MARY KAY O'CONNOR PROCESS SAFETY CENTER
TEXAS A&M ENGINEERING EXPERIMENT STATION

19th Annual International Symposium
October 25-27, 2016 • College Station, Texas

Are We Missing any Detonations?

Author(s):

Max Kolbe, mkolbe@GenesisOilandGas.com [1]

Vinicius Simoes, vinicius.simoes@GenesisOilandGas.com [1]

[1]Genesis, 11750 Katy Freeway, Houston TX 77079

Keywords: Detonations, VCE, explosion modeling, explosion prediction

Abstract

The common rift between academia and industry has existed in all fields of engineering. However, ultimately the rift can be seen as more of a lag; it is not so much a question of "academia is not the real world" but rather "academia is research which ends up finding its way into the practical world of industry years if not decades later". On the topic of detonations or vapor cloud explosions (VCE), this is indeed a true statement. A little more than a decade ago the common belief in the chemical process industry was that detonations were not really possible unless you had some very reactive process materials such as hydrogen or acetylene. When some industry and consulting experts began to challenge this view they soon found out that a more common and less reactive process material such as ethylene could in fact be made to detonate as well. The key was that the environment had to be just right in order for an ignited flame to accelerate and transition to a detonation. In fact, academia had known this since the early 1960s and so the question remains, what else can we learn?

Industry has retuned itself and made use of a several common explosion modeling tools which for some can be made to predict detonations. In others, they must be inferred and only very knowledgeable users can determine detonations. This paper will review the basics of detonations, the academic perspective and the industrial applications. Additionally several of the various and commonly used models for explosion prediction will be reviewed.

Explosions, background

As is well known, there are two distinct paths for a combustion process to undertake. The first path is the most common one known as a deflagration; where the combustion occurs via heat conductivity and diffusion within the flame front. An acoustic wave travels ahead of the flame and generates a turbulent field ahead of the flame. If the system is in motion (traveling flame front) then the acoustic wave is traveling through an unburned mixture of fuel-air and the mixing process prior to combustion is enhanced via turbulence. The flame front in this system sees all the action since the rate of combustion is determined by the surface area of the flame front; therefore the more surface area or wrinkling of the flame front, the higher the rate of combustion and therefore speed of the flame. Naturally the acoustic wave provides this well mixed fuel-air as well as turbulent flows where the flame speed will benefit by enhancing its surface area. As can be guessed, provided that there is fuel-air and turbulence, this process will continue to rapidly accelerate; the flame will go faster and faster and push the acoustic wave ahead of it harder and harder. These are the basics as described in the turbulent flame propagation models and instabilities (Markstein, 1955), (Kelvin, 1871) (von Helmholtz, 1868).

The second mechanism of combustion is known as a detonation. During this mechanism heat and pressure are applied to the unburned mixture through a shock wave that has been created, ignition of the flame is now occurring through auto ignition via this heating and compressing mechanism. Effectively the flame and shock are somewhat coupled and travel at supersonic speeds unlike the deflagrations which travel at subsonic speeds but still occur at high speed relative to our perception. This is the basis from the well-known ZND model for detonation process of an explosion (Zel'dovich, 1940), (von Neumann, 1942), (Doring, 1943).

Originally, the study of detonations took place in laboratory sized tubes and vessels. Therefore, these were fully closed systems where venting was not permitted. These “detonation tubes” began to study flame acceleration first in smooth tubes, then in obstacle laden tubes (typically in the form of orifice plates). These initial detonation studies took place in the mid to late 1900s where parameters such as Chapman-Jouguet (CJ) Velocity, Critical Tube Diameter (d_c), Cell Size (λ) and Critical Energy (E_c) were all being categorized (Chapman, 1899), (Jouguet, 1905). Indeed these defined and descriptive detonation characteristics are unique to all gaseous explosive mixtures (Teodorczyk, 2006). These parameters, although important in detonation physics, will not be discussed further in this paper but can be found in a number of readily available databases (Shepherd, 2005).

