogram TNT. For hydrogen explosive, *E* can be calculated

$$E = m_{H2} \cdot 120 \cdot 10^6 J / kg \tag{6-22}$$

where  $m_{H2}$  is the total mass of hydrogen assumed to be burn. Heat released from one kilogram hydrogen, therefore, corresponds to the energy of about 26 kg TNT.

Alternatively, the duration of shock overpressure phase can be defined according to Landau and Lifshitz (1986). We can now express gas pressure behind the shock wave as

$$p_2 = \frac{2\rho_1 u_1^2}{\gamma + 1} \tag{6-23}$$

If we assume a situation where the shock wave overpressure has totally decayed, we have,  $p_2 = p_0$ , and substituting Eqs. (6-2) and (6-3) into Eq. (6-23) we can solve the **total time of the overpressure phase** 

$$t_{dur,2} = E^{1/3} \rho_1^{1/2} \left[ \frac{8}{25} \cdot \frac{\beta^2}{p_0(\gamma+1)} \right]$$
(6-24)

The time dependency of shock overpressure decay can be solved from equation

$$p(t) = p_{\max}(1 - t/t_{dur,1})e^{-\zeta t/t_{dur,1}}$$
(6-25)

where  $p_{\text{max}}$  is the maximum overpressure obtained e.g. from Eq. (6-16) or (6-18), and  $\zeta$  is the wave form parameter. In order to find the wave form parameter, we must first calculate the <u>impulse per unit area</u> given by Kinney and Graham (1985) for chemical explosions as

$$\frac{I}{A} = \frac{0.067\sqrt{1 + (Z/0.23)^4}}{Z^2\sqrt[3]{1 + (Z/1.55)^3}}$$
(6-26)

<u>The wave form parameter</u>  $\zeta$  can now be solved iteratively by integration of Eq. (6-25)

$$\frac{I}{A} = \int_0^{t \, dur} p \, dt = p_{\max} t_{dur} \left[ \frac{1}{\zeta} - \frac{1}{\zeta^2} (1 - e^{-\zeta}) \right] \tag{6-27}$$

Conclusively, the wave form parameter  $\zeta$  in Eq. (6-25) is calculated according to following procedure:

- 1) Calculate equivalent energy release from Eq. (6-21)
- 2) Calculate scaling distance from Eq. (6-20)
- 3) Calculate impulse per unit area from Eq. (6-26).
- 4) Calculate the duration of "2/5" overpressure phase from Eq. (6-19)
- 5) Solve iteratively the wave form parameter  $\zeta$  from Eq. (6-27) using the Newton Raphson method. The maximum value of the wave form parameter was limited to the value of 4.

The overpressure decay, i.e. pressure-time curve, is evaluated according to Figure 6-5.



Figure 6-5. The principal of evaluation of pressure-time curve.

In order to estimate the threat of shock wave on structures, at least three independent variables must be known: the shock intensity (e.g. peak overpressure), the duration of shock wave overpressure, and the rate of decay of overpressure. Based on these parameters total impulse for the pressure forces can be calculated.

The duration of the exponential decay  $t_{dur,1}$  is calculated from Eq. (6-19) and the corresponding pressure-versus time curve (from point 1 to 2 in Table 6-5) from Eq. (6-25). During this time period the shock pressure was assumed to decay from maximum peak pressure  $p_{max}$  to 2/5 of the pressure of incident shock. This approximation is based on Landau & Lifshitz (1986) proposing that for air the pressure in the strong explosion centre is about 2/5 of that just behind the spherical shock front. Taking into account this approximation the corresponding pressure-versus time curve of the "2/5" overpressure phase (from point 1 to 2) is calculated as

$$p(t) = (p_{\max} - \frac{2}{5}p_{shock}) \cdot (1 - t/t_{dur,1})e^{-\zeta t/t_{dur,1}} + \frac{2}{5}p_{shock}$$
(6-28)

where  $p_{shock}$  is the incident shock pressure just before reflection.

The total duration of shock overpressure phase  $t_{dur,2}$  is obtained according to Eq. (6-24). A simple approximation for linear pressure decay is used from point 2 to 3.

The time period needed to achieve the pressure maximum is not calculated. The pressure rise is assumed to start at the time when the shock wave impacts the wall according to Eq. (6-2). After that the pressure is assumed to increase to its maximum value during one time step.

After the maximum peak overpressure, the duration of overpressure phase and the decay of overpressure is solved, the total impulse for pressure forces caused is integrated numerically according to pressure-time curve.

6.2.2 Detonation Overpressure According to Chapman-Jouguet Theory

If the detonation and shock waves are induced by strong external source, the corresponding end state can be at any point on the upper part of the Rankine-Hugoniot adiabatic curve in Figure 3-2 (region for strong or overdriven detonation). Within this region, the pressure of burned gases may be significantly greater than that of the C-J detonation. According to the strong explosion theory mainly used in this study, the velocity of the shock wave is bounded by the total energy release of explosion. If the explosion energy is very high and the distance from the explosion centre is relatively small, the velocity of shock wave and the corresponding pressure can therefore be much higher than obtained by C-J theory. It is well known that in most typical cases the spontaneous one-dimensional planar or spherical propagation of detonation wave occurs at a fairly constant, supersonic velocity, which is equal to the local velocity of sound relative to the gas behind the detonation front (Strehlow, 1991, Landau & Lifshitz, 1986). This velocity corresponds to the upper Chapman-Jouguet point of the detonation adiabatic curve in Figure 3-2. The overdriven detonations are observed experimentally, if the overdriven shock in exothermic reactive system is supported e.g. by a highvelocity piston. This suggests that in a well-confined situation, like a reactor building room for example where several shock reflections are bound to occur, the real pressure spikes lie somewhere between the classical C-J pressures and the maximum pressures obtained by the strong explosion/reflected shock wave theory.

