# NEW PARADIGMS IN HYDROGEN EXPLOSION MODELLING USING AN INDUSTRIAL CFD CODE

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## ABSTRACT

It is well-known that deflagration to detonation transition (DDT) may be a significant threat for hydrogen explosions. This paper presents a summary of the work carried out for the development of models in order to enable the industrial computational fluid dynamic (CFD) tool FLACS to provide indications about the possibility of a deflagration-to-detonation transition (DDT). The likelihood of DDT has been expressed in terms of spatial pressure gradients across the flame front. This parameter is able to visualize when the flame front captures the pressure front, which is the case in situations when fast deflagrations transition to detonation. Reasonable agreement was obtained with experimental observations in terms of explosion pressures, transition times, and flame speeds for several practical geometries. The DDT model has also been extended to develop a more meaningful criterion for estimating the likelihood of DDT by comparison of the geometric dimensions with the detonation cell size. The conclusion from simulating these experiments is that the FLACS DPDX criterion seems robust and will generally predict the onset DDTs with reasonable precision, including the exact location where DDT may happen. The standard version of FLACS can however not predict the consequences if there is DDT as only deflagration flames are modelled. Based on the methodology described above, an approach for predicting detonation flames and explosion loads has been developed.

The second part of the paper covers new paradigms associated with risk assessment of a hydrogen infrastructure, such as a refueling station. In particular, approaches involving one-to-one couplimng between CFD and FEA modelling are summarized. The advantages of using such approaches are illustrated. This can have wide-ranging implications on the design of things like protection walls against hydrogen explosions.

## 1.0 INTRODUCTION – DDT

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. This rapid turbulent flame acceleration can lead to DDT when sufficiently intense turbulent mixing is achieved at the reaction zone. The determination of the conditions for the transition from deflagration to detonation has been a subject of several studies for hydrogen explosion safety. Also, considerations of mixture sensitivity and geometric dimensions are important as a stable detonation front will only be formed if the concentration lies within the detonability limit and the geometric dimensions exceed the detonation cell size. Even if it is possible to initiate detonation directly, this is not a cause of worry for typical safety applications as explosions normally start as a result of weak ignition sources e.g. an electrical spark. Under certain conditions, the flame can accelerate and undergo a transition to detonation. The flame acceleration phenomenon is separate from the actual initiation of detonation and is equally important to study.

Transition to detonation can occur in a variety of situations, many of which are commonly employed in industrial settings. These include flame propagation in smooth tubes or channels (e.g. [1]), flame acceleration as a result of repeated obstacles (e.g. [2]), and jet ignition (e.g. [3]). This is a common problem in industrial process piping as it is typically designed to withstand only moderate over-pressurization (due to cost reasons) and catastrophic failure is mitigated by the use of venting devices. However, these devices are insufficient to limit the rapid pressure rise from a fast flame and/or detonation and therefore, it is important to understand and avoid the conditions for a transition to

detonation. A common feature of any future "hydrogen economy" will be a hydrogen filling station. If a significant hydrogen release were to occur, it could form an explosive hydrogen-air mixture. The possibility of a transition to detonation upon ignition must be accounted for when planning for the location of the filling station in relation to other facilities and buildings. Further, the actual design of the storage facility and handling procedures all require the issue of DDT to be understood in a quantitative manner. The nuclear industry has also been very interested in these investigations as the consequences from nuclear accidents are global as opposed to offshore oil exploration accidents, and it is very important to keep confinement in case of a hydrogen explosion. 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 [4]. 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. Thankfully, a transition to detonation (DDT) did not occur in this case but this accident led many countries with nuclear power plants to initiate extensive research programs investigating hydrogen detonation related phenomena.

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 (e.g. [5,6]). It is very challenging to fully understand the phenomena behind high-speed turbulent deflagrations and the transition to detonation (Shepherd & Lee, 1992). There have been several experimental studies in recent years. Some of them have been basic studies of high-speed turbulent flame propagation in detonation tubes (e.g. [7,8]). The goal of these studies is to show that the maximum steady-state turbulent flame speed that can be achieved in the experiments depends only on the properties of the mixture and is governed only by the chemical kinetics and energetics. A transition to detonation (or quasi-detonation since losses may result in a speed less than the CJ velocity) can occur for more "sensitive" mixtures. These speeds can then form a basis for the development of models for understanding DDT. 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. These have mostly been performed by Dorofeev and coworkers [9-11]. Several other large-scale tests in a congested area have been carried out to simulate the conditions of a process facility. These tests are often not directly useful for the development of models as detailed measurements of e.g. turbulence parameters is not carried out.

