Effect of Initial Temperature on FA and DDT in H_2-air mixtures: CFD Simulations & Validation against Experimental Data

Prankul Middha
GexCon AS
Bergen, Norway

1 Introduction

There has been a continuous and increasing interest in studying hydrogen safety in recent years. One of the motivating factors is handling the safety concerns in the nuclear industry as the consequences from nuclear accidents are global, and it is very important to maintain confinement in case of a hydrogen explosion. Hydrogen can be produced during a nuclear accident involving core degradation and may lead to a strong explosion that could compromise the integrity of the containment building. In particular, during the Three Mile Island accident, there was a partial meltdown of the reactor core resulting in the production and release of a large amount of hydrogen gas into the containment building [1]. During the accident, the combustion of the hydrogen resulted in several pressure spikes but the pressure rise was fortunately not large enough to compromise the integrity of the containment. This may have occurred if the hydrogen deflagration had transitioned to a detonation. It is well-known that deflagration to detonation transition (DDT) may be a significant threat for hydrogen explosions. Due to the high reactivity of hydrogen, DDT is likely in a variety of scenarios involving H_2-air mixtures and result in large-scale damage. The situation is exacerbated in the presence of obstacles, which induce turbulence that accelerates flames to a high speed.

Transition to detonation in an explosive mixture has been studied for more than 65 years to obtain a qualitative and quantitative understanding of the phenomenon [2]. There have been several experimental studies in recent years. Some of them have been basic studies of high-speed turbulent flame propagation and DDT in detonation tubes [3,4]. Other studies have focused on the development of necessary criteria for “effective flame acceleration”. These have examined the effect of basic flame parameters (expansion ratio, Lewis number, Zeldovich number, etc.) and geometry (tube diameter, blockage ratio, etc.) on the possible development of fast combustion regimes that can eventually transition to a detonation [5]. Several other large-scale tests in a congested area have been carried out to simulate the conditions of a process facility.

Calculations have shown that certain accident scenarios can be characterized by high local compartment temperatures. However, there are not many DDT experiments carried out at temperatures higher than the ambient. The experimental tests used in this article were carried out to generate DDT data at high temperatures, up to 650 K. This data can also be valuable for carrying out safety analyses for gas turbines where hydrogen is used as fuel. For this purpose, a well-documented experimental test series was carried out in the High-Temperature Combustion Facility (HTCF) at the Brookhaven National Laboratory (BNL) in the United States [6]. The present experiments were much better controlled than previous experiments by Beauvais et al [7]. The entire length of the test vessel was

Correspondence to: prankul@gexcon.com

filled with orifice plates in order to allow a steady-state velocity. The objective of the present set of experiments was to characterize the effect of the initial temperature of the mixture on flame acceleration and the potential for DDT. The applicability of the proposed DDT limit criteria $d/\lambda = 1$, where λ is the detonation cell size and d is the tube diameter, is also tested at elevated initial temperatures using cell size data for Ciccarelli et al. [8].

These experiments have been simulated using the Computational Fluid Dynamics (CFD) tool FLACS. FLACS is a commercial special-purpose CFD tool that is developed by GexCon and has been designed for modelling gas explosions in industrial-scale geometries [9]. It has previously been extensively validated for hydrogen safety applications for dispersion, explosion as well as combined dispersion and explosion studies [10-12]. The test geometry has been implemented in FLACS and simulations have been carried out for the entire concentration range as well as all three temperatures.

2 Experimental Details

The DDT experiments were carried out in the BNL HTCF which is a 27 cm inner diameter, 21.3 m long heated detonation tube. A detailed description of the HTCF detonation tube and the associated measurement and gas handling equipment is found in [6]. An array of obstacles in the form of orifice plates with the outer diameter equal to that of the tube and an inner diameter of 20.6 cm (blockage ratio = 0.43) are placed inside the entire length of the tube with a spacing of one tube diameter (i.e. 27 cm). The values of these obstacle parameters are based on previous experiments by McGill University to provide the optimum configuration for FA and DDT. The tube was filled with premixed hydrogen-air mixture at various concentrations that was ignited by a standard diesel engine glow plug mounted centrally on one of the end plates. The temperature of the gas was maintained uniformly at 300, 500 and 650 K to investigate the effect of temperature on the FA and DDT process. The tube was equipped with instrumentation ports located every 61 cm along the length that consisted of ionization probes, photo diode detectors, and fast response thermocouples in order to measure the flame time-of-arrival data. Combustion front pressure was measured using one piezoelectric transducer located near the end of the tube. A schematic of the orifice plate geometry and dimensions is shown in Fig. 1.