In the following, the simplified formulas of calculating the pressures according to C-J theory are presented. Strehlow (1991) has formulated a simple treatment of detonation propagation in a hydrogen-air mixture at initial pressure of 1 atm using the <u>working</u> **fluid heat addition model**. He determines the equilibrium Hugoniot curve over pressure range from 1 to 20 atm and curve fits it to the hyperbola to determine the constants  $\beta_1$  and  $\beta_2$ .

$$\left(\frac{\nu_2}{\nu_1} - \beta_1\right)\left(\frac{p_2}{p_1} + \beta_1\right) = \beta_2 \tag{6-29}$$

where

$$\beta_1 = \frac{\gamma - 1}{\gamma + 1} \tag{6-30}$$

and

$$\beta_2 = \frac{4\gamma}{(\gamma+1)^2} + \frac{2q}{p_1 v_1} \left(\frac{\gamma-1}{\gamma+1}\right)$$
(6-31)

where q is the heat of reaction per unit mass of reactant, and v is the specific volume. Curve fit constants (within error rate 0.25%) for hydrogen-air mixture at stoichiometric mixture conditions are:

33.89 for  $\frac{q}{p_1v_1}$ , and 1.173 for  $\gamma$ .

If the combustion process is assumed to be a simple heat addition to a polytropic gas, the **ratio of AICC pressure to initial pressure** can be expressed

$$\frac{p_{AICC}}{p_{init}} = \frac{(\gamma - 1)q}{p_1 v_1} + 1$$
(6-32)

Using this heat addition model, the <u>Chapman-Jouguet Mach number</u> of the detonation is obtained from the equation (Strehlow, 1991)

$$M_{CJ} = \sqrt{\left(\frac{\gamma^2 - 1}{\gamma} \frac{q}{p_1 v_1} + 1\right)} + \sqrt{\left(\frac{\gamma^2 - 1}{\gamma} \frac{q}{p_1 v_1} + 1\right)^2 - 1}$$
(6-33)

The <u>ratio of Chapman-Jouguet pressure to initial pressure</u> can be calculated from the equation

$$\frac{p_{CJ}}{p_{init}} = \frac{1 + \gamma M_{CJ}^2}{\gamma + 1}$$
(6-34)

### 6.3 Application of DETO Code to Reactor Building Room B.60-80

#### 6.3.1 Initial and Boundary Conditions

The initial conditions of detonation analyses are based on the earlier MELCOR and FLUENT calculations performed at VTT. The accident progression (station blackout) was calculated by the MELCOR 1.8.4 code (Lindholm, 1998). All metallic Zr of core was conservatively assumed to oxidise leading to about 1900 kg hydrogen release into the containment (Sairanen, 1999). The containment was assumed to leak into Olkiluoto reactor building room B.60-80 from the pipe penetrations located in the upper part of the containment. The two leak sizes considered were 2 mm<sup>2</sup> (containment design leakage) and 20 mm<sup>2</sup>. The total mass of leaking hydrogen into the reactor building was 3 kg and 30 kg, respectively.

The leak into the reactor building is assumed to occur before the start of containment filtered venting at containment pressure 0.6 MPa. After start of the venting, the leak rate would decrease and finally stop. The total amount of hydrogen leak into the reactor building is actually independent of the Zr oxidation fraction, if the containment is vented. With less Zr oxidation the containment pressurisation would only take a longer time. It was also assumed conservatively that the hydrogen leak from the containment occurs to one reactor building room. More realistic assumption would be that the leak is diffused to several locations of the reactor building.

The MELCOR calculation was used to provide the initial conditions for more detailed hydrogen distribution studies in reactor building rooms performed by the FLUENT CFD code (Manninen and Huhtanen, 1998). The geometry of the computational volume for the room used in the FLUENT calculations is shown in Figure 6-6. The FLUENT calculations suggested that hydrogen accumulates to the upper parts of rooms and a rather stable stratification was built up. Similar behaviour was observed in all cases studied.

Noticeable hydrogen release from containment to reactor building started at about 4000 s, which was the start time for FLUENT calculations. The instants of times presented in the following text refer to time of the FLUENT calculations i.e. are calculated from the start of hydrogen release into the reactor building.

The Olkiluoto reactor building room B.60-80 has a total volume of  $897 \text{ m}^3$ . The height of the room is 33 m. The cross sectional dimensions of the room are shown in Figure 6-7 (Manninen & Huhtanen, 1999). The location of room B.60-80 is illustrated in Figure 6-1.



**Figure 6-6.** Geometry of computational volume for room B.60-80 used in the FLUENT calculations (Manninen & Huhtanen, 1999).



Figure 6-7. Cross-sectional dimensions of room B.60-80.

Due to very strong stratification of hydrogen at the top of the room B.60-80, it is prudent to estimate, which amount of the hydrogen is at combustible, detonable region. According to the FLUENT combustion calculations, the flame acceleration occurs rapidly, in millisecond time scale. Furthermore, the propagation of detonation will also occur in millisecond scale in the narrow shaft of room B.60-80. Based on this knowledge, it can be assumed that turbulent mixing is too slow a process to bring in fresh oxygen to the detonation front from the lower parts of the room. Thus, detonation can propagate as long as initial mixture is in the detonation region. The detonable region based on current experimental data is in terms of  $H_2$  molar fraction from 0.1 to 0.78. Since the additional nitrogen mass released from the drywell is rather small, we can assume that the gas region of room B.60-80 consists of a mixture of hydrogen and air. The stoichiometric mixture of hydrogen in air is 29.6 % hydrogen, 14.8 % oxygen and 55.6 % nitrogen, if we approximate that air is a mixture of 21 % oxygen and 79 % nitrogen.