Within smooth tubes, it was found that once a fuel air mixture was ignited, there was a continuous flame acceleration until detonation was abruptly achieved. This deflagration to detonation transition is also commonly referred to as DDT (Teodorczyk, 2006). In obstacle laden or “rough” tubes several regimes of steady flame propagation can be observed. Another parameter that was observed was the distance from ignition to this DDT point, this distance was to be known as the “run-up length”, although it is very difficult to in fact quantify as it is dependent on the physical environment surrounding the flame acceleration and this will be discussed further on as it becomes an important defining point between methods used to predict explosion strength and detonations.

With regards to the physical surroundings, in the field of detonations and deflagrations, there are two types of environments; confined and unconfined. In the confined events, there are several phenomena that occur and greatly enhance the deflagration and detonation processes. One of these phenomena is called venting; if venting is allowed to occur, the combustion processes are weakened and thus over pressure build-up is not so easily achieved. For example, a simple vessel of given volume filled with a flammable mixture and completely smooth inside is capable of generating over pressures of 7-10 times the initial pressure (Benoit, 1965), (McAllister, 2011). This is due to several reasons such as turbulence inducing acoustic wave reverberations and continuous compression and heating of the unburned mixture occurring from the burned products. In the case of long tubes, detonations are achieved and allowed to form simply due to the length and accelerating process or (in the case of rough tubes) through the addition of turbulence. Regardless of the type of confinement, all of these detonation parameters have been studied and predicted from nearly all flammable gases and gas mixtures that are in use for industry and recorded.

Unconfined explosions are those that occur in the open and do not have the benefit of these turbulence inducing reverberations or heating and compressing caused by the burned combustion products. These explosions require more turbulence in the surroundings in order to propagate so that the unburned fuel is well mixed with the surrounding air. Therefore with respect to over pressure generation, unconfined fuel air explosions are far weaker and require much greater volumes to generate significant overpressures than in confined cases; however with respect to equipment and structural damage, very little overpressure is in fact required in order to achieve appreciative levels of destruction. What is important however, is that if the material released in air is a flammable one, and if it is released in a confined or unconfined environment and ignited, then given enough turbulence it will progress into an explosion and depending on the release size or turbulence generated it can achieve a detonation state.

Turbulence, where does it come from?

The best known mechanism for uniformly mixing gases or liquids is through turbulent mixing. The advent of better performance internal combustion engines was in fact from the efficient mixing of fuel and air (carburetors, fuel injectors, compressors and other devices). Therefore when a fuel is released from its storage vessel or process piping into the atmosphere it begins as a homogenous fuel mixture and gradually mixes with air. If the release occurs in the open without any physical obstruction the mixing will be dependent on the hydrodynamic properties or release parameters of the jet release (pressure, temperature, orifice size etc,). From the images in **Error! Reference source not found.**, the turbulence effect can be seen **Error! Reference source not found.**by the generation of vortices, beginning moderately on the left and far more intense on the right most image (Bulat, 2016). In this case, as back pressure was increased, the vortices production increased and so does the mixing of the flow with ambient air.

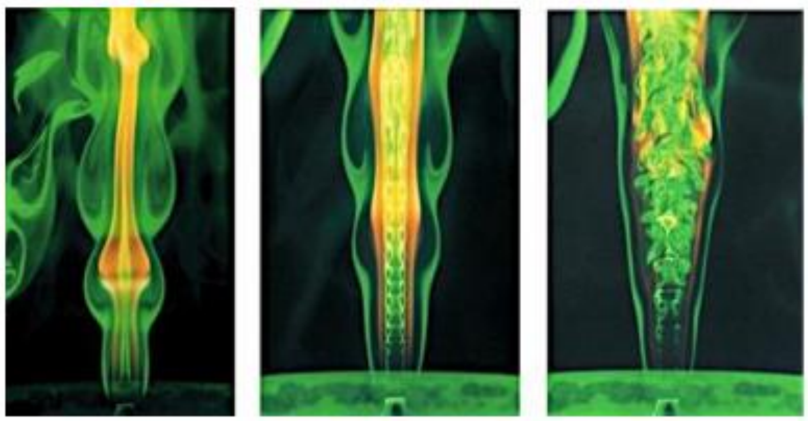

Figure 1. Laminar, Transient and Turbulent Regimes of Fluid Flow – Courtesy Bulat 2016

