Detonations in pipes and in the open

Kees van Wingerden
Dag Bjerketvedt[1]
and Jan Roar Bakke[2]
Christian Michelsen Research
Bergen, Norway

INTRODUCTION

A detonation is the most devastating form of gas explosion. Unlike the deflagration, a detonation does not require confinement or obstructions in order to propagate at high velocity. Particularly in an unconfined situation, the behaviour of a detonation is quite different from a deflagration. A detonation is defined as a supersonic combustion wave (i.e. the detonation front propagates into unburned gas at a velocity higher than the speed of sound in front of the wave). The gas ahead of a detonation is therefore undisturbed by the detonation wave. In fuel-air mixtures at atmospheric pressure, the detonation velocity is typically 1500 – 2000 m/s and the peak pressure is 15-20 bar.

Transition to detonation, propagation and transmission of detonation waves, depend strongly on the reactivity of the gas cloud as well as on the geometry/environment in which the gas cloud is located. There are two extremes regarding the geometry/environment: a gas cloud inside a pipe and a gas cloud in the open.

In this paper several aspects of detonations will be discussed with an emphasis on the environment in which the detonation takes place.

DETONATION WAVES

Detonation waves were observed experimentally more than 100 years ago. Chapman and Jouguet were the first to present a theory describing this supersonic combustion wave, propagating at a unique velocity. The C-J (Chapman-Jouguet) theory (Fickett and Davis, 1979) treats the detonation wave as a discontinuity with infinite reaction rate. The conservation equations for mass, momentum and energy across the one-dimensional wave gives a unique solution for the detonation velocity (CJ-velocity) and the state of combustion products immediately behind the detonation wave. Based on the CJ-theory it is possible to calculate detonation velocity, detonation pressure etc. if the gas mixture is known. The CJ-theory does not require any information about the chemical reaction rate (i.e. chemical kinetics).

---

[1] Telemark Høgskole, Porsgrunn, Norway
[2] GexCon, Bergen, Norway

Table 1. CJ-pressure and CJ-detonation velocity for some fuel-air mixtures. Initial conditions 25°C and 1.013 bar (Baker et al. 1983).

	Hydrogen	Ethylene	Propane	Methane
CJ-Pressure (bar)	15.8	18.6	18.6	17.4
CJ-Velocity (m/s)	1968	1822	1804	1802

During World War II, Zeldovich, Döring and von Neumann improved the CJ-model by taking the reaction rate into account. As shown in Figure 2 the ZND-model describes the detonation wave as a shock wave, immediately followed by a reaction zone (i.e. flame). The thickness of this zone is given by the reaction rate.
The ZND-theory gives the same detonation velocities and pressures as the CJ-theory, the only difference between the two models is the thickness of the wave.

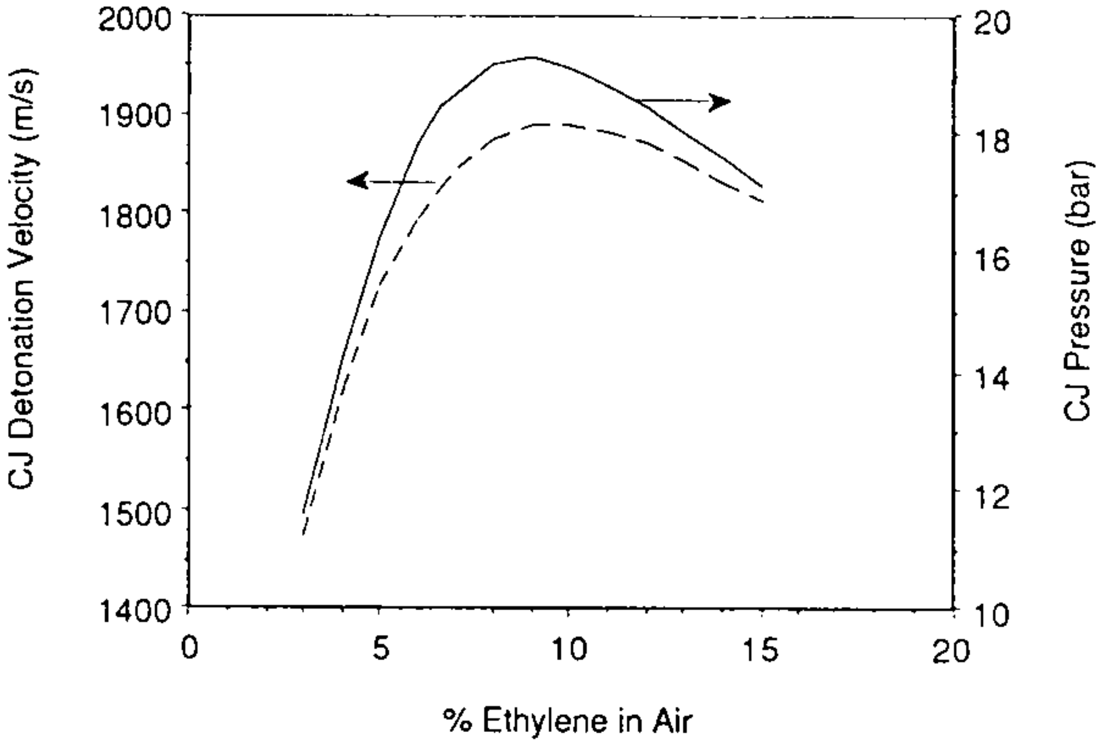
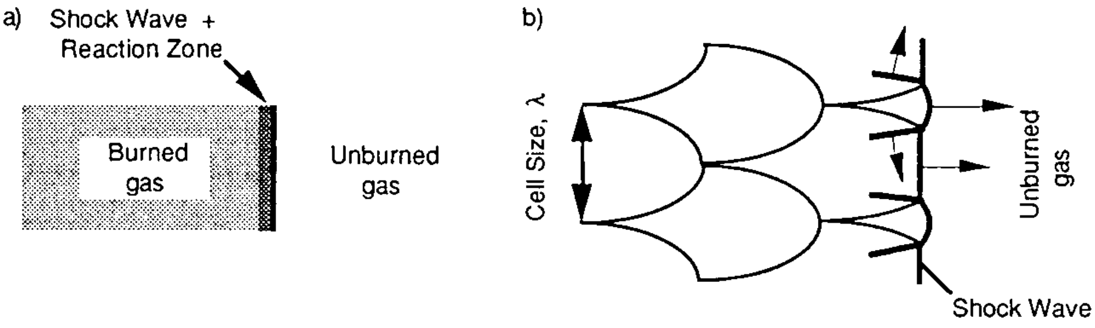


Figure 1 CJ detonation velocity and pressure for ethylene-air.