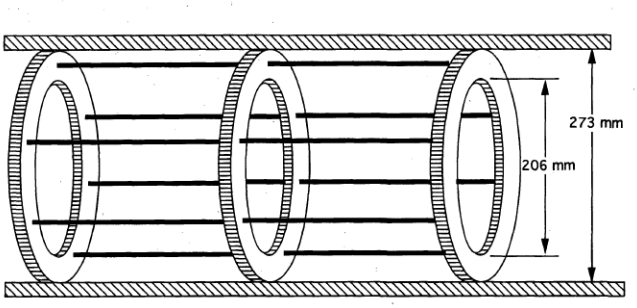


Figure 1. Schematic of orifice plate Geometry and dimensions

3 Simulation Details

The CFD tool FLACS has been used for modelling the experimental tests. FLACS is a computational fluid dynamics (CFD) code solving the compressible conservation equations (mass, momentum and energy) on a 3-D Cartesian grid using a finite volume method. The inherent capability of FLACS has been performing explosion and dispersion calculations to help in the improvement of oil and gas platform safety with initial focus on the North Sea. Significant experimental validation activity has contributed to the wide acceptance of FLACS as a reliable tool for prediction of natural gas explosions in real process areas offshore and onshore. It has previously been extensively validated for hydrogen safety applications for dispersion, explosion as well as combined dispersion and explosion studies [10-12].

A distributed porosity concept is applied, which enables FLACS to simulate all kinds of complicated geometries using a Cartesian grid [13]. Large objects and walls are represented on-grid, and smaller objects represented sub-grid. Sub-grid objects contribute with flow resistance, turbulence generation and flame folding. FLACS uses a standard k-ε model in order to model the convection, diffusion, production, and dissipation of turbulence. Several important modifications are however implemented, including a model for generation of turbulence behind sub-grid objects.

FLACS contains a combustion model that assumes that the flame in an explosion can be regarded as a collection of flamelets. One-step reaction kinetics is assumed, with the laminar burning velocity being a measure of the reactivity of a given mixture. Since a grid size that is significantly finer than realistically possible is needed to fully resolve the flame, a β flame model is used in FLACS that artificially thickens the flame so that its structure is fully resolved and coarse grids may be used [13]. The flame model gives the flame a constant flame thickness (equal to 3–5 grid cells) and makes sure that the flame propagates into the reactant with the specified velocity (with a number of other modifications). Models for laminar and quasi-laminar burning velocities (to account for flame wrinkling) implemented in the FLACS code, depending on among others the concentration, composition, flame radius, and Lewis number, are described in detail in [13]. The model has been modified to include the effect of higher initial temperature. The turbulent burning velocity model is based on a broad range of experimental data from Leeds University and the empirical correlation by Bray [14], $\frac{S_T}{S_L} = 0.875K^{-0.392}\frac{u'}{S_L}$. Here, K is the Karlovitz stretch factor, S_T is the turbulent burning velocity, and S_L is the laminar burning velocity.