There are several different mechanisms that have been propounded to explain the DDT phenomenon. In the CJ theory, the detonation wave is treated as a discontinuity with infinite reaction rate. Based on this one-dimensional theory, it is possible to calculate detonation velocity, pressure, etc. if the composition of the gas mixture is known. The values calculated from this simple theory agree surprisingly well with observations. Therefore, a detonation front was initially thought to be one dimensional and the 3D structure was discovered only later. However, understanding the actual mechanisms for the formation of the detonation wave is much more complex. The widely prevailing "Gas Dynamic" explanation for DDT is essentially one-dimensional wherein the volume expansion of hot burned gases move into the unburned gas and generate shock waves. These shock waves preheat the unburned mixture, thus increasing the burning rate and forming further shock waves. The resultant shock fronts can merge into a wave that is strong enough to cause a local explosion that transforms into a steady detonation [12]. Under this scenario, the study of the flame acceleration leading to the development of the "right" conditions leading up to detonation initiation is as important as the actual onset of the detonation event. Oppenheim [13] have shown an additional mechanism to be prevalent in many cases wherein the transition begins with a local explosion in a region of high turbulence, even though the compression heating of the unburned gas due to shock waves is not sufficient. The interactions of flame with the wall have also been found to be important. Lee, Knystautas & Yoshikawa [14] have propounded the shock-wave amplification by the coherent energy release (SWACER) mechanism where induction time gradients associated with temperature and pressure gradients in the system produce a compression wave that can gradually get amplified into a strong shock wave. This shock wave can auto-ignite the mixture and produce DDT. Instabilities near the flame front as well as interaction between the flame and another flame, a shock wave or a secondary explosion (local quenching and then re-ignition), may also lead to

DDT. Further details and a fairly exhaustive list of references for the mechanisms involved in DDT can be found in [15] and [16].

Although there has been a strong debate on the mechanisms underlying the transition to detonation and it is still an active research area, there is no doubt that it is very important to study this phenomenon from a process safety perspective. Detailed description of all processes following ignition that may lead to DDT is extremely challenging. This is due to a complicated interaction of compressible flow, chemical reaction, and turbulence that needs to be described at very high spatial and temporal resolution. Therefore, much theoretical effort has been focused on development of criteria for DDT [15]. As described above, researchers have tried to establish the initial and boundary conditions, and geometric and process parameters under which a transition to detonation can be expected. However, these criteria and scaling arguments are difficult to apply in a process setting where exact numerical results are much more valuable.

## 2.0 CFD MODELLING

With the advance in scientific computing, research on DDT has been shifted toward the use of computational approaches. Numerical simulations can be a powerful tool to obtain detailed analyses of the underlying phenomena and can provide a picture of the basic DDT process from flame ignition, acceleration and transition to detonation. One such numerical simulation tool is FLACS.

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 been extensively validated for hydrogen safety applications for dispersion, explosion as well as combined dispersion and explosion studies [17-19].

A distributed porosity concept is applied, which enables FLACS to simulate all kinds of complicated geometries using a Cartesian grid [20]. 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 [20]. 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 [20]. 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 [21], $\frac{S_T}{S_L} = 0.875K^{-0.392}\frac{u'}{S_L}$. Here, *K* is the Karlovitz stretch factor, *ST* is the turbulent burning velocity, and *SL* is the laminar burning velocity.

Before the beginning of this work, the standard versions of the CFD tool FLACS could only handle the deflagration mode of combustion, in which the flame propagates because hot flame products heat and ignite the unburned gas ahead. In situations with very fast flames and/or very strong pressure waves a deflagration to detonation transition (DDT) may change the propagation mode so that shockwaves will ignite unburned gas and lead to faster flame propagation (1500–2000 m/s). In this work, the use of

FLACS to simulate hydrogen explosions in different geometries and get indications about the likelihood of DDT is described. The study of this phenomenon is very critical as the overpressures in detonation front can cause losses which are much more severe as compared to those seen with blast waves produced by a deflagration.

## 3.0 DDT MODELLING IN FLACS

### 3.1 Spatial pressure gradient

The DDT phenomena can be usually divided into two separate phases [5,22]: (1) the creation of conditions for the onset of detonation by processes of flame acceleration, mixing of products and reactants, etc. and (2) the actual formation of the detonation wave itself or the onset of detonation. Processes in the first phase are particular to the specific initial and boundary conditions of the problem. Different physical mechanisms dominate the process of flame acceleration in obstructed channels, smooth tubes or large volumes filled with combustible mixtures. However, the actual formation of the detonation appears to be a more universal phenomenon and the basic structure of the detonation front is well known. The methodology used is based on this underlying structure of a detonation front. The structures of deflagration and detonation waves are contrasted in Figure 1 [23,24].