An actual detonation is a three-dimensional shock wave followed by a reaction zone. The leading shock consists of curved shock segments. At the detachment lines between these shock segments, the shock wave interacts in a Mach stem configuration. A two-dimensional illustration of the actual structure is given in Figure 2.

The size of the fish shell pattern generated by the triple point (Mach stem) of the shock wave is a measure of the reactivity of the mixture representing a length scale characterising the overall chemical reaction in the wave (Lee, 1984). This length scale, λ, is often the cell size or the cell width. The more reactive the mixture, the smaller the cell size. Figures 3 and 4 show the detonation cell size versus fuel concentration for several fuel-air mixtures.



ZND theory

Pattern of an Actual Structure

Figure 2 ZND structure and pattern of an actual structure of a detonation front. The characteristic length scale of the cell pattern, the cell size, l, is shown in the figure.

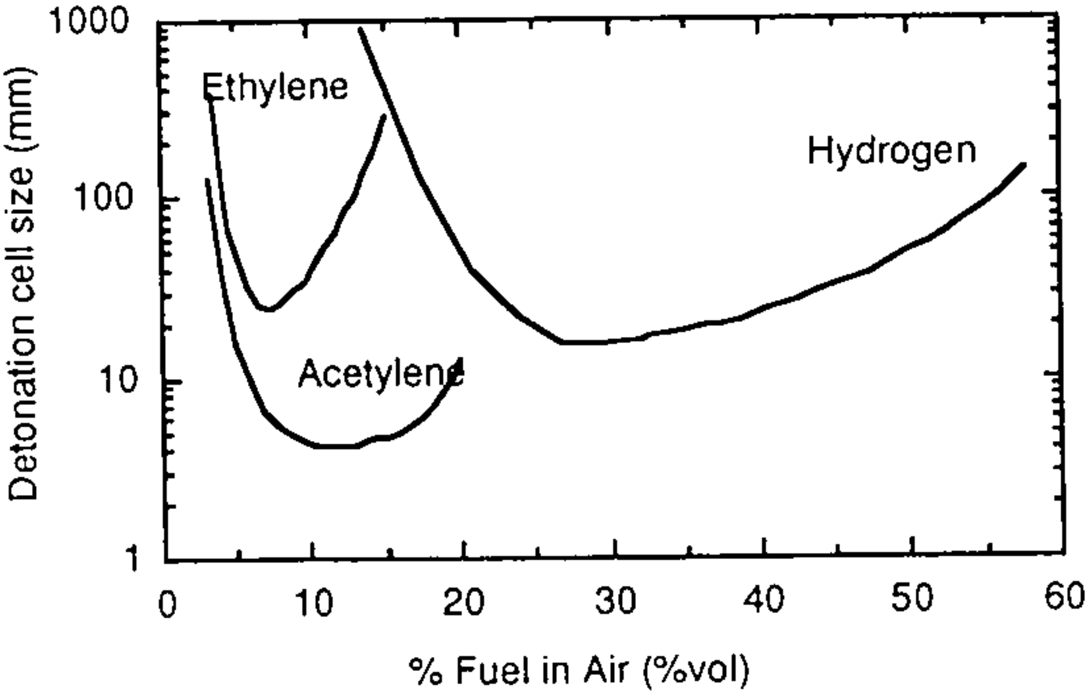


Figure 3 Cell size vs. fuel concentration for acetylene, ethylene and hydrogen in air (25°C and 1 atm) (Shepherd et al., 1991).

The cell size is measured experimentally and there are some variations in the reported results. Variations of a factor of two are not uncommon.

The cell size, λ, is a parameter which is of practical importance. The transition from deflagration to detonation, propagation and transmission to detonation can to some extent be evaluated based on the knowledge of the cell size of the mixture. This will be discussed in the following sections.