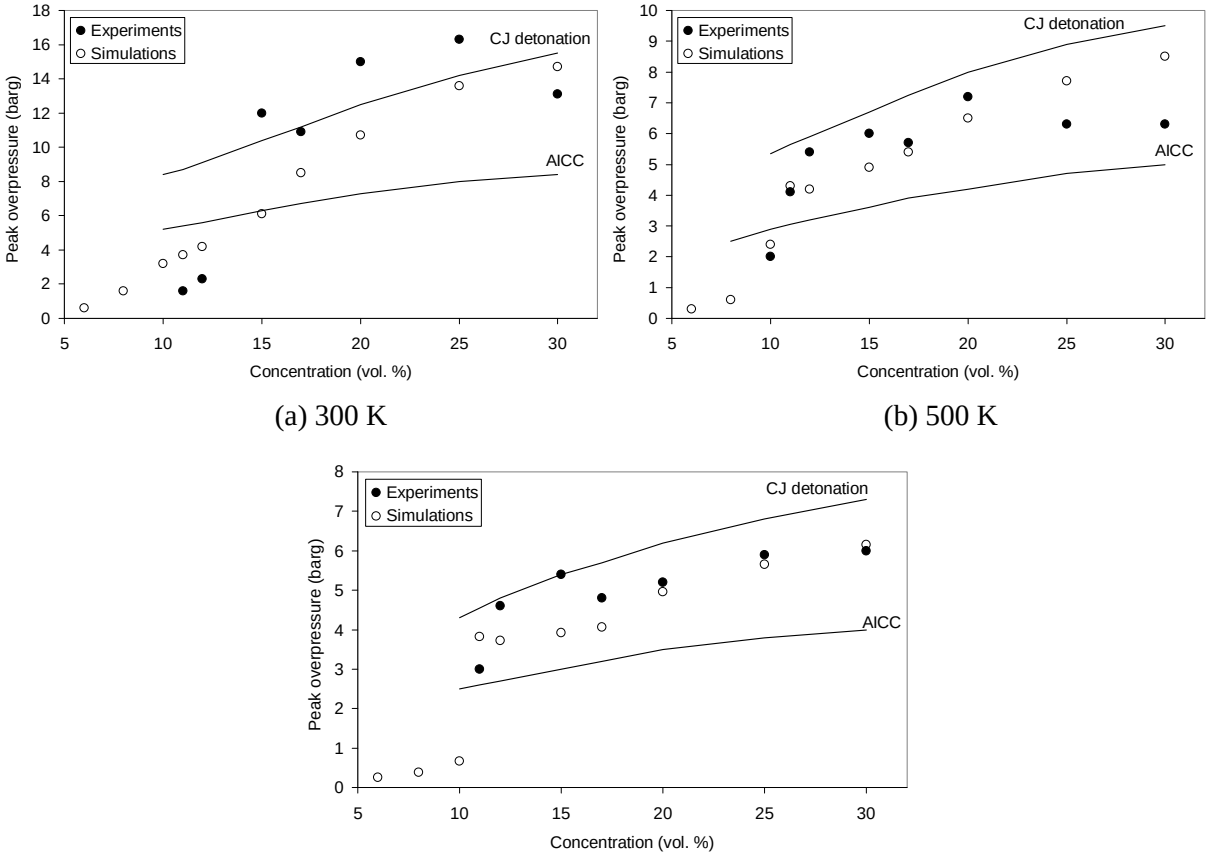
FLACS cannot simulate a transition to detonation directly as that requires resolution of very small scales. The likelihood of DDT is indicated in terms of a normalized spatial pressure gradient across the flame front $\left.\frac{dP}{dx}\right|_{normalized} = \left.\frac{dP}{dx}\right|_{actual}\frac{X_{CV}}{P_0}$ (where X_{CV} is the grid size and P_0 is the initial pressure) as this parameter is able to visualize when the flame front and the pressure front are only separated by the reaction length, which is the case in situations when fast deflagrations transition to detonation [15,16]. A shock wave may propagate through a flame without causing DDT and this method cannot distinguish between a propagating shock and a DDT event. Rather, it presents the magnitude of the normalized spatial pressure gradient as a criterion for determining the likelihood of a transition to detonation. Comparison of the characteristic geometrical dimensions with the detonation cell size is also carried out in order to ensure that the geometrical dimensions are sufficient for the propagation of any initiated detonation front. Many different experiments have been simulated and the simulations are able to match the observations reasonably well. This has included diverse experiments such as detonation tube experiments at McGill University, large-scale channel experiments at the Sandia FLAME facility, jet ignition experiments at the KOPER facility and Fh-ICT lane geometry [15,16]. However, FLACS has no shock ignition model which means that the speed of the flame front is expected to be somewhat lower than that seen in the experiments.

The geometry has been implemented using the FLACS pre-processor CASD. Appropriate boundary and initial conditions are defined. The grid resolution used was 2.7 cm. All the simulations have been carried out using the most recent version of FLACS v9.1 r2 (June 2010) for the entire concentration range as well as all three temperatures.

4 Results and Discussion

The experiments were carried out for hydrogen-air mixtures with concentrations ranging from 6-30 % hydrogen for three different temperature, 300, 550 and 650 K. FLACS was used to simulate several of these tests for all three temperatures. Fig. 2 presents the experimental and simulated overpressures as a function of hydrogen concentration for all three temperatures. It can be seen that the simulations agree

reasonably well with experimental data in all cases. The figure also presents a comparison with theoretical AICC and CJ detonation pressures. The goal of the experiments was to determine the not only the variation of combustion overpressures as a function of concentration but also to determine concentration limits above which a transition to detonation could be expected. It can be seen that DDT occurs for a concentration of 15 % H_2 at a temperature of 300 K. The cell size for a 15 percent hydrogen mixture at 300K and 0.1 MPa is about 21.8 cm [8], and the inner diameter of the rings is 20.6 cm. Therefore, the ratio d/λ equals 1.0.