To apply the gas component mass fraction curves from the FLUENT calculation, we transform the molar fractions into the mass fractions according to the simple formula

$$xm_{y} = \frac{X_{y} \cdot M_{y}}{X_{H_{2}} \cdot M_{H_{2}} + X_{O_{2}} \cdot M_{O_{2}} + X_{N_{2}} \cdot M_{N_{2}}}$$
(6-35)

where  $xm_y$  is the mass fraction of gas y,  $M_y$  is the molecular weight of gas y, and  $X_y$  is the molar fraction of gas y. Gas y is hydrogen, nitrogen, or oxygen.

The stoichiometric mass fractions of hydrogen and oxygen in air are 0.0283 and 0.2266, respectively. In the same way, we get the mass fractions of hydrogen at the lower and upper detonation limits to be 0.009946 and 0.19548, respectively. The oxygen mass fraction at the lower detonation limit is 0.30077 and at the upper detonation limit 0.1889.

Three different hydrogen distribution situations from previous FLUENT calculations in room B.60.80 were selected for closer assessment.

# Case 1:

The end state of the case with 20 mm<sup>2</sup> leakage corresponding to time t  $\approx$  13 000 s in the FLUENT calculation (Figure 6-8).

# <u>Case 2:</u>

The state of the case with  $20 \text{mm}^2$  leakage at t  $\approx 7500$  s corresponding to the situation, where the average gas molar fractions are near stoichiometric (Figure 6-9).

# <u>Case 3:</u>

The third case was selected to be the end state of FLUENT calculation in 2 mm<sup>2</sup> leakage case at t  $\approx 12500$  s (Figure 6-10).



**Figure 6-8**. Vertical profile of the mass fraction of hydrogen in room B.60-80 at  $t = 13\ 000\ s.\ 20\ mm^2$  leakage.



**Figure 6-9.** Vertical profile of the mass fraction of hydrogen in room B.60-80 at  $t = 7500 \text{ s. } 20 \text{ mm}^2$  leakage



Figure 6-10. Vertical profile of the mass fraction of hydrogen in room B.60-80 at  $t = 12500 \text{ s. } 2 \text{ mm}^2$  leakage

The hydrogen and oxygen mass fractions as functions of room elevation were taken from the FLUENT data at the defined moments of time. A curve fit was produced by the Table Curve 2D-program package. The fitted curves are the following:

#### <u>Case 1:</u>

End state of room B.60.80 in 20 mm<sup>2</sup> leak case, t  $\approx$  13 000 s.

 $xm_{H_{2}} = \frac{a}{\left(1 + e^{\frac{-(x - c \cdot \ln(2^{-d} - 1) - b)}{c}\right)^{d}}},$ (6-36) where  $xm_{H_{2}}$  = hydrogen mass fraction x = elevation in room B.60.80 (-2 m ... 31 m) a = 0.23330274 b = 24.421958 c = 0.29001771 d = 0.25312889

Respectively the fit for oxygen mass fraction is

$$xm_{O_2} = a + \frac{b}{\left(1 + e^{\frac{-\left(x - d \cdot \ln\left(2 - e_{-1}\right) - c\right)}{d}\right)^e},$$
(6-37)

where

$$xm_{O2}$$
 = oxygen mass fraction,  
x = elevation in room B.60.80 (-2 m ... 31 m)  
a = 0.23162894  
b = -0.1567779  
c = 24.376762  
d = 0.27688061  
e = 0.22193718

# **Case 2:**

State at t = 7500 s (near stoichiometric average mass fractions) in room B.60-80 with 20 mm<sup>2</sup> leakage.

$$xm_{H2} = a + b \cdot x + c \cdot x^{2} + d \cdot x^{3} + e \cdot x^{4} + f \cdot x^{5} + g \cdot x^{6} + h \cdot x^{7} + i \cdot x^{8} + j \cdot x^{9} + k \cdot x^{10}$$
(6-38)

where

$$a = 3147.4034$$
  

$$b = -565.3291$$
  

$$c = 32.228007$$
  

$$d = -0.02822013$$
  

$$e = -0.066950582$$
  

$$f = 0.002696525$$
  

$$g = -5.8180609e-5$$
  

$$h = 2.2085808e-6$$
  

$$i = -9.0610234e-8$$
  

$$j = 1.8217528e-9$$
  

$$k = -1.3586225e-11$$

For oxygen mass fraction a polynomial of order 9 was obtained with coefficients being:

### <u>Case 3:</u>

The end state of room B.60-80 with 2 mm<sup>2</sup> leakage.

The hydrogen mass fraction was fitted with a 10<sup>th</sup> order polynomial with the coefficients being:

The oxygen curve fitting was not needed in the case 3, because the mass fraction of hydrogen was below the stoichiometric point in the whole room.

For each case the elevations corresponding to hydrogen mass fraction at the lower and upper detonation limit and at the stoichiometric mixture point were defined by iteration. Then the mass fraction curves were integrated (numerically in case 1) along the hydrogen curve below stoichiometric point and along the oxygen curve above the stoichiometric point. Multiplying by the cross-sectional area 25.86 m<sup>2</sup> and by average density of gas in the integrated height, one gets the masses of hydrogen and oxygen that are assumed to be detonable. The hydrogen integral in the upper region was calculated from the respective oxygen integral.

In case 1, the lower detonation limit is at the elevation 21.58 m, the stoichiometric point is at the elevation 22.78 m and the upper detonation limit is reached at the elevation 25.12 m. The total amount of hydrogen that is detonable is 1.428 (536 g below and 892 g above stoichiometric point). This result indicates that at the stabilised end state about 95 % of hydrogen is at region where detonation can not propagate.

The average conditions, where the maximum amount of detonable mixture is found (case 2), are near stoichiometric. This state is reached after about 2 hours leakage (20 mm<sup>2</sup>) to the room B.60-80. At this time moment (t = 7500 s in FLUENT simulation) the lower limit of detonable concentration is at the elevation 25.82 m, the stoichiometric point is at elevation 27.98 m and the upper detonation limit is not exceeded. In this case, the total amount of detonable hydrogen is 3.15 kg (1.39 kg below the stoichiometric point and 1.76 kg above it).