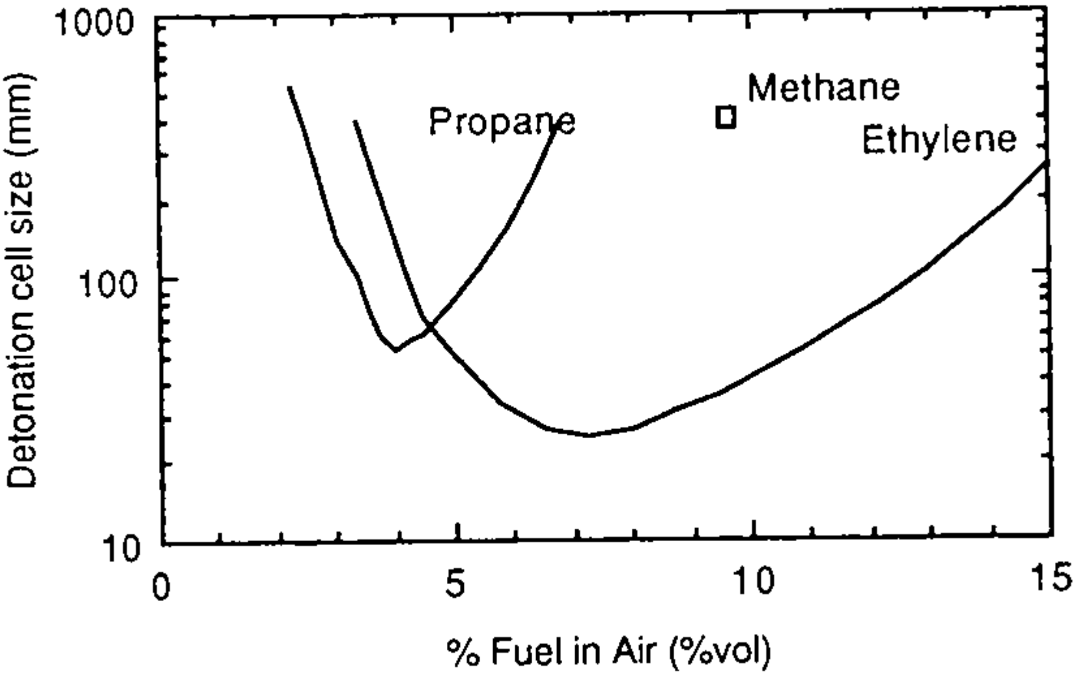


Figure 4 Cell size vs. fuel concentration for ethylene, propane and methane in air (25°C and 1 atm) (Shepherd et al., 1991).

DEFLAGRATION TO DETONATION TRANSITION (DDT)

When a deflagration becomes sufficiently strong, a sudden transition from deflagration to detonation can occur.
This has been observed in several experiments, especially in those involving very reactive mixtures, such as acetylene-air, hydrogen-air or fuels with oxygen-enriched atmospheres.

In addition to closed vessels, pipes (including channels and tunnels) are also typical simple geometries where internal explosions can occur. In pipes, the pressure generated by the flame has the possibility to propagate away from the combustion front. For long pipes or open-ended pipes, a high flame speed is required to generate high explosion pressure. The main mechanism causing the flame to accelerate in pipes, is turbulence. When the gas burns, it expands and pushes unburned gas ahead of the flame front. The flow ahead of the flame will cause a turbulent boundary layer to grow and the turbulence will enhance the burning rate. This is illustrated in Figure 5.

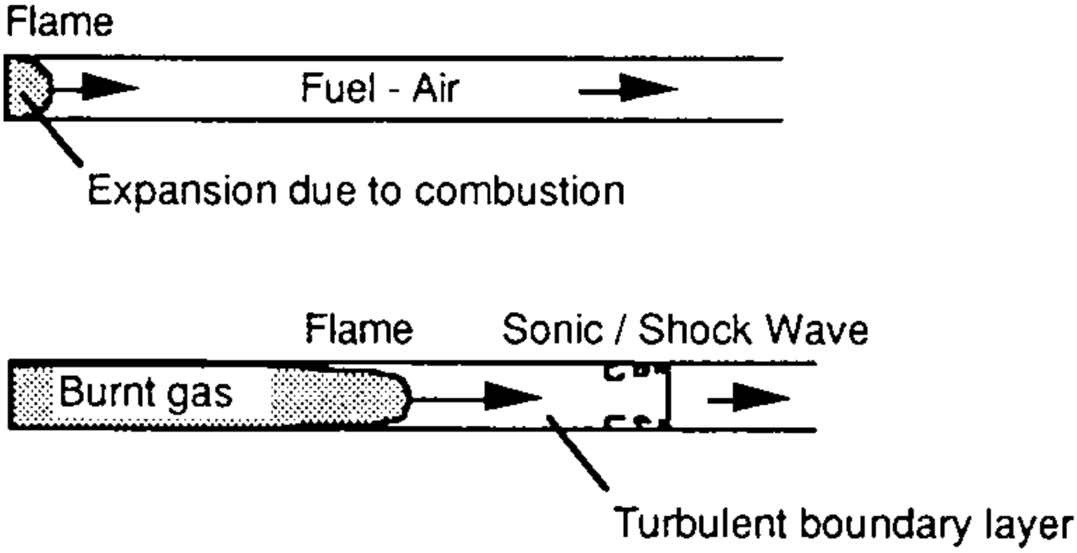


Figure 5 Flame acceleration in a pipe.

Bartknecht (1971) has measured flame velocities in a 1.4 m diameter pipe with methane-air at 1 atm. The pipe was 40 m long and the end was either closed or open. The results are shown in Figure 6. The highest flame speed was observed when the gas was ignited in the closed end and the other end was open. In that case the gas ahead of the flame was pushed through the pipe and a lot of turbulence was generated. When the pipe was closed in both ends, the flame accelerated fast in the beginning, but after 15-20 m the flame started to decelerate, because the closed end obstructs the flow ahead of the flame. Since the pipe is closed in both ends, the pressure will increase like in a closed vessel. In the third case the ignition is at the open end and the other end is closed. Here, the flow velocity and the turbulence level ahead of the flame are very low and the flame propagates at low velocities through the pipe. These experiments show the importance of boundary conditions for the flame acceleration in a pipe. The boundary conditions in a pipe will be similar to ignition at the closed end of a pipe if the gas cloud is ignited in the