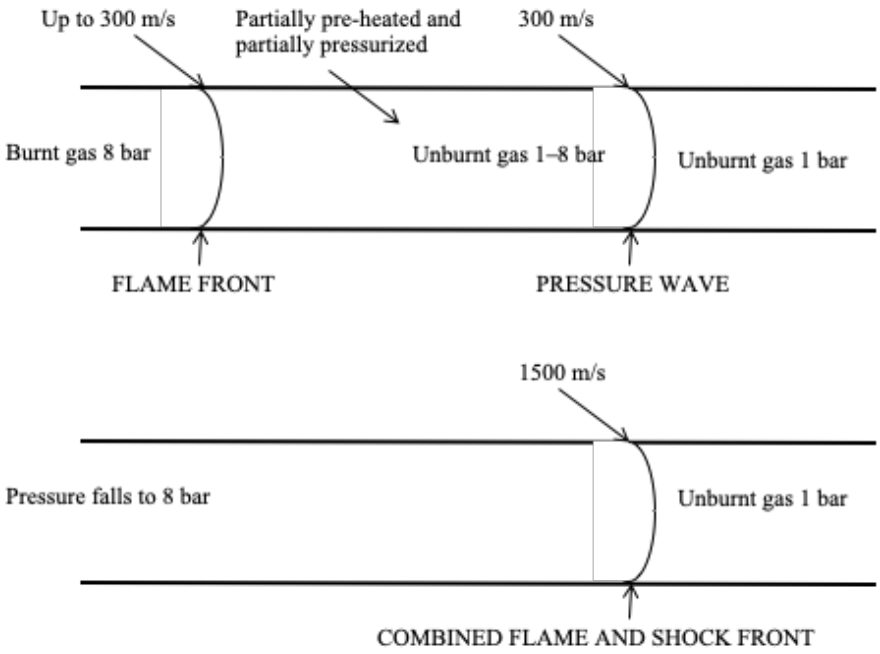


Figure 1. A schematic diagram showing the underlying structure of a detonation front.

In a detonation, a high-pressure shock front travels only about 1 to 10 mm ahead of the reaction zone / flame (in a fast deflagration, the reaction zone lags much further behind the shock front). Therefore, for all practical purposes, it can be assumed that the flame and pressure front travel together. Early work by Bone and Frazer [25] has also indicated that a shock wave, independently started, should precede the flame and observed that, as the accelerated flame front caught up with the shock wave, detonation set in ahead of the flame.

Based on the discussion above, the likelihood of DDT is illustrated in terms of a parameter proportional to the spatial pressure gradient across the flame front [5,26]. This parameter is able to visualize when the flame front captures the pressure front, which is the case in situations when fast deflagrations

transition to detonation. It is proposed that the presence of these spatial pressure gradients represents the indication of a possibility of the deflagration front transiting to detonation.

The methodology has been validated against several experiments, including hydrogen explosion tests in the FLAME facility [12], McGill detonation tubes [2], a smooth tube [11], KOPER facility [27] and FhICT lane geometry [28,29].

Putting the current DDT work into perspective, the description of DDT by FLACS can only be characterized as an "average" description. Some authors criticize this approach. Ng and Lee [30] have the following comment: "Unfortunately, the current directions of numerical studies tend to reproduce the effects in a so-called realistic accidental scenario. As a result, too many unknown constants have to be adjusted to permit these codes to produce data to match with often-crude ill-defined large-scale test data. Such resulting models can sometimes provide the right answers even if the correct mechanisms are not in the model." It is correct that the exact mechanisms of DDT are not accounted for, but the study focuses on the possibility of the shock and flame front travelling together. However, it must be remembered that high-speed turbulent deflagration and DDT are extremely complex phenomena involving a multitude of physical mechanisms which are strongly coupled in a non-linear manner. Exact representation of DDT in a typical hazardous industrial scenario involves scales that can differ by up to 10 orders of magnitude [16]. An exact simulation for such a 3*D* system will take many years using current computational power. There are tools that aim to simulate the transition to detonation directly (a review is given in [31]) but these are mostly confined to small, 2*D* systems and require special, multidimensional numerical simulations that cannot be carried out for risk analyses. If we were to proceed further in understanding and avoiding this phenomenon in realistic process geometries, the approach developed here is very valuable. It is believed that useful results can be obtained using this approach 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. As the validation work described below will show, the results obtained are remarkably consistent with experimental observations in terms of overpressures and location/time of the occurrence of DDT.