In case 3, the hydrogen concentration in the mixture is below the stoichiometric value in the whole volume at the end of FLUENT calculation. At this point, 1.94 kg hydrogen was released from the containment and a total of 1.4 kg of it is in detonable region. The detonable mixture starts from elevation 27.09 m and goes all through to elevation 31 m.

The average gas density, temperature, and hydrogen molar fractions in the detonable region were obtained from the FLUENT calculations by integrating over all computational cells in the detonable gas region considered. Summary of the initial conditions for three base cases considered are listed in Table 6-1.

Case	Hydrogen mass burned	Start time *)	Leak area [mm <sup>2</sup>	Pres. [Pa]	Temp. [K]	Density [kg/m <sup>3</sup> ]	X <sub>H2</sub> [%]	X <sub>N2</sub> [%]	X <sub>O2</sub> [%]	X <sub>H2</sub> 0 [%]
1	1.428	13000	20	1.274e5	307.7	0.841	43.7	44.7	10.3	1.3
2	3.15	7500	20	1.065e5	301.2	0.9	27.8	57.5	13.6	1.1
3	1.4	12500	2	1.035e5	300.4	1.021	15.5	66.9	17.2	0.4

**Table 6-1.** Initial conditions of detonation calculations by computer program DETO.

\*) Calculated from the beginning of leakage to the reactor building.

 $X_{H2}$ ,  $X_{N2}$ ,  $X_{O2}$ ,  $X_{H2O}$  are initial average vol-% for hydrogen, nitrogen, oxygen, and steam, respectively

### 6.3.2 Results

### Case 1

The calculated pressures at different angles of shock incident on the concrete wall in room B.60-80 in 20 mm<sup>2</sup> leakage case are shown in Figure 6-11. The pressure histories at different locations (with different angles of incidence) were calculated to facilitate the scoping analyses of structural response to overpressure spikes to be performed later. A total amount of 30 kg hydrogen was released into the room B.60-80, from which 1.428 kg hydrogen was assumed to burn as detonation instantaneously.

The pressure-time curves are plotted as functions of angle of incident shock  $\alpha_1$  (see Figs. 6-3 and 6-4). The normal distance  $R_0$  of explosion centre from the concrete wall was assumed to be 2.0 m corresponding to the situation where the ignition occurs near the hydrogen leakage location close to the containment wall.

The maximum pressure spike of about 12.6 MPa was obtained in the case of normal shock reflection (angle = 0 degrees). Corresponding pressure impulse was about 2.3 kPa-s. The total duration of pressure spike, and also the duration of total overpressure phase, in all angle positions was very short, in order of four milliseconds. As the incident angle increased, the distance from explosion centre to wall also increased (*R* in Fig.6.3), and hence, the incident shock impacted to the wall later. In the strong ignition theory, the pressure of incident shock decreases with distance according to relation  $p \sim$ 

 $\frac{E}{R^3}$ . Therefore, the maximum pressure spike after reflection also decreased as the

incident angle and distance to wall increased. When the incident angle exceeded the Mach stem limit value, the pressure spike became much lower than that for reflected shocks (see Figure 6-11 angle of 40 degrees).



Figure 6-11. Calculated detonation shock pressures in 20 mm<sup>2</sup> leak case (Case 1) as functions of incident angle,  $t = 13\ 000\ s$ .

#### Case 2

The calculated pressures as functions of incident angle in case 2 (20 mm<sup>2</sup> leakage) are shown in Figure 6-12. The total amount of 3.57 kg hydrogen was released into the room B.60-80, from which 3.15 kg hydrogen was assumed to burn. Average density of gas mixture in case 2 was higher and the molar fraction of hydrogen lower than in case 1 due to earlier time considered i.e. less hydrogen was released into the reactor building room B.60-80 in case 2.

The maximum pressure spike was about 38.7 MPa in the case of normal shock reflection, and the corresponding pressure impulse was about 9.4 kPa-s. Duration of the overpressure phase was about seven milliseconds. Once again, Mach stem formation was observed at angle about 40 degrees leading to significantly lower pressure maximum than that for reflected shocks at smaller angles.



Figure 6-12. Calculated detonation shock pressures in 20 mm<sup>2</sup> leak case (Case 2) as functions of incident angle, t = 7500 s.

The influence of the distance of explosion centre from the wall ( $R_o$  in Fig 6-3) is shown in Figure 6-13. In this figure, only normal shock reflection was considered i.e. the incident angle was zero. The maximum pressure was strongly dependent on the distance. If the distance was small, the strong explosion theory gave very high pressure. But on the other hand, this seems reasonable when considering that 3.15 kg of H<sub>2</sub> compares to 80 kg of high explosive. The maximum peak pressure increased from 16 MPa to 106 MPa as the distance of explosion centre from concrete wall decreased from 2.5 to 1.5 m. Corresponding impulses ranged from 1.7 kPa-s to 30 kPa-s.



**Figure 6-13.** Calculated detonation shock pressures in 20 mm<sup>2</sup> leak case (Case 2) as functions of distance from explosion center to wall, t = 7500 s.

#### Case 3

In case 3, a total amount of 1.94 kg hydrogen was released into the room B.60-80, from which 1.4 kg hydrogen was assumed to burn during detonation.

The calculated pressures as functions of incident angle are shown in Figure 6-14. The pressure behaviour was nearly similar to case 1 (Figure 6-11) having the maximum pressure of about 13.2 MPa, and the maximum pressure impulse of about 2.8 kPa-s.



**Figure 6-14.** Calculated detonation shock pressures in  $2 \text{ mm}^2$  leak case (Case 3) as functions of incident angle,  $t = 12\ 000\ \text{s}$ .