As the release parameters are varied, the turbulent mixing is either enhanced or diminished and in an open environment these (and the weather stability) are the only contributing factors to promote mixing of two fluids (in the case of a hydrocarbon release, fuel and the ambient air). A practical example of this can be the release of a gas or from a wellhead or pipeline in an open field (see Figure 2).

Figure 2. Anhydrous Ammonia Pipeline Release-National Transportation Safety Board

However when a release occurs in an area containing physical obstructions (process piping, equipment, buildings, cars or even vegetation such as brushes or trees) the turbulent mixing is greatly enhanced as the release flows wrap and flow over a number of physical objects causing vortices of all sizes and therefore mixing with the ambient air far better. In Figure 3, we see how the flows over obstacles can cause extensive vortices and eddy production, each allowing for the enhanced mixing of two fluids. Naturally, the smaller the obstacles the smaller the produced vortices therefore if the field contains a few larges obstacles the turbulence produced will be less than if the field contained many small obstacles. So if we were to imagine a very densely packed process unit such as the one in Figure 4) we can see that a gas flowing through it would generate a significant amount of turbulence.

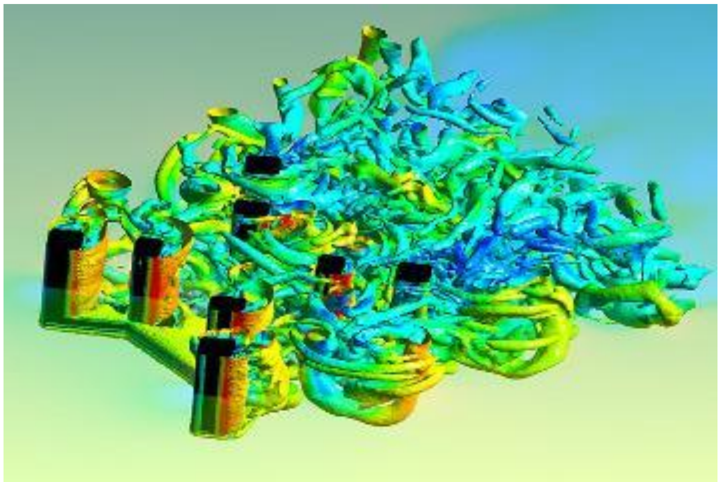

Figure 3. CFD Simulation of flows over obstacles - Courtesy Los Alamos National Laboratories

Figure 4. Bank of heat exchangers in refinery – Courtesy The Process Technology and Operator Academy

Blast Prediction Methodologies

One point that requires extensive highlighting is that in order to predict detonations it is important to have a deep understanding of their inner workings and the same can be said of all the models available in industry that are used to predict blast strength. The old adage, of “garbage in garbage out” is clearly valid and in this case and however not correctly predicting blast over pressures can have disastrous consequences. Other than their physical-chemical differences, deflagrations and detonations have differences that are very important for the design of process plant buildings. To begin with, there are two parameters that are of importance when considering blast design; overpressure and impulse (related to the duration of the explosion event). Although this paper will not discuss the implications of these parameters on buildings it is important to note that when designing for blast resistance the over pressure and the under pressure (expansion phase) are both important since structural elements that resist in compression do not always resist in tension. And the impulse or duration of the event is of equal importance to over pressure since a low pressure blast event that is applied for a long period of time can cause more damage than a high pressure event that is of very short duration.