(a) 300 K (b) 500 K

(c) 650 K

Figure 2. Comparison of the measured and simulated peak overpressures for hydrogen-air mixtures at 0.1 MPa and the theoretical AICC and CJ detonation pressure for three different initial temperatures

At a temperature of 500 K, mixtures of 12 % or higher show measured pressures larger than the corresponding AICC pressure but lower than the CJ detonation pressure for both simulations and experiments. Mixtures with less than 12 percent hydrogen exhibit pressures consistently below the AICC pressure. The cell size for a 12 percent hydrogen mixture at 500K and 0.1 MPa is about 13.5 cm which yields a value of 1.5 for the ratio d/λ. The value of this ratio can be considered as satisfying the d/λ = 1 criterion for DDT transition, considering the uncertainty in the experimentally measured detonation cell size. The above figure (and supporting evidence from the front velocity, see Fig. 3) show that 11 percent is the minimum hydrogen composition which results in a DDT at a temperature of 650 K. The cell size for an 11 percent hydrogen mixture at 650K and 0.1 MPa is about 3.7 cm. This yields a value of 5.5 for the ratio d/λ. Although this result does not violate the d/λ >1 criterion for the possibility of DDT, it is at variance with the DDT limit of d/λ = 1 which was found to apply at the other initial conditions. One of the explanations for this seems to be the fact that the transition seems

"more sudden" and the mixture seems to go directly from very low velocities to detonation speeds (see Fig. 3). The lower maximum pressure that gives lower expansion ratios can also play a significant role. However, this is still an open issue.

The simulations use a normalized spatial pressure gradient across the flame front in order to indicate the likelihood of DDT (where a value higher than 1 indicates significant chance of a transition of detonation). This criterion also fully supports the conclusions described regarding the limits for DDT for all three temperature values. An example of the spatial pressure gradients seen in the simulations is shown in Fig. 4 for 30 % H_2-air mixture at 300 K. The simulations are unable to predict the exact run-up distance to a detonation that can be observed in the experiments as a transition to detonation is not actually modeled but a run-up distance can be indicated by the distance before a significant value of the pressure gradients occur. For a concentration of 30 %, the detonation transition was observed to occur between 2-3 m from ignition while the simulations predict a value between 1.5-3 m for the three temperatures. For a concentration of 20 %, the run up distance in the experiments was seen to be between 3-6 m that was again in a good agreement with the simulation values between 2-6 m.

Fig. 3 presents a comparison between the observed and simulated average flame front velocity as a function of concentration for the initial temperature of 650 K. The theoretical isobaric products sound speed as well as the CJ detonation velocity is also presented. It can be seen that while the experiments approach the CJ detonation velocity for concentrations above the DDT transition limit, the simulated values do not exceed the isobaric products sound speed (choking regime). FLACS still lacks a shock ignition model, which means that a detonation front cannot actually propagate, and the speed of the front is limited by the speed of sound in products. However, a model is currently under development in order to replicate the propagation of a detonation front for the cases that DDT is indicated and the geometrical dimensions are sufficient.

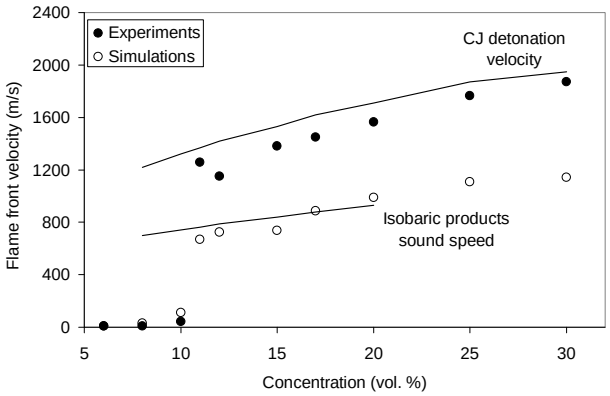


Figure 3. Comparison of the measured and simulated average flame front velocity for hydrogen-air mixtures at 0.1 MPa and 650 K and the theoretical isobaric products sound speed and CJ detonation velocity