The calculated pressures (as functions of incident angle) in different base cases are summarised in Table 6-2. The value of  $p_{shock}$  corresponds to the pressure behind the incident shock on the wall just before the reflection. Value of  $p_{max}$  is the reflected shock pressure. Table 6-2 also includes the calculated impulses *I* for pressure forces on concrete wall. The first time point in  $t_{dur,1}$  in Table 6-2 is the theoretical time during which the shock pressure has decayed to the value 2/5 of the incident shock pressure. The total duration of the overpressure phase is  $t_{dur,2}$ . The pressure decay between the points  $t_{dur,1}$  and  $t_{dur,2}$  is assumed to be linear. The last column of Table 6-2 consists of calculated velocity of the shock wave at the instant of time when it impacts the wall structure.

Case 1:	p <sub>shock</sub> [Pa]	$p_{max}$ [Pa]	t <sub>dur,1</sub>	t <sub>dur,2</sub>	Ι	U <sub>1</sub>
1.428 kg H <sub>2</sub>			[ms]	[ms]		[m/s]
0 °	$17.6 \cdot 10^5$	$126.5 \cdot 10^5$	0.3	4.2	$2.26 \cdot 10^3$	1508.
10 °	$16.8 \cdot 10^5$	$115.8 \cdot 10^5$	0.3	4.1	$2.13 \cdot 10^3$	1474
20 °	$14.6 \cdot 10^5$	$88.4 \cdot 10^5$	0.3	4.1	$1.80 \cdot 10^3$	1374.
30 °	$11.4 \cdot 10^5$	55.6·10 <sup>5</sup>	0.4	3.9	$1.38 \cdot 10^{3}$	1216.
40 °	$7.8 \cdot 10^5$	$19.1 \cdot 10^5$	0.6	3.6	$8.51 \cdot 10^2$	1011.
Case 2:						
3.15 kg H <sub>2</sub>						
0 °	$38.8 \cdot 10^5$	$387.1 \cdot 10^5$	0.5	7.0	$9.37 \cdot 10^3$	2166.
10 °	$37.1 \cdot 10^5$	$357.0 \cdot 10^5$	0.5	6.9	$8.69 \cdot 10^3$	2117.
20 °	$32.2 \cdot 10^5$	$279.0 \cdot 10^5$	0.4	6.9	$6.97 \cdot 10^3$	1973.
30 °	$25.2 \cdot 10^5$	$181.8 \cdot 10^5$	0.4	6.8	$4.91 \cdot 10^3$	1745.
40 °	$17.4 \cdot 10^5$	$42.3 \cdot 10^5$	0.4	6.6	$2.70 \cdot 10^3$	1452.
Case 3:						
1.4 kg H <sub>2</sub>						
0 °	$17.1 \cdot 10^5$	$132.4 \cdot 10^5$	0.3	5.5	$2.80 \cdot 10^3$	1356.
10 °	$16.3 \cdot 10^5$	$121.4 \cdot 10^5$	0.3	5.5	$2.66 \cdot 10^3$	1325.
20 °	$14.1 \cdot 10^5$	$93.0 \cdot 10^5$	0.4	5.4	$2.30 \cdot 10^3$	1235.
30 °	$11.0 \cdot 10^5$	$58.9 \cdot 10^5$	0.5	5.2	$1.81 \cdot 10^3$	1092.
40 °	$7.6 \cdot 10^5$	$31.2 \cdot 10^5$	0.8	4.9	$1.30 \cdot 10^3$	909.

**Table 6-2.** Calculated peak pressures, duration of overpressures phases, impulses on structure surface, and shock velocities.

The highest pressure spike of 38.7 MPa and impulse of 9.37 kPa-s are obtained in case 2 assuming normal reflections. As the incident angle increases the pressure spikes decrease. When the incident angle exceeds about  $40^{\circ}$ , the shock wave forms a Mach stem which results in significantly lower pressure spikes than predicted for reflected shocks.

Considering all calculated cases, the maximum pressure spikes range from 38.7 MPa to 1.9 MPa as the incident angle increases from  $0^{\circ}$  to  $40^{\circ}$ . Corresponding impulses range from 9.37 kPa-s to 0.85 kPa-s.

It is, however, observed experimentally that in most typical cases the spontaneous propagation of detonation wave occurs at a fairly constant, supersonic velocity which is equal to the local velocity of sound relative to the gas behind it corresponding closely to the upper Chapman-Jouguet point. If we apply the heat addition model and use the curve fit constants for stoichiometric hydrogen-air mixture as presented by Strehlow (1991)

 $\frac{q}{p_1 v_1}$  =33.89, and  $\gamma = 1.173$ ,

we can calculate the corresponding ratio of AICC pressure to initial pressure, C-J Mach number and the ratio of C-J pressure to initial pressure from Eqs. (6-32), (6-33), and (6-34), respectively. We get

$$\frac{p_{AICC}}{p_{init}} = 6.86\tag{6-39}$$

$$M_{CI} = 4.87$$
 (6-40)

$$\frac{p_{CJ}}{p_{init}} = 13.24$$
 (6-41)

This calculations yield AICC pressure of  $7.3 \cdot 10^5$  Pa and C-J pressure of  $14.1 \cdot 10^5$  Pa for case 2 where the initial state corresponds closely to stoichiometric conditions.

Rough estimates for the C-J pressures can also be obtained with the aid of Figure 4-11 and Eq. (6-34) using following procedure. Firstly, C-J velocity as a function of hydrogen concentration can be found from Figure 4-10 where NTP conditions are assumed. Secondly, sound of speed at initial conditions can be calculated, and the corresponding C-J Mach number is obtained from Eq. (6-4). After that, C-J pressure is calculated from Eq. (6-34). Detailed chemical equilibrium calculations should be needed to solve the specific heat ratio  $\gamma$  in different conditions, but that is not possible in this context. Hence, a constant value of 1.2 is used for  $\gamma$ . According to Landau and Lifshitz (1986), the peak reflected pressure of planar 1-dimensional detonation front can be assumed to be approximately 2.55 times the C-J pressure using the value of 1.2 for  $\gamma$ .