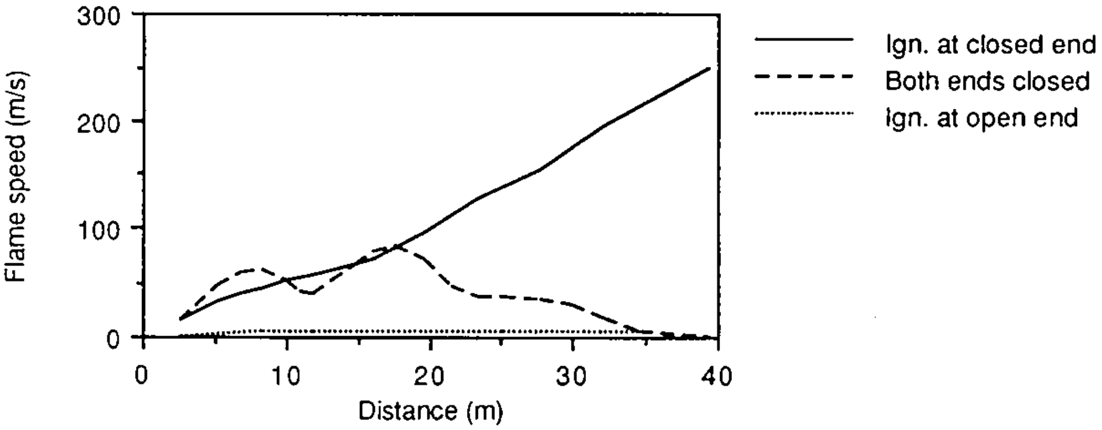


Figure 6 Flame speed in a 1.4 m diameter pipe with methane-air. (Bartknecht 1971)

centre of the cloud. In that case the flame will propagate in both directions and there will be zero flow velocity where the ignition took place (i.e. symmetry plane).
In a pipe the flame can continue to accelerate until it becomes a detonation (a supersonic combustion wave propagating at 1500-2000 m/s in fuel-air). We have only a qualitative understanding of the mechanism of transition from deflagration to detonation. We are therefore not capable of predicting this phenomenon. Experimental data is all that is available. The transition phenomenon is characterised by very high local pressures, pressures of 50 times the initial pressure have been measured when transition to detonation has occurred. In accidental situations, very strong damage can be observed at the location of transition to detonation. A case history from a gas explosion in a pipe is illustrated in Figure 7. At one particular location the pipe was expanded radially. That was the place where the transition to detonation took place. When the detonation propagated further down it stabilised at a so-called CJ-condition, which gives lower pressure. In the case history, the pipe did not rupture. If the pipe had ruptured, a high-pressure reservoir would have been released. This shows that transition to detonation in pipes, channels and tunnels is a hazardous phenomenon, which should be recognised as being possible.

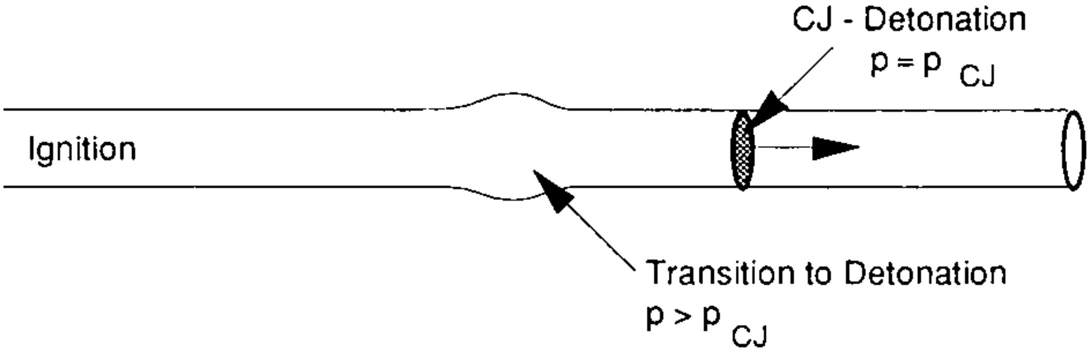


Figure 7 A case history. Deformation of a pipe by a transition to detonation.

The run-up distance, i.e. the distance from ignition to transition to detonation in pipes is an experimental value giving some indication of the likelihood of transition to detonation. Steen and Schampel (1983) have reviewed experimental investigations of the run-up distance of gaseous detonations in large pipes. The experimental conditions, i.e. pressure, temperature and gas mixture, are limited compared with the actual conditions in the industry. The data presented by Steen and Schampel are mainly for 1 atm. and fuel-air mixtures. Figure 8 shows the run-up distance for stoichiometric ethylene and propane/air versus pipe diameter. The run-up distance increases with increasing pipe diameter. The turbulent boundary layer ahead of the flame is filling a relatively larger portion of the tube in small pipes than in large pipes. The fuel concentration is also an important factor for the run-up distance. This can be seen in Figure 9.

Several other factors also influence the run-up distance. Experiments show that it decreases with

- increasing initial pressure

- decreasing initial temperature, and
- increasing turbulence in the pipe (i.e. obstructions in the pipe).

In general we can say that the run-up distance in a smooth pipe depends on the reactivity and cell size. The smaller the cell size and the more reactive the mixture (burning velocity), the shorter is the run-up distance.