As a part of this work, the parameter spatial pressure gradient (*dP/dx* or DPDX) described above has been normalized, in order to remove dependence on grid and initial conditions. The dimensionless spatial pressure gradient can be expressed as:

$$\left.\frac{dP}{dx}\right|_{normalized} = \left.\frac{dP}{dx}\right|_{actual} \frac{X_{CV}}{P_0} \tag{1}$$

where $P_0$ is the initial pressure and $X_{CV}$ represents the grid resolution. The DPDX ranges and their qualitative likelihood with respect to DDT are shown in the figure below. Current guidelines are as follows:

- DPDX < 0.5 DDT is not considered likely
- 0.5 < DPDX < 5 DDT may happen if hot-spot region in flame front is significant (see below)
- DPDX > 5 DDT is likely if hot-spot region in flame front is significant (see below)

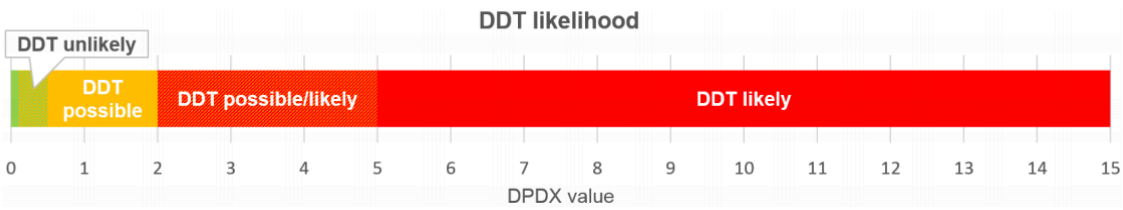


Figure 2. Illustration of the DPDX value range and the likelihood of DDT.

This model has been validated against a range of experiments with hydrogen (as described above), and more recently also ethylene (MERGE experiments, BakerRisk experiments), propane (Buncefield experiments) and even natural gas (NIOSH pipe).

However, a high enough DPDX value is not the only criterion that should be checked to conclude whether a detonation is likely; rather, at the same time the flame front also has to cover a large enough area compared to the detonation cell size of the gas. The reason for the size requirement is that the detonation front consists of a cell pattern, whose characteristic length scale λ sets requirements for the minimum geometrical dimensions to enable the detonation front to propagate, e.g. transverse size of passage ($d > \lambda$) and minimum distance for detonation formation ($L > 7\ \lambda$). To verify if the size of the region where significant values of DPDX are present is "large enough" (on the order of a certain multiple of cell size), a quantitative criterion ('DDT length scale') based on a length scale ratio has been developed. The methodology is illustrated for the FhICT lane geometry [28,29] in Figure 3 below.