Following the procedure described above, the approximative C-J values can be found for all computational cases. In case 1, average initial concentration of hydrogen was 43.7%. Corresponding C-J velocity is about 2000 m/s obtained from Fig. 4-10. The speed of sound for the initial gas mixture is about 423 m/s. This results in C-J Mach number of 4.7 from Eq. (6-4), and corresponding C-J pressure of about  $16.0 \cdot 10^5$  Pa from Eq. (6-34) (the initial pressure is  $1.274 \cdot 10^5$  Pa). Peak reflected C-J pressure is 2.55 times the C-J pressure, and hence, about  $41.0 \cdot 10^5$  Pa.

In case 2, the average initial concentration of hydrogen was 27.8% and the sound of speed 374 m/s. Corresponding C-J velocity is about 1940 m/s and C-J Mach number about 5.2. The C-J pressure is about  $16.2 \cdot 10^5$  Pa (initial pressure is  $1.065 \cdot 10^5$  Pa). Note that this value is greater than obtained from Eq. (6-41) due to larger value of  $\gamma$  and smaller sound of speed used. Shock reflection peak pressure according to the C-J theory is about  $41.3 \cdot 10^5$  Pa.

In case 3, the average initial concentration of hydrogen was 15.5% and the sound of speed 348 m/s. The C-J velocity is about 1545 m/s and C-J Mach number 4.4. The C-J pressure is about  $11.4 \cdot 10^5$  Pa and the shock reflection peak pressure about  $29.0 \cdot 10^5$  Pa.

Comparing the approximative C-J values to the results in Table 6-2, we can conclude following. In case 1, the incident shock pressures predicted by the DETO code are about 0.5 to 1.1 times higher than the C-J pressures when the incident angle ranges from  $40^{\circ}$  to  $0^{\circ}$ , respectively. Predicted values for reflected shock peak pressures are about 0.5 to 3 times higher than the theoretical values. In case 2, the DETO code predicts about 1.1 to 2.4 higher incident shock pressures and about 1 to 9.4 higher reflected peak pressures than approximated by the C-J theory. In case 3, the incident shock pressures are about

0.7 to 1.5 and peak reflected pressures about 1.1 to 4.6 times higher than approximated C-J values.

6.3.3 Sensitivity and Uncertainties of the Results

Large uncertainties of the results are caused by the fact that only the first reflection of 1-D shock wave is considered. In addition, the effect of propagating combustion front on the shock wave ahead of it is not modelled.

The reflected shock pressure predicted by the DETO code was maximally (in case 2) about 9.5 times higher than approximated by the C-J theory. This is due to the fact that the shock velocity predicted by the strong explosion theory can under certain circumstances significantly exceed the C-J velocity. In addition, the ratio of reflection pressure to incident shock pressure was maximally about 10 according to the model used in the DETO code. However, we know that the theoretical pressure ratio of the reflection shock pressure to the incident detonation pressure is about 2.3 to 2.6 depending on the specific heat ratio used (Landau & Lifshitz, 1986). Conclusively, the normal reflection shock pressures estimated by the DETO code exceed the theoretical C-J values in all cases considered, and the corresponding end state can be somewhere on the upper part of Rankine-Hugoniot curve of Fig. 3-2. This represents the region for strong (or overdriven) detonation.

The spontaneous one-dimensional propagation of detonation wave is generally considered to correspond to the C-J point. However, this conclusion is not universally valid. C-J theory assumes a steady, uniform, and one-dimensional detonation wave without any information of wave structure and chemical reaction kinetics. In reality, the detonation wave is an unsteady process with a three-dimensional structure. Under real circumstances also the over-compressed detonation wave can occur spontaneously e.g. when a detonation wave propagates from a wide pipe into a narrow one (Landau & Lifshitz, 1986). We also know that the pressures of incident and reflected shock waves may exceed the C-J pressure. The situation is even more complicated in 3-D geometries where the transverse wave collision and possible focusing of multiple shock may still increase the local pressure loads (inside the detonation front) compared to the C-J state. Because the duration of shock pressure is normally very short, the C-J pressure has often been considered more important (Strehlow, 1991). On the other hand, the C-J pressure exists only at the detonation front and the pressure of over-passing front has a very small duration. In closed volumes, such as reactor building rooms for example, the shock reflections from the structures probably dominate the loads. These complicated interactions and 3-D phenomena can not be modeled by the DETO code. But, on the other hand, a simple shock wave approach can give applicable rough estimates of the damage factor of the first, and highest, pressure pulse.

As can be seen in Figs (6-8) to (6-10) the FLUENT calculations suggested that hydrogen accumulates to the upper parts of the reactor building rooms leading to a rather stable stratification, and hence, inhomogeneous, stratified atmosphere. This may have an important effect on detonation propagation and shock reflections. The computer program DETO is based on an idealised theory of a strong ignition assuming a **homogeneous** gas mixture. Hence, the constant, average values for relevant input parameters, such as gas initial density, temperature, and hydrogen molar fraction, have
to be used (and is used) in the calculations. Also the specific heat ratio is assumed to be constant during the shock propagation. This is not actually the case in reality and the specific heat ratio is a function of temperature and density due to the dissociation and ionisation which take place at high temperatures (Zel'dovich & Raizer, 1996).

Table 6-3 shows the results of some additional sensitivity studies performed by program DETO. Case 2 was selected as a reference case. The first column of the table tells the sensitive parameter changed.