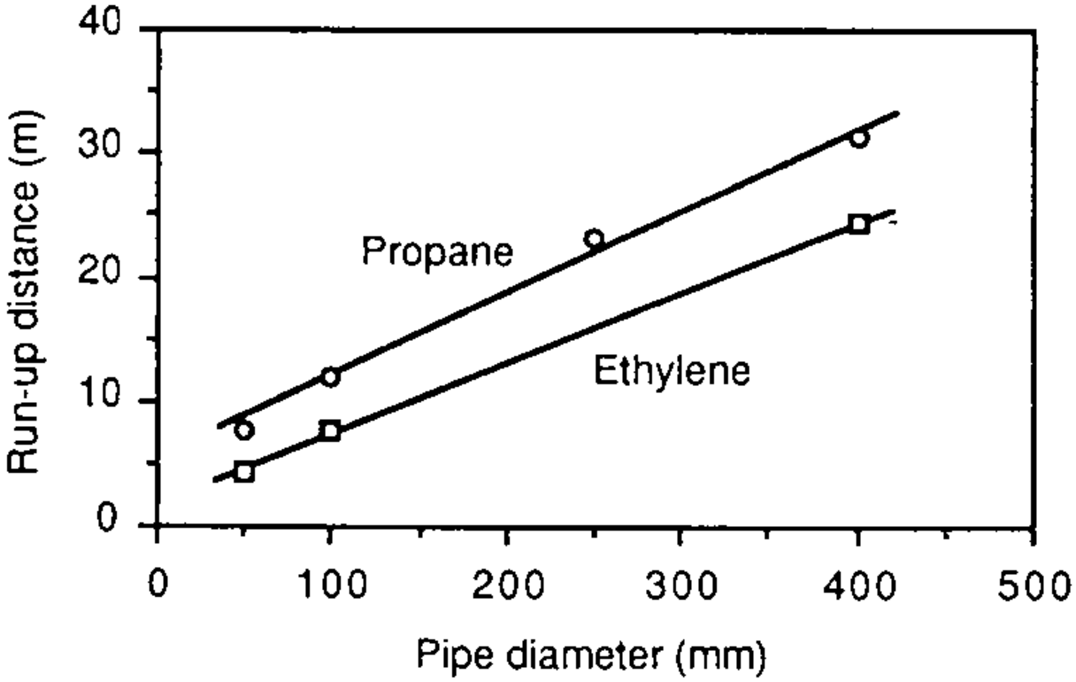


Figure 8 Run-up distance to detonation versus pipe diameter. (Steen and Schampel, 1983).

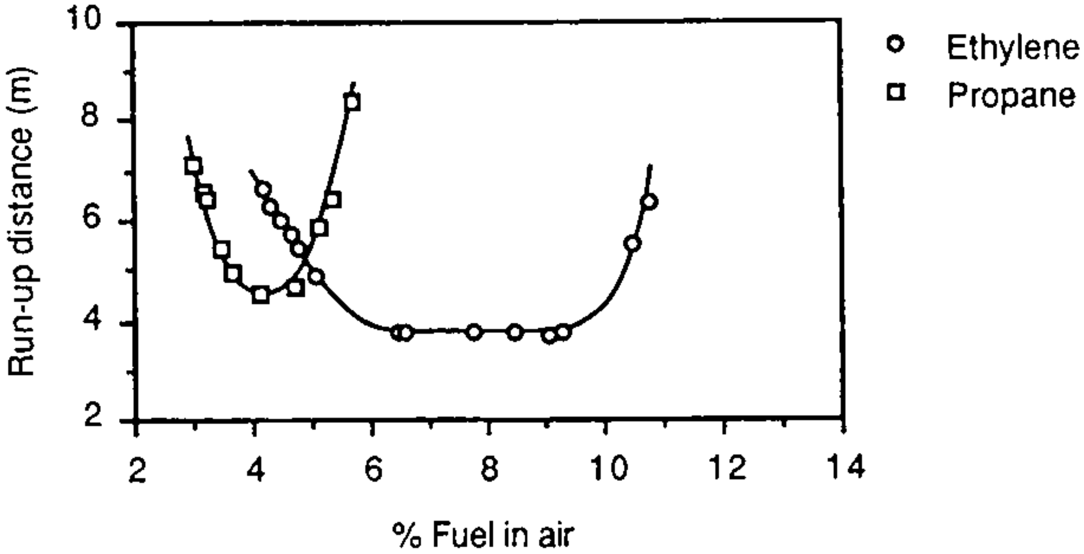


Figure 9 Run-up distance for ethylene- and propane-air. Pipe diameter 50 mm. (Steen and Schampel, 1983).

The effect of obstructions can be demonstrated by comparing the run-up distance for propane in a smooth pipe (Steen and Schampel (1983, see Fig. 9)), to a propane experiment reported by Hjertager et al. (1984) performed in an obstructed 50 m^3 pipe. In the 50 m^3 pipe pressures close to detonation pressures were measured indicating that a DDT was not far away. The pipe had a length-to-diameter ratio of 4. The results reported by Steen and Schampel (1983) suggest a DDT after approximately 94 pipe diameters in a smooth pipe.

Nevertheless the experimental evidence shows that a transition to detonation in a pipe can occur in any gas mixture as long as the pipe is sufficiently long to allow the flame to accelerate to conditions where DDT can occur and when the geometry allows for a detonation to sustain. Reactive mixtures will reach these conditions, however, much easier than less-reactive mixtures.

Also in geometries deviating from pipes, DDT can occur even for fuel-air mixtures with moderate reactivity.

In an experiment reported by Bjørkhaug and Hjertager (1984) in a 10 m long wedge-shaped vessel with stoichiometric propane-air, 100% top confinement and circular obstructions, transition to detonation was observed. This experiment shows that a propane-air explosion initiated with a weak ignition source can accelerate to a detonation in less than 10 m, if sufficient confinement and obstructions are present.

Moen et al. (1985 and 1989) have observed transition to detonation due to jet flames. In one test they reported transition to detonation in a lean mixture of acetylene-air (5% C_2H_2) in an essentially unconfined situation. The transition to detonation was caused by a jet-flame shooting into the unconfined cloud. These experiments demonstrated that detonations could be induced in an unconfined fuel-air cloud with moderate reaction rates as long as the size of the cloud is large.

Acton et al. (1990) report a DDT in a pipe rack geometry for propane-air. Transition to detonation occurred after 15 m. This experiment showed that in relatively "open" situations, such as a pipe bridge, the geometry can support flame acceleration to detonation.

Recent full-scale explosion experiments performed in a geometry representing an offshore module (Al-Hassan and Johnson, 1998) showed than when the flame is allowed to propagate and accelerate over a large distance in a fairly obstructed geometry DDT is even possible for natural gas.

The mechanism of transition to detonation is not fully understood. Presently there is no theory which can predict conditions for deflagration to detonation transition. We have only a qualitative understanding of the phenomenon; it is likely that local explosions within explosions cause transition to detonation. The size of these localised explosions must be of the order of 10 times the cell size λ (Moen, private comm.).

From a practical point of view, it is important to recognise that transition to detonation will cause extremely high pressures in the area where the transition takes place.