Deflagrations or subsonic explosions typically yield over pressures of 13-15 psig or less whereas detonations yield over pressures of 15 psig or more. The bulk of explosions are known as weak deflagrations and typically yield over pressures of about 5-7 psig, strong deflagrations between 7-15psig and are less common. Detonations in the process industry do not appear to be very common however further assessment of past events have lately yielded a better view on this and we will discuss this later on in the paper.

There are essentially two approaches of blast modeling, one is known as the Computational Fluid Dynamic (CFD) method and the other is using blast severity curves and calculated using a one dimensional hydrodynamic code and Sach’s scaling law. Both approaches have several methods and tools but all of them have been developed using field tests of various sizes. The parameters of importance to all of them are the obstacle or congestion density, the confinement and the fuel reactivity.

Originally, blast curves were calculated using the TNT equivalency method where a given mass of hydrocarbon is equated to an equivalent yield of TNT then an over pressure was calculated. This method is not appropriate for the process industry unless a solid explosive is involved and the reason is that TNT will detonate 99% of the time (because it is designed to do so) and thus will be a high over pressure and short duration. Hydrocarbons are not designed to detonate since they have other applications and therefore work as to be done to them in order for them to achieve detonation state. Calculating vapor cloud explosions (VCE) via this method is nearly always misleading, as the calculations are normally overly conservative in the near field and lose this conservatism in the farfield.

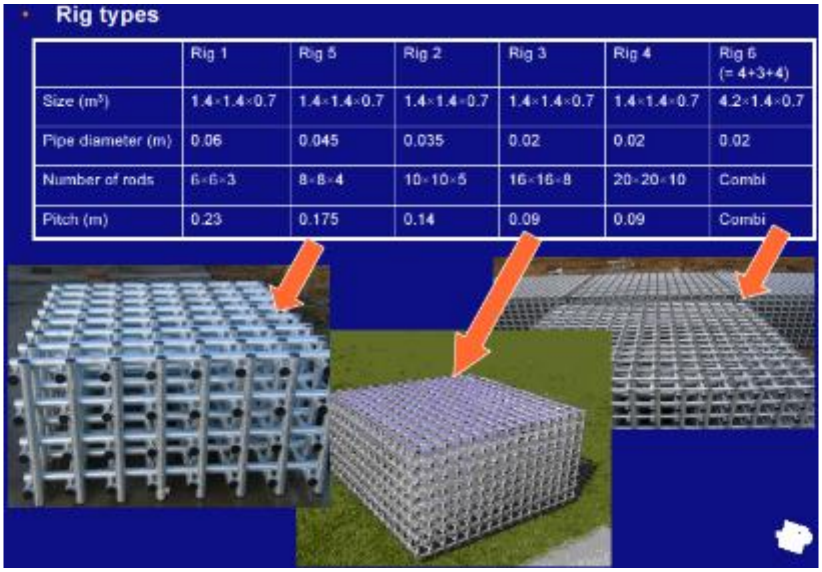

Figure 5. Test Rigs used in the Development of the TNO Multi Energy Method – Courtesy TNO

TNO Methodology

After some time, it was realized that a better approach would be needed in order to account for the conservativeness. The Multi Energy Method (MEM or TNO) developed from field tests using rigs of various sizes filled with a flammable mixture and then ignited ; pressure gauges placed in various positions of the test field recorded over pressures and this data was tabulated against various fuels and flammable volumes and congestion (obstacle) configuration (TNO, 1996). The TNO method eventually developed in a series of blast severity curves (1-10 with increasing severity) which associated the predicted blast with the obstacle complexity of a given process plant environment (Figure 7). Depending on what fuel would be possibly released in the area also determined the blast severity curve or TNO rating, so for example portions of an LNG facility, although they may have the same congestion level as a Gas Fractionation plant, may not have the same TNO rating given that the hydrocarbons that could be accidentally released in each plant are not of the same reactivity. In other words the potential to detonate is not uniquely determined by the fuel released and as a result there is no real way of restricting a detonation to occur.