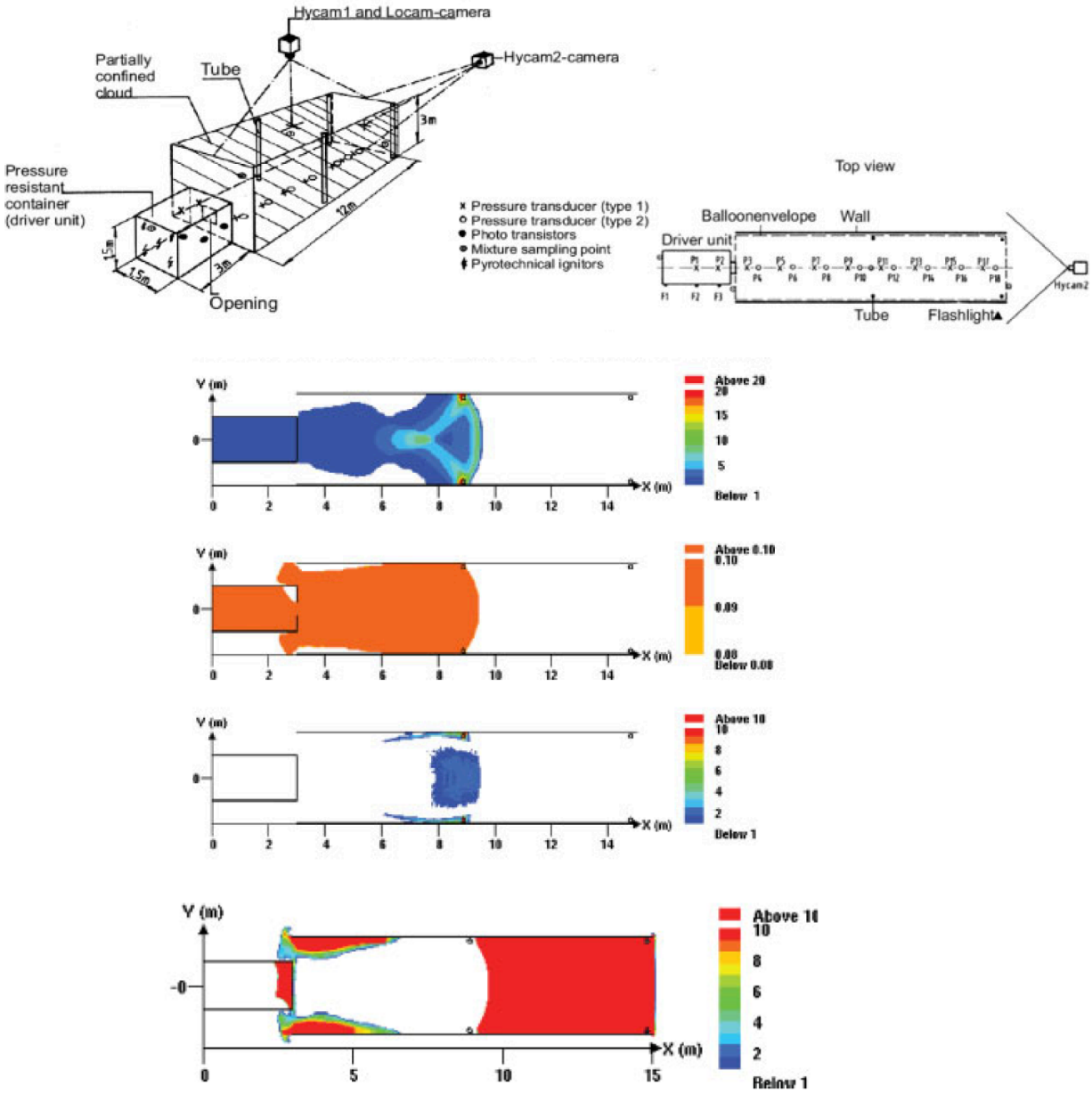


Figure 3. Illustration of methodology to determine DDT likelihood within FLACS for the FhICT lane geometry. The simulation contours show the overpressure (top), flame (second), DPDX (third) and the 'DDT length scale' (bottom).

## 3.2 Detonation Model

A “shock-ignition / detonation model” has also been implemented in FLACS as a part of this work in order to represent a detonation front. This has been implemented by modeling ignition ahead of the merged shock-flame front (based on the criteria described above). The ignition is implemented by artificially increasing the burning rate in the grid cells ahead of the flame front. This shock ignition model has been tested in the RUT facility geometry [32]. The schematic of the geometry used is shown in Figure 4.

Figure 5 shows the flame front and the pressure front during the simulations, as well as the propagation of flame front as a function of time. Each sensor point is 1 m apart and it can be seen that a constant velocity (equal to approximately 1800 m/s) is achieved. The maximum overpressures achieved in this case are around 15 bar. These values are in reasonably good agreement with the theoretical C-J values.

The conclusion from simulating these experiments is that the FLACS DPDX criterion seems robust and will generally predict the onset DDTs with reasonable precision, including the exact location where DDT may happen. The standard version of FLACS can however not predict the consequences if there is DDT as only deflagration flames are modelled.

Based on the methodology described above, Hansen and Johnson [33] have developed an approach for predicting detonation flames and explosion loads. By adjusting input parameters to FLACS flame speeds ~1500 m/s and flame front explosion pressures of 10-15 bar could be predicted. Both the flame speeds and pressures are sufficiently close to those seen in a detonation to predict explosion loads with fairly good precision. By combining this approach with the DDT-prediction approach, it was possible to predict explosion loads from DDT scenarios by a) simulating a deflagration with FLACS to predict initial flame propagation and time and location for DDT and store the temporary results at the moment of DDT, and b) restart the simulation from the moment of DDT using settings or detonation flames. In [33], this approach is used to simulate existing large-scale experiments with natural gas (BFETS Phase 3A Test 4) and propane (Buncefield Tree experiments Test 2), in both cases the simulations can reproduce experimental results quite well. It can be applied in a similar fashion to hydrogen explosions.

## 4.0 3D RISK ASSESSMENT

When carrying out risk assessment for e.g. a hydrogen refueling station, protection measures such as blast walls may be recommended to protect surrounding structures against the effect of a potential explosion on site. The risk is typically expressed in terms of exceedance curves and the design is based on an acceptance frequency, typically $10^{-4}$ or 1 every 10000 years.