Figure 10 shows a pressure-time profile from an experiment where transition to detonation occurred. The first pressure rise at t = 2510 μs is the shock wave which compresses the unburned gas. The pressure continues to rise after the shock wave, and subsequently a transition to detonation occurs. Due to this pre-compression, the detonation pressure in the transition process is much higher than the pressure in a stabilised detonation wave (i.e. CJ-pressure).

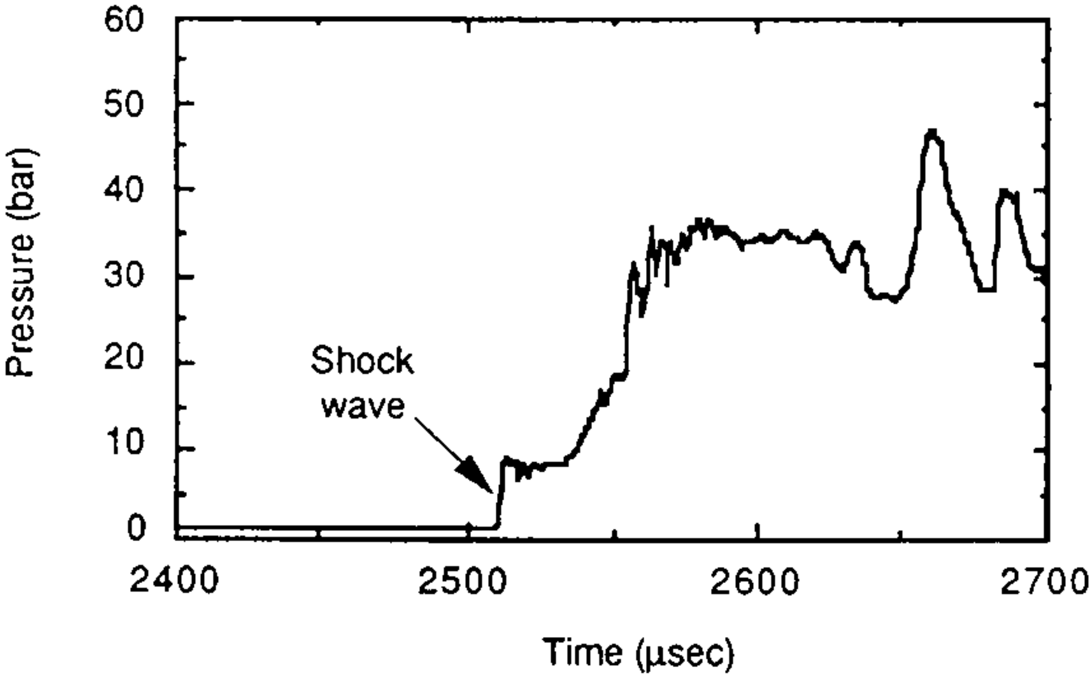


Figure 10 Pressure-time profile from a pressure transducer located close to an area of transition to detonation (Engebretsen, 1991).

PROPAGATION AND TRANSMISSION OF DETONATION WAVES

The propagation and transmission of a detonation are limited by geometrical conditions. As mentioned before a detonation cannot propagate in any pipe. The limited conditions are controlled by the sensitivity of gas mixtures and length scale of the geometry. As discussed before, the cell size is a length scale characterising the reactivity of the mixture. By using this length scale, the conditions for successful propagation and transmission can be evaluated. By transmission is meant the possibility for a detonation to propagate further into an unconfined cloud.

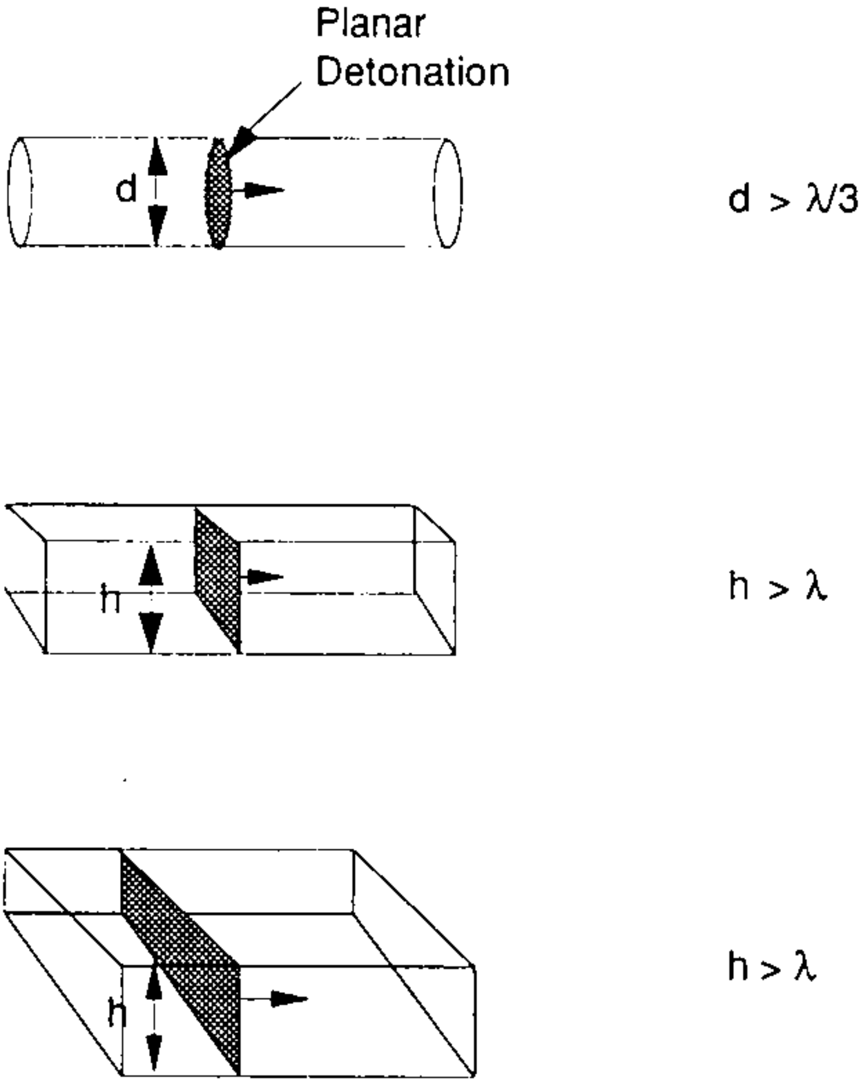


Figure 11 Requirements for successful propagation of a planar detonation in pipes and channels.