Figure 6. BakerRisk Vapor Cloud Explosion Test Rig – Courtesy BakerRisk

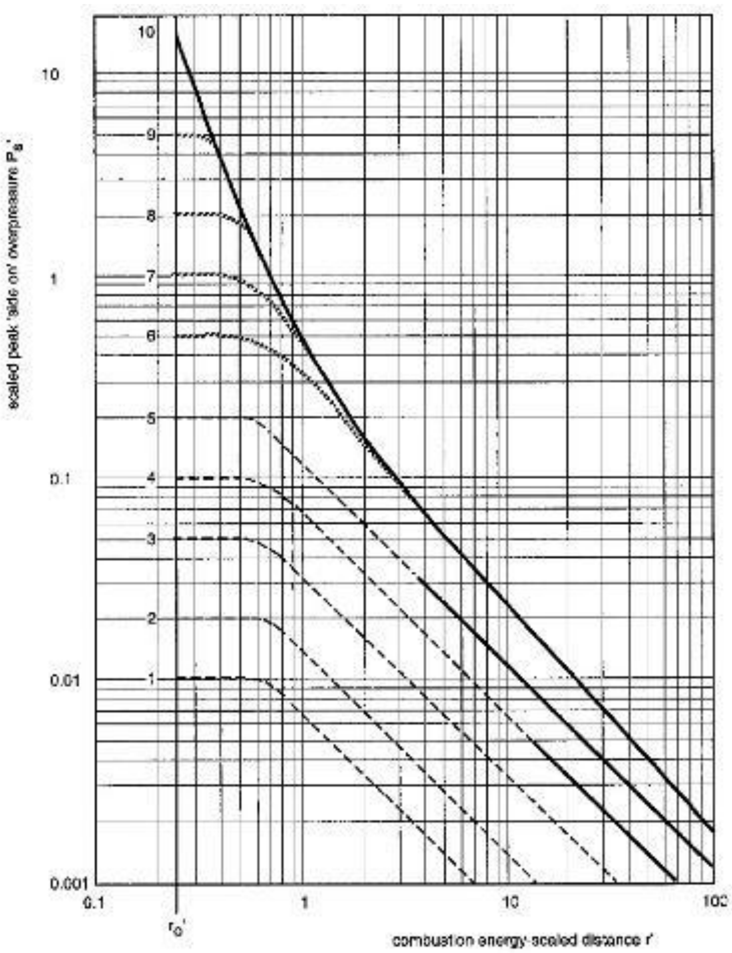

Figure 7. Blast Severity Curves - TNO

BST Methodology

The other more common blast prediction method is known as the BST method. Also developed through the use of blast curves, the BST method uses flame speeds and not severity levels to determine blast strength and has also been generated by a series of field tests (Figure 6) with given congestions and volumes and fuel variations (Pierorazio, J., 2004). In the BST methodology however a given volume is determined as having a certain level of congestion and confinement and then depending on what type of fuel is ignited in it, it would yield a blast strength. Essentially the BST uses a Flame Speed table from which the calculations are carried out in order to determine a flame speed and then from there obtain over pressures from the blast curves. However observing the flame speed table closely one can see that only high reactivity fuels are allowed to detonate in the BST methodology (Table 1). In the table below, Confinement represents the confining planes (walls or decks), the Congestion is the obstacle density (based on volume blockage ratio) and the Reactivity is based on the fuel's laminar burning velocity or burning rate. DDT signals that the data in the field tests (or derived data) has achieved a detonation.

Table 1. Flame Speeds in Mach Number (BST), where the values represent Mach speeds of the flame front.