The explosion loads, particularly for large targets such as blast walls, may vary spatially so providing a single value for the design load may be overly conservative. Large objects are typically represented by a discretised array of monitor panels within the CFD model, and by using Simulation Data Management (SDM) tools to automatically compile individual exceedance curves for each panel in the array and read off the explosion load corresponding to the allowable frequency of interest, it is possible to investigate the spatial variation of the explosion load corresponding to that frequency across the target.

This is demonstrated for a blast wall in Figure 6. In this case, the design explosion load (this is a natural gas explosion scenario, but it would similarly apply to a hydrogen explosion) from the exceedance curve on the left of the figure is 2 barg, but it is immediately obvious from the plot on the right of the figure that the 2 barg load is localised at the bottom right corner of the blast wall, which in this example was adjacent to a heavily congested module operating at high pressure. This insight can help the structural engineers to design a more effective blast wall.

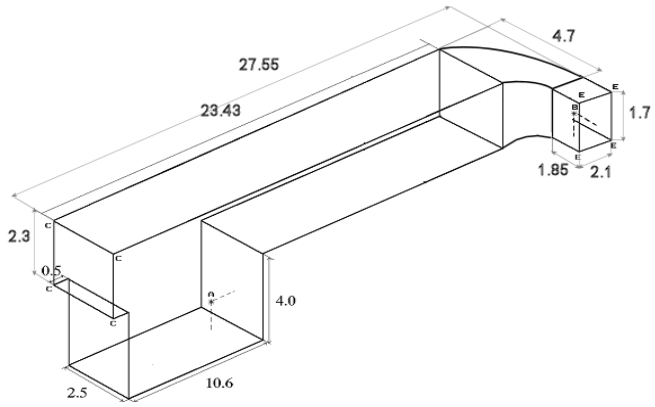


Figure 4. Schematic of the RUT facility.