Figure 11 shows detonation propagation limits within pipes and channels. We see that a pipe is more supportive of detonation propagation than a channel.

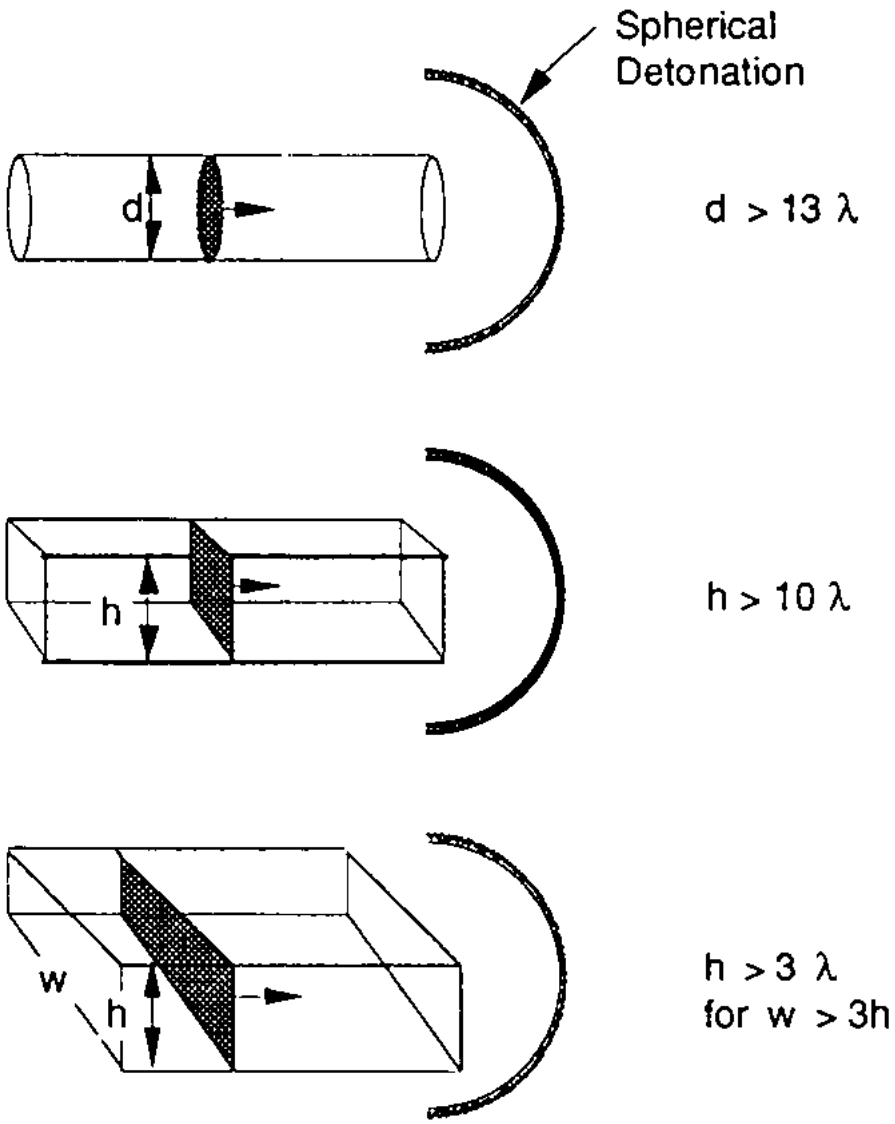


Figure 12 Requirements for successful transmission of a planar detonation into an unconfined three-dimensional spherical detonation wave.

Figure 12 shows requirements for a successful planar detonation transmission from a pipe or channel into an unconfined situation (i.e. three-dimensional spherical detonation wave). In order to make a successful transmission, there is a need for more cells than for the planar propagation mode. The information in Figure 12 is useful in evaluating the possibility for transmission of a detonation from a confined area, like a building, ventilation duct, culvert etc. into an unconfined situation.

The requirement for propagation in an unconfined cloud is shown in Figure 13.

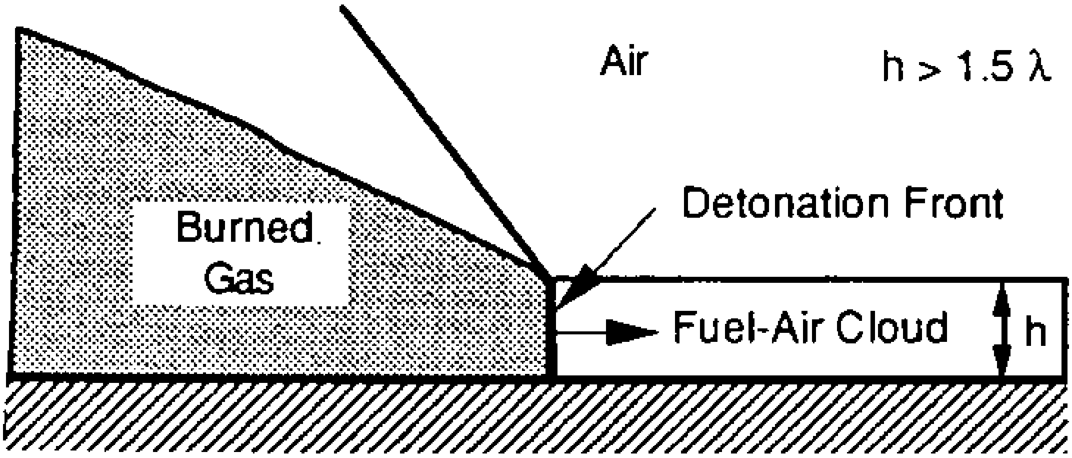


Figure 13 Limit for propagation of detonation waves in an unconfined fuel-air cloud.