The relevant input values for the reference case (case 2) were following:

$m_{H2} = 3.15 \text{ kg}$	(hydrogen mass burned)
$p_1 = 1.065e5 Pa$	(initial pressure),
$T_1 = 301.2 \text{ K}$	(initial temperature)
$X_{H2} = 0.278$	(hydrogen molar fraction)
$\rho_1 = 0.9 \text{ kg/m}^3$	(initial gas density)
R = 2.0  m	(distance from explosion center to wall)
$\gamma = 1.2$	(specific heat ratio)
$\beta = 0.89$	(numerical parameter)
$\alpha = 0$	(angle of incident shock)

Case	Usound	U <sub>1</sub>	$M_1$	M <sub>ref</sub>	<b>p</b> <sub>shock</sub>	p <sub>max</sub>	Ι
	[m/s]	[m/s]			[Pa]	[Pa]	[Pa-s]
1) Reference case	374.1	2165.3	5.8	3.0	38.8e5	387.1e5	9.37e3
2) R = 1.5 m	374.1	3334.4	8.9	3.3	92.2e5	106.2e5	37.0e3
3) R = 2.5 m	374.1	1549.7	4.1	2.8	19.8e5	161.5e5	3.93e3
4) $m_{H2} = 2.36 \text{ kg}$	374.1	1874.6	5.0	2.9	29.1e5	268.6e5	5.70e3
5) $m_{H2} = 3.94 \text{ kg}$	374.1	2422.2	6.5	3.1	48.6e5	508.2e5	14.08e3
6) $X_{H2} = 0.1$	338.2	1957.5	5.8	3.0	38.8e5	387.3e5	9.37e5
$(\rho_1 = 1.12 \text{ kg/m}^3)$							
7) $T_1 = 323 \text{ K}$	387.4	2242.3	5.8	3.0	38.8e5	387.1e5	9.37e5
$((\rho_1 = 1.85 \text{ kg/m}^3))$							
8) Air:	347.9	2706.0	7.8	2.5	75.0e5	551.2e5	18.5e3
p <sub>1</sub> = 1.065e5 Pa							
$T_1 = 301 \text{ K}$							
$\rho_1 = 1.23 \text{ kg/m}^3$							
$\gamma = 1.4$							
$\beta = 1.033$							

**Table 6-3**. Sensitivity study for case 2 as calculated by the DETO code.

 $U_{sound}$  = speed of sound in undisturbed gas mixture

 $U_1$  = velocity of incident shock at distance *R* from the explosion centre

 $M_1$  = Mach number before the incident shock

 $M_{ref}$  = Mach number for reflected shock

 $p_{shock}$  = pressure of the incident shock

 $p_{max}$  = maximum pressure behind the reflected shock

I = pressure impulse

Predicted pressure behind the incident shock is strongly dependent on the distance *R* from the explosion centre according to relation  $p \sim \frac{1}{R^3}$  (first three rows in Table 6-3).

In addition, the corresponding pressure is directly dependent on the total amount of energy *E* released (or mass of hydrogen burned) in the explosion (rows 4 and 5 in Table 6-3). The specific heat ratio  $\gamma$  and the numerical parameter  $\beta$  depend on each other. The values of about 1.2 and 0.89, respectively, correspond to the Hugoniot curve fit values for detonation in near stoichiometric hydrogen-air mixture (Strehlow, 1991). Values 1.4 and 1.0333, respectively, are typical values for pure air. The predicted reflected shock pressure for pure air ( $\gamma = 1.4$ ,  $\beta = 1.033$ ) is about 40% higher than that for near stoichiometric hydrogen-air mixture (last row in Table 6-3). The shock pressures predicted by the DETO code are not directly dependent on the initial gas density (rows 6 and 7 in Table 6-3). This is due to the assumption of the theory used that both the shock velocity and the speed of sound in unreacted gas mixture have a similar

relation to density  $U \sim \frac{1}{\sqrt{\rho_1}}$ . Consequently, the initial Mach number before the incident

shock does not change as the gas density changes, because the specific heat ratio is assumed to be constant. The dependence of the specific heat ratio on temperature and density is not taken into account in this study.

## 6.4 Testing of DETO Code to a Balloon Experiment

The capability of DETO code to assess the incident shock pressure of (hemi)spherically propagating shock wave under detonation conditions is assessed against a Balloon experiment performed at Fraunhofer-Institut fuer Chemische Technologie in Germany (Pförtner, 1991; Breitung & Redlinger, 1994). The facility consists of hemispherical balloons of diameter of about 6 m and the volume of 50 m<sup>3</sup>. The balloon was initially filled with premixed hydrogen-air mixtures, which was centrally ignited with high explosive. The pressure spikes were measured at several distances from the ignition point. The test arrangements were designed to obtain data for detonation pressures in a simple 1-D spherical geometry without reflections.

Figures 6-15 shows a set of pictures from one experiment (Pförtner, 1991). The few upper pictures represents very luminous combustion products of high explosive which were overtaken by the gaseous detonation front in the lower pictures. Test number 1 was selected as comparison case. The initial conditions of the test are shown in Table 6-4.



**Figure 6-15.** *Propagation of detonation front in a hemispherical balloon test* (Pförtner, 1991).

Volume [m <sup>3</sup> ]	Pressure[ Pa]	Temperature [K]	Hydrogen concentration [%]	Gas density [kg/m <sup>3</sup> ]	Energy from explosive [J]
53.	$0.999 \cdot 10^5$	304.	29.05	0.8318	$2.63 \cdot 10^5$

The measured and calculated shock peak pressures at three different distances from the ignition centre are compared in Table 6-5. All hydrogen (1.2182 kg) was assumed to burn in the ignition centre in the DETO calculation. Total energy of ignition used in the calculation was the energy of explosive plus the energy release from the hydrogen burn. The reaction energy of hydrogen-oxygen reaction is 120 MJ/kg, and hence, the total explosion energy used was 146.2 MJ.