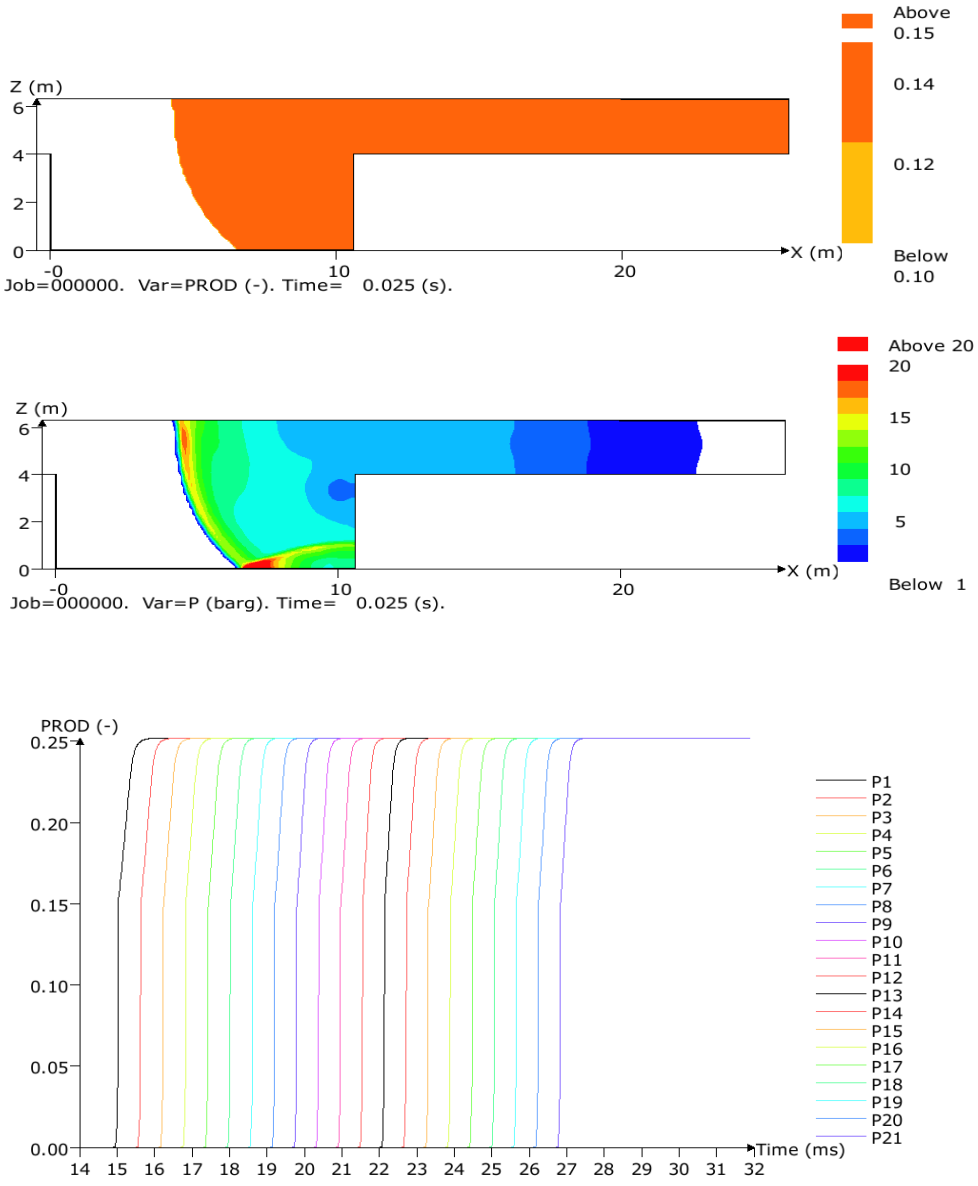


Figure 5. Flame front (top), pressure front (middle) and flame arrival times (bottom) for detonation simulations in the RUT facility.

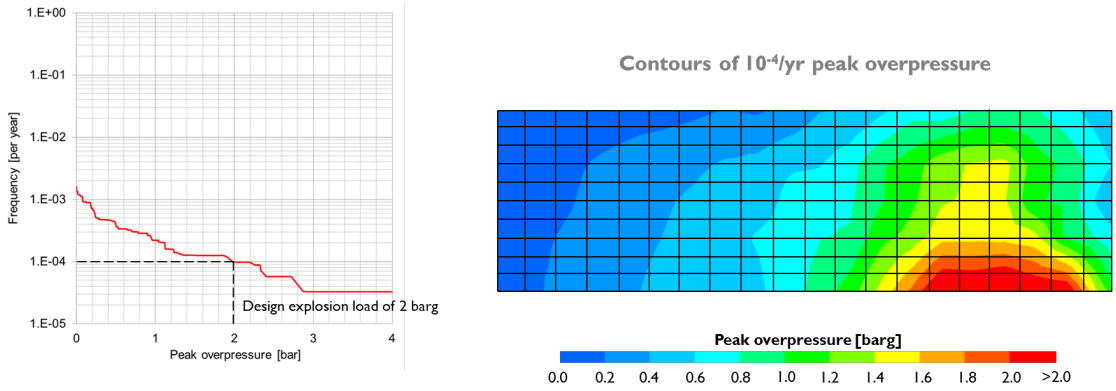


Figure 6. The spatial variation of the design explosion load may vary significantly across a large structure, such as a blast wall

When it comes to the structural design activities, it is typical to identify and/or construct representative blast events that can be used as the basis of the design. Rather than trying to identify representative explosion events from those within the simulated dataset, or constructing a representative pseudo-event by somehow combining multiple simulated events, another method is to directly simulate the response of the structure for each simulated explosion using non-linear finite element analysis (NLFEA), enabled through one-to-one coupling between the explosion CFD and structural FEA codes as part of an effective SDM tool.

The direct one-to-one coupling approach is attractive because it is a fundamental approach – it does not introduce any new assumptions. Whilst traditionally this may have been prohibitive in terms of computational effort, it is Abercus' assertion that with effective SDM tools and improving computing facilities, this approach is now feasible and could become more widespread. As part of our activities, Abercus has learned that the computational effort required for the NLFEA of selected structures can be comfortably undertaken alongside the rest of the probabilistic assessment (it is often the dispersion phase of the assessment which is the bottleneck), and that not all explosion events necessarily need to be simulated using NLFEA – by starting with the larger events and working towards smaller events, a point is reached where the frequency-based measures of interest (for example, damage or deflection) stop changing.

This approach is illustrated in Figure 7 below. It is clear is that the **traditional approach** with a uniformly applied $10^{-4}$/yr load is **overly conservative** when compared to the probabilistic structural response approach. More details of the approach can be found in [34].

## 5.0 FINAL REMARKS

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. With the advance in scientific computing, research on DDT has been shifted toward the use of computational approaches. Before the beginning of this work, the standard versions of FLACS could only handle the deflagration mode of combustion, in which the flame propagates because hot flame products heat and ignite the unburned gas ahead. In this work, the use of FLACS to simulate hydrogen explosions in different geometries and get indications about the likelihood of DDT is described. The study of this phenomenon is very critical as the overpressures in detonation front can cause losses which are much more severe as compared to those seen with blast waves produced by a deflagration. The likelihood of DDT is illustrated in terms of a parameter proportional to the spatial pressure gradient across the flame front. This parameter is able to visualize when the flame front captures

the pressure front, which is the case in situations when fast deflagrations transition to detonation. The methodology was then validated against available experimental data using several practical systems. In general, the modelling results are able to capture the experimental observations, including pressure traces and locations of DDT, reasonably well. The current model, when coupled with the additional features currently that have been proposed recently, can be used by the process industry to get a fair idea of the danger of DDT.