Confinement	Reactivity	Congestion Low	Congestion Medium	Congestion High
2-D	**High**	0.59	DDT	DDT
	Medium	**0.47**	0.66	**1.6**
	Low	0.079	0.47	0.66
2.5-D	**High**	**0.47**	**DDT**	**DDT**
	Medium	**0.29**	**0.55**	**1.0**
	Low	0.053	**0.35**	**0.50**
3-D	**High**	**0.36**	**DDT**	**DDT**
	Medium	**0.11**	**0.44**	**0.50**
	Low	0.026	**0.23**	**0.34**

Despite the many updated and leading edge test programs, the BST method is confined by the most fundamental parameter of laminar burning velocity (LBV) which defines the fuel reactivity. In the BST method, low reactivity represents fuels that have an LBV of 30 cm/s or less (Methane, Ammonia, Methanol etc) , medium reactivity is for fuels with an LBV of 30-75 cm/s and high reactivity is reserved for fuels having an LBV of 75cm/s or more. These high reactivity fuels consist of Hydrogen, Acetylene, Ethylene and of course many hydrocarbon-oxide combinations that yield an LBV of 75 cm/s or greater.

Either method above will yield over pressure contours overlaid on a facility plot plan and provide pressure and impulse data from which to assess process buildings and equipment as seen in Figure 8.

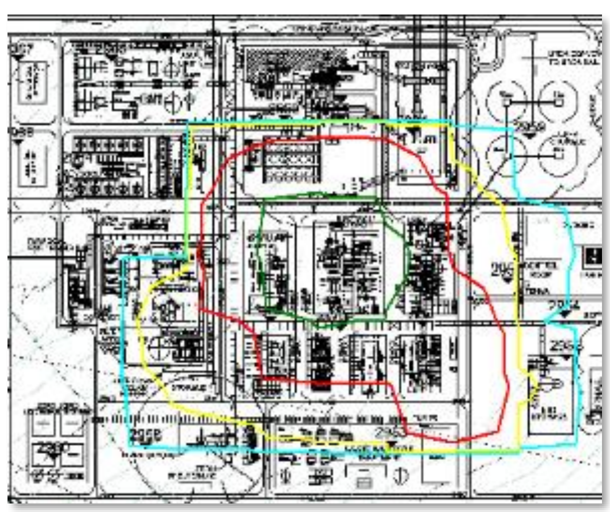

Figure 8. Over pressure contours from typical TNO or BST methods.- Courtesy Genesis

CFD Modeling

In CFD modeling, there are two well-known types of methods, one employs a turbulence model and the other utilizes the reaction kinetics. The main point here is that the dispersions and explosion pressure waves interact with physical geometries to provide a dynamic modeling of blast waves with wrapping and turbulence effects from both the dispersion and the blast wave accounted for.

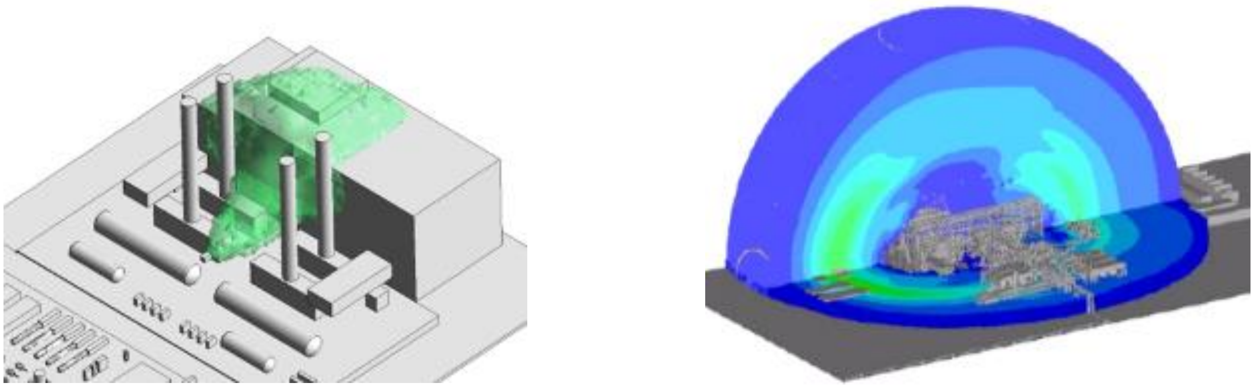

Figure 9. Dispersion and Blast Wave Simulations using CFD codes – Courtesy Genesis