Table	6-5. Comparis	son of measured	d and calculated	l results in ballooi	n test number 1
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Distance [m] *)	P <sub>exp</sub> [Pa]	P <sub>calc</sub> [Pa]	t <sub>d,exp</sub> [ms]	t <sub>d,calc</sub> [ms]	t <sub>h,exp</sub> [ms]	t <sub>h,calc</sub> [ms]	v <sub>calc</sub> [m/s]
0.75	$29.5 \cdot 10^5$	$281.4 \cdot 10^5$	1.8	5.4	0.6	0.05	6088
1.50	$20.6 \cdot 10^5$	$35.1 \cdot 10^5$	2.1	5.1	1.0	0.3	2152
3.25	$8.8 \cdot 10^5$	$3.4 \cdot 10^5$	3.4	3.5	~1.9	1.9	675

\*) calculated from the ignition centre

 $P_{exp}$  = measured shock pressure

 $P_{calc}$  = calculated shock pressure

 $t_{d,exp}$  = measured duration of shock overpressure phase

 $t_{d,calc}$  = calculated duration of shock overpressure phase

 $t_{h,exp}$  = measured time when the shock wave reaches the certain distance from ignition centre

 $t_{h,calc}$  = calculated time when the shock wave reaches the certain distance from ignition centre

 $v_{calc}$  = calculated velocity of shock wave

The theoretical detonation speed in the experiment was about 1950 m/s. According to strong explosion theory (Eqs. 6-2 and 6-3), the velocity and shock pressure approach infinity as the distance from the centre goes to zero. On contrary, as the distance approaches infinity, the shock velocity and pressure go to zero. This leads to a conclusion that the explosion theory clearly overpredicts at small distances and underpredicts at large distances the shock velocity and pressure. Somewhere between, the lines through the DETO results and the measured detonation pressures probably intersect each other (Figure 6-16). It is interesting that this intersection occurs in the Balloon test number 1 near the distance of about 2 m, which was also the basic distance used in the DETO applications to Olkiluoto reactor building room B.60-80. The total amount of hydrogen that burned in the Balloon test 1 (1.2182 kg) was also fairly close to the hydrogen mass used in calculation cases 1 (1.428 kg) and 3 (1.4 kg) for Olkiluoto reactor building.



Figure 6-16. Calculated and measured shock pressures as a function of distance from the ignition centre (Balloon test 1).

## 7. SUMMARY AND RECOMMENDATIONS

This report consists of the literature study of detonation dynamics in hydrogen-air-steam mixtures, and the assessment of shock pressure loads to Olkiluoto 1 and 2 reactor building under detonation conditions using the computer code DETO. The code is developed during this work at VTT. The code results are assessed approximately against a Balloon experiment performed at Germany, and the classical Chapman-Jouguet detonation theory. The work was carried out as a part of the Nordic SOS-2.3 project, dealing with severe accident analysis.

The initial conditions of the detonation calculations were based on previous severe accident analyses made by the MELCOR and FLUENT codes. The detonation shock pressure loads were analysed in three different base cases. The average hydrogen concentrations and gas densities were obtained from previous FLUENT calculations. The flammability region for detonations in hydrogen-air mixtures was assumed to lie between 10 and 78 volume per cent of hydrogen. The containment leak area was similar in the first two cases, but two different instants of time were considered: the end of simulation and the moment of time when the average conditions were closely stoichiometric. Detonable hydrogen masses in the reactor building room B.60-80 were 1.428 kg and 3.15 kg, respectively. The third case considered 2 mm<sup>2</sup> leak area (containment design leakage) in which the calculated detonable hydrogen mass was evaluated to be 1.4 kg. It was assumed conservatively that the hydrogen leak from the containment occurs to one reactor building room. More realistic assumption would be that the leak is diffused to all parts of the reactor building. The distance from the explosion origin to wall was assumed to be 2.0 m in all base cases.

The peak pressure maximum after normal shock reflection from the concrete wall ranged from about 12.6 MPa to 38.7 MPa at the distance of 2.0 m from the explosion centre. Corresponding maximum pressure impulses to the concrete wall ranged from about 2.3 kPa-s to 9.4 kPa-s. The duration of overpressure phase ranged from about 3.6 ms to 7 ms. The shock pressure spikes and corresponding impulses decreased as the angle between the incident shock wave and the wall surface increased. Furthermore, the results were sensitive to the initial distance of the explosion centre from the wall. For example, the decrease of initial distance from 2.0 m to 1.5 m leaded to increase of peak maximum pressure from 38.7 MPa to 106 MPa. Predicted shock pressure was also dependent on the total amount of hydrogen assumed to be burned during explosion, and the properties of undisturbed gas medium just before the arrival of shock wave.

Uncertainties of the model is primary caused by the fact that only the first reflection of 1-D shock wave is considered in the DETO code. Other simplification is that total energy is instantly released in the explosion origin. The local explosion is then assumed to induce a freely propagating spherical shock wave without modelling of propagation of combustion front typical under real detonation conditions. Neither, the multiple shock wave reflections, collisions, and possible focusing e.g in three-dimensional corners, which may lead to high local pressure in the detonation front can be modelled by DETO code. More detailed, three-dimensional numerical analyses with a specific detonation code is, therefore, recommended in order to assess these complicated interactions and their influences on pressure loads under detonation conditions.

Due to lack of modeling of propagating combustion front in the DETO code, the shock wave is assumed to propagate "freely", and the incident shock velocity and pressure are very sensitive to the distance from the explosion centre. Consequently, estimated shock pressure may be very high at very small distances from the explosion centre. Comparison of the DETO results to the classical C-J theory and the Balloon experiments indicated that the DETO overestimated the maximum pressure spike after the normal shock reflection from the wall. This conclusion can be justified by the fact that the predicted peak pressure of normally reflected shock and corresponding incident shock waves exceeded the C-J value (by factor 1.1 to 9.4) in all cases considered in the application for Olkiluoto reactor building. Also the comparison of the DETO results to the Balloon experiment showed that DETO overpredicted the incident shock pressure at small distances (< 2 m).

In spite of the limitations and simplification, the computer program DETO is found to be a beneficial tool for simple first-order assessments of the structure pressure loads under the first reflection of detonation shock waves.

The work on assessment of detonation loads will continue in the future with full 3dimensional simulations with detailed DET3D computer code. Development of interface between the DETO code and ABAQUS structural analysis code is also under way.

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