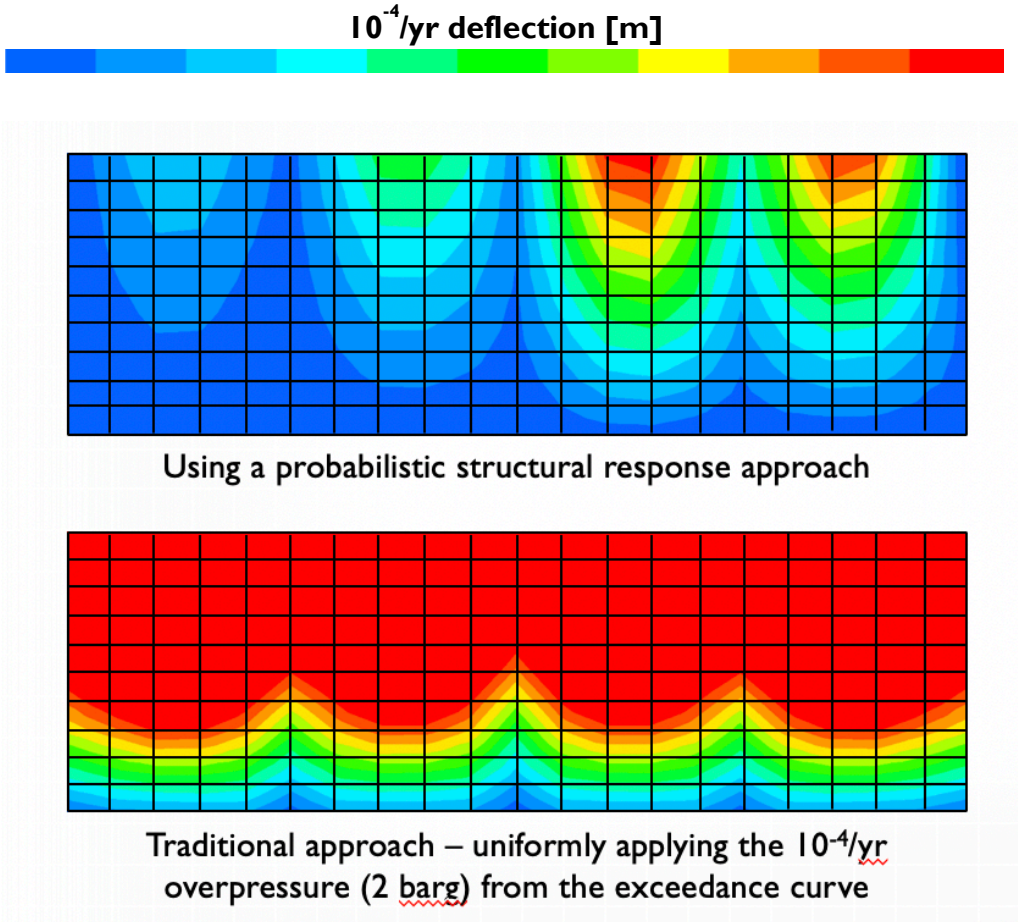


Figure 7. Comparision of the $10^{-4}$/year deflection of a blast wall using the traditional approach and the probabilistic structural response approach. Red represents high deflection and blue represents low deflection.

When carrying out risk assessment for e.g. a hydrogen refueling station, protection measures such as blast walls may be recommended to protect surrounding structures against the effect of a potential explosion on site. The explosion loads, particularly for large targets such as blast walls, may vary spatially so providing a single value for the design load may be overly conservative. Large objects are typically represented by a discretised array of monitor panels within the CFD model, and by using Simulation Data Management (SDM) tools to automatically compile individual exceedance curves for each panel in the array and read off the explosion load corresponding to the allowable frequency of interest, it is possible to investigate the spatial variation of the explosion load corresponding to that frequency across the target. The direct one-to-one coupling approach is attractive because it is a fundamental approach – it does not introduce any new assumptions. Whilst traditionally this may have been prohibitive in terms of computational effort, it is Abercus' assertion that with effective SDM tools and improving computing facilities, this approach is now feasible and could become more widespread. It is clear is that the **traditional approach** with a uniformly applied $10^{-4}$/year load is **overly conservative** when compared to the probabilistic structural response approach.

This can have wide-ranging implications on the design of things like protection walls against hydrogen explosions.

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