As can be seen in Figure 9. CFD modeling is more realistic and allows for more accuracy in determining the blast loads on equipment and buildings. However there is a drawback in CFD modeling, essentially the modeling is accurate in determining nearfield over pressures and determining the blast loads of targets within the flammable cloud however in the far field the predictions are not as accurate as the TNO and BST models. Additionally, the CFD codes have a difficult time predicting detonation, although they do indirectly allow for the onset of detonation as can be observed in the pressure rise rates. From here a proper blast effects analyst can determine if the explosion is in fact transitioning to a detonation or not (DDT).

Appropriate Application of Methodologies and Case Studies

The application of appropriate methodology is important for a variety of reasons. Traditionally, CFD modeling has taken significant computing power requiring multiple machines running codes for weeks. Now with the advent of more powerful computers CFD studies are becoming more prominent. In the case of offshore facilities, the density and compact nature of the facility makes it so that any accidental release of hydrocarbon will almost always engulf living quarters or some building requiring blast analysis and design. As a result, the CFD models are more accurate in determining these blast loads where the explosion surrounds the buildings to be assessed.

With respect to onshore facilities, there is far more space between units and buildings and distance is available. So the far field blast load calculations are more reliable coming from the TNO and BST type methods. Additionally, the processes involved on onshore facilities are often more complex and larger than those occurring on offshore facilities and involved more complex chemicals. Therefore, when carrying out risk assessments it is more convenient to run thousands of calculations on flammable, toxic and blast scenarios not through CFD as they would take several months to complete.

However, lately there have been some cases where there has been debate on what in fact has occurred on process plant accidents and whether the explosions were detonations or strong deflagrations (Mannan, 2009). Much of this debate is stemmed from not fully understanding both the damage indications as well as the explosion physics involved. For example, the Buncefield Tank farm explosion is one such case. Here the damage indicators were confusing since there were some indications that showed simple glass breakage and moderate structural deformations and yet other locations not far from there indicated extreme high pressures (parked car damage). The initial thoughts were that it was simply a large cloud explosion with significant impulse, however after some analysis of damage indication it was determined that there could have been pockets of detonations (UK, 2009).

Figure 10. Vehicle damage and vegetation proximity at the Buncefield site – Courtesy HSE UK Report

The common misconception is that detonation must yield tremendous damage indicators due to the high pressures generated. However not all of a flammable cloud will detonate, even in experimental settings, unless the flammable volume is directly initiated (Alekseev, 1996) there will be portions of the cloud that do not contribute to a detonation. Additionally, detonations can fail once established either due to fuel-air fluctuations or some physical environments that promote quenching (Zakaznov, 1967).

Another such case was the Flixborough incident in 1974 where an accidental release of about 30 tons of Cyclohexane was released from a process unit in the UK. Recent analyses of both the review of damage indication and CFD modeling show that the over pressures generated on the scene were of detonation scale (Hoiset, 2000).

For both examples, the use of CFD was pivotal in determining the effect of congestion on the flame acceleration however several modeling trials and careful examination of damage structural indicators had to be carried out. With respect to more simplistic methodologies such as TNO and BST the issue is not so simple. In the case of the TNO method, the modeling would have to have been done in such a way that all severity points were accounted for; meaning that process equipment and other turbulence generating features were accounted for such as the dense vegetation (trees and brushes) and confining channels between tanks and sleeper racks (in the Buncefield case). In the BST method taking into account the extra congestion would still not have yielded the correct answer since the fuels that were released in both Buncefield and Flixborough were of medium reactivity category (LBVs between 30-75 cm/s) (Frassoldati, 2010).