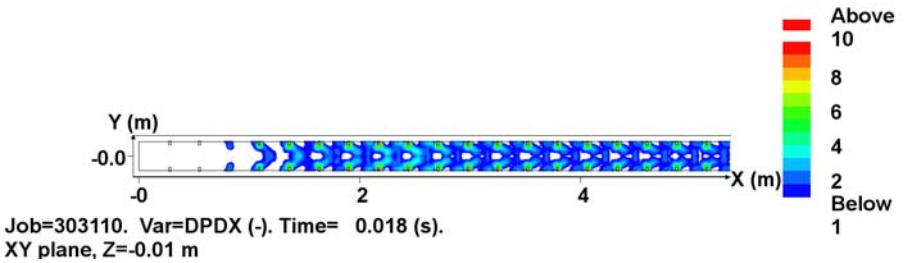


Figure 4. The simulated spatial pressure gradients in the XY plane at the centre of the geometry for 30 % H_2-air mixture at 300 K and 0.1 MPa.

5 Conclusion

In general, the simulations compare reasonably well with experimental predictions for the observed overpressures, DDT limits and run-up distances even if the combustion front velocities are underestimated. This points to the value of FLACS as a useful tool that can be employed in a predictive capacity in a process setting. FLACS can thus be applied to relevant problems in the nuclear industry. Even though the description of DDT described above is approximate, we believe that useful results can be obtained and this represents an important first step to be able to bridge the gap between CFD simulations and realistic process safety studies involving the possibility of a transition to detonation.

References

[1] Henrie JO, Postma AK. (1983). Analysis of the Three Mile Island (TMI-2) Hydrogen Burn, In: Thermal-Hydraulics of Nuclear Reactors, Vol. 2, ANS Order No 700081.

[2] Lee JHS, Moen IO. (1980). The mechanism of transition from deflagration to detonation in vapor cloud explosions. Proc. Energy Comb. Sci., 6: 359.

[3] Chao J, Lee JHS. (2003). The propagation mechanism of high-speed turbulent deflagration. Shock Waves 12: 277.

[4] Lee, JHS, Knystautas, R, Freiman, A. (1984). High-speed turbulent deflagrations and transition to detonation in H2–air mixture. Comb. Flame, 56: 227.

[5] Dorofeev SB, Kuznetsov MS, Alekseev VI, Efimenko AA, Breitung W. (2001). Evaluation of limits for effective flame acceleration in hydrogen mixtures. J. Loss Prevent. Proc. Ind., 14: 583.

[6] Ciccarelli G, Boccio JL, Ginsberg TC, et al. (1998). The Effect of Initial Temperature on Flame Acceleration and Deflagration-to-Detonation Transition Phenomenon. Brookhaven National Laboratory, NUREG/CR-6509, BNL-NUREG-52515.

[7] Beauvais B, Mayinger F, Strube G. (1993). Severe Accident in a Light Water Reactor: Influence of Elevated Initial Temperature on Hydrogen Combustion," ASME/JSME Nuclear Engineering Conference, Volume 1, 425.

[8] Ciccarelli G, Ginsberg TC, Boccio JL, et al. (1997). Detonation Cell Size Measurements in High-Temperature Hydrogen-Air-Steam Mixtures at the BNL HTCF. NUREG/CR-6391, BNL-NUREG-52482.

[9] FLACS Software, GexCon AS, http://www.gexcon.com/index.cfm?id=268677.

[10] Middha P, Hansen OR. (2009). Using computational fluid dynamics as a tool for hydrogen safety studies. J. Loss Prevent. Proc. Ind., 22: 295.

[11] Middha P, Hansen OR, Storvik IE. (2009). Validation of CFD-model for hydrogen dispersion. J. Loss Prevent. Proc. Ind., 22: 1034.

[12] Middha P, Hansen OR, Grune J, Kotchourko A. (2010). Validation of CFD calculations against ignited impinging hydrogen jet experiments. J. Haz. Mat., 179: 84-94.

[13] Arntzen BJ. (1998). Modelling of turbulence and combustion for simulation of gas explosions in complex geometries. Dr. Ing. Thesis, NTNU, Trondheim, Norway.

[14] Bray KNC. (1990). Studies of the turbulent burning velocity. Proc. R. Soc. Lond. A, 431: 315.

[15] Middha P, Hansen OR, Storvik IE. (2006). Prediction of deflagration to detonation transition in hydrogen explosions, In: Proceedings of 40th Annual Loss Prevention Symposium.

[16] Middha P, Hansen OR. (2008). Predicting deflagration to detonation transition in hydrogen explosions. Proc. Safety Prog. 27: 192.