Conclusion

The research community for detonation physics has for nearly a century been investigating the phenomenon of detonations. To date, there have been many advances in understanding the structure and behavior of these severe blast waves allowing us to better understand past incidents and correctly label detonations where they have occurred and were perhaps over looked. Statistics of course is based on data of what was determined at the time. So in fact there may be more detonations that have occurred in the history of process plant operations but were overlooked or incorrectly labeled. Nowadays with better software and methodologies and more power computers we are able to review past incidents and update our current methods in order to better predict the occurrence of detonations.

The academic database from over 50 years of experimentation suggests that detonations are possible for nearly every flammable gas that the process industry is currently using given certain physical or thermodynamic boundary conditions. Therefore it is to our benefit to conduct facility blast assessments with methods and tools that in fact utilize as much of the research data that has been gathered on detonations and apply them to industrial facilities for incident mitigation and protection.

References

Alekseev, V. D. S. S. V., 1996. *Direct Initiation of Detonations in Unconfined Gasoline Sprays.* s.l., Springer Verlag.

Benoit, A. G. J., 1965. Thermodynamic and Composition Data for Constant Volume of Stoiciometric Mixtures of Hydrogen-Oxygen Diluted with Helium or Hydrogen.

Bulat, P. V. K. N., 2016. The History of the Study of Detonation. *International Journal of Environmental Science Eduction.*

Chapman, D., 1899. On the Rate of Explosion in Gases. *Philosophical Magazine*.

Doring, W., 1943. Detonation Processes in Gases. *Annalen de Physik.*

Frassoldati, A. G. R. C. A. F. T. R. E., 2010. *A Wide Range of Kinetic Modelling Study of Laminar Flame Speeds of Reference Fuels and their Mixtures.* s.l., s.n.

Hoiset, S. H. B. S. T. M. K., 2000. Flixborough Revisited - An Explosion Simulation Approach. *Journal of Hazardous Materials.*

Jouguet, E., 1905. On the Propagation of Chemical Reactions in Gases. *Journal of Pure and Applied Mathematics*.

Kelvin, W., 1871. Hydrokinetic SOlutions and Observations. *Philosophical Magazine*.

Mannan, S. M., 2009. *A Technical Analysis of the Buncefield Explosion and Fire.* s.l., IChemE.

Markstein, G. S. W., 1955. On the Stability of a Plane Flame Front in Oscillating Flow. *Journal of American Acoustic Society.*

McAllister, S. C. J. F. A., 2011. *Fundamentals of Combustion Processes.* s.l.:Springer.

Pierorazio, J., 2004. *An Update to the Baker-Strehlow-Tang Vapor Cloud Explosion Prediction Methodology Flame Speed Table.* s.l., s.n.

Shepherd, J., 2005. *Detonation Database.* [Online]
Available at: www.shepherd.caltech.edu/detn_db/html/db.html

Teodorczyk, A., 2006. *Fast Deflagrations, Deflagration to Detonation Transition and Direct Detonation Initiation in Hydrogen-Air Mixtures,* s.l.: University of Warsaw.

TNO, 1996. *Methods for the Calculation of Physical Effects.* s.l.:s.n.

UK, H., 2009. *Buncefield Explosion Mechanism Phase 1,* s.l.: s.n.

von Helmholtz, H., 1868. *On the Discontinuous Movements of Fluids,* s.l.: Monthly Reports of the Royal Prussion Academy of Philosophy in Berlin.

von Neumann, J., 1942. Theory of Detonation Waves. *Progress Report to the National Defense Research Committee Div. B.*

Zakaznov, V. R. A. S. I., 1967. Quenching of Detonation and Some Characteristics of its Propagation in Narrow Channels. *Combustion, Explosion and Shock Waves.*

Zel'dovich, Y., 1940. On the Theory of the Propagation of Detonations on Gaseous System. *Eksp. Teor. Fiz.*