VAPOUR CLOUD DETONATIONS

The above shows that detonations in the open are possible. Initiation is possible from more confined areas such as a culvert or just by flame accelerations in congested areas. This may have consequences for predicting the consequences of vapour cloud explosions; i.e. explosions of clouds in landbased petrochemical installations such as refineries. Methods for blast prediction such as the Multi-Energy method (Van den Berg, 1985) assume that blast is only generated in the congested parts of the cloud. As a result the blast prediction methods use the combustion energy in these congested areas only. In case of a detonation also the unconfined parts of the cloud will contribute to the blast possibly causing it to be much stronger at larger distances. The fact that a vapour cloud detonation can be expected even for the relatively low reactive fuels may make blast prediction methods such as the Multi-Energy method unreliable. On the other hand it should be emphasised that low reactive fuels will be able to reach detonations over a relatively small fuel concentration region only whereas more reactive fuels such as ethylene, ethylene-oxide, acetylene and hydrogen have a more wider explosive area with high reactivity concentrations. This will make it unlikely that low reactive fuel will reach detonations in reality. For the more reactive fuels a detonation may however, be possible also in realistic clouds.

DETONATION LOADING

Considering loading due to detonations one has to consider the full pressure-time history and not just the maximum pressures. So far we have discussed the detonation pressure (i.e. CJ-pressure) of a detonation front only. After the detonation front (CJ-plane) the combustion products will expand, i.e. the pressure will fall. How fast this expansion will take place, i.e. how fast the pressure will fall will depend on the boundary conditions.

The expansion of the combustion products forming a detonation wave propagating in a tube (i.e. one-dimensional propagation) is illustrated in Figure 14. The tube is closed at x = 0 and propagates from left to right. When the detonation is at x = L, the tail of the expansion wave will be located at approximately
x = L/2 which means that the tail of the expansion wave propagates at half of the detonation velocity for this boundary condition. The expansion process between the wave front (CJ-conditions) and tail of the expansion wave can be approximated as being isentropic.

In this case the pipe is closed at x = 0. The boundary condition at x = 0 is therefore gas velocity equal to zero (u = 0 m/s). For this boundary condition the pressure will expand to P » 0.4 PCJ. Note that this pressure is approximately the same as the constant volume combustion pressure. This pressure will be constant from x = 0 to the tail of the rarefaction wave (i.e. x » L/2).

For other boundary conditions, u ¹ 0 m/s, the pressure will vary with the boundary conditions. The mode of propagation for the detonation, i.e. spherical or planar mode, will influence the expansion slope behind the wave.

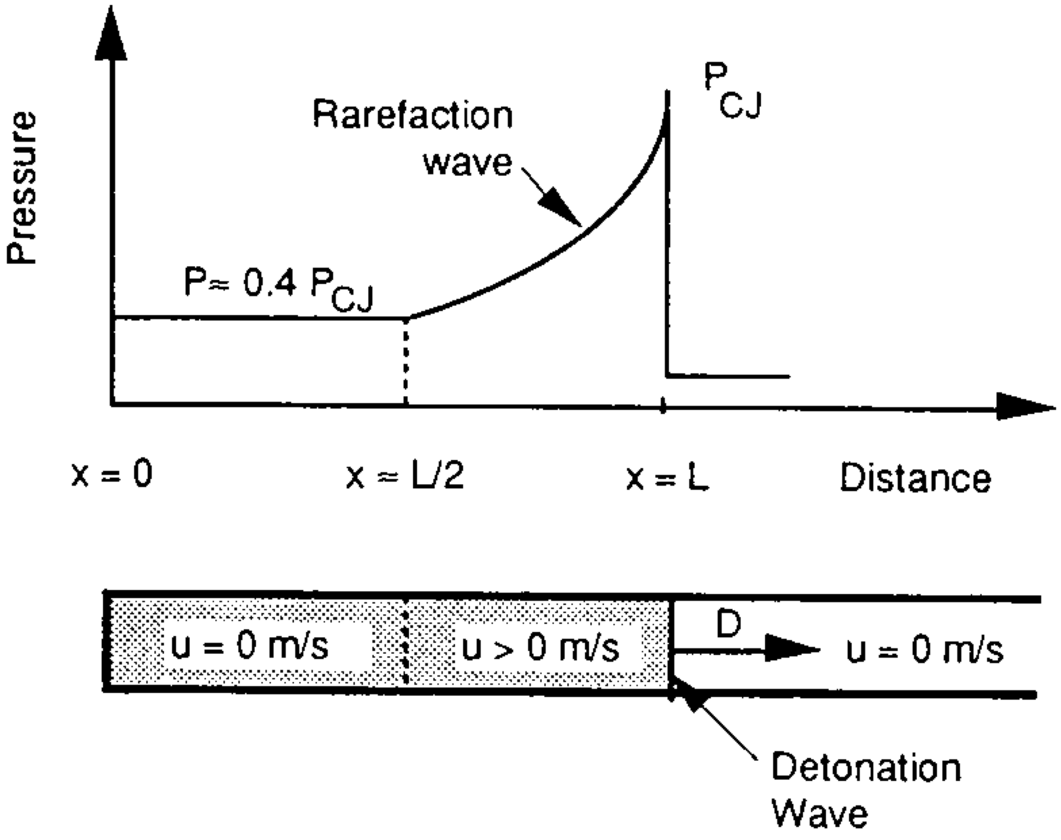


Figure 14 Pressure-distance profile for a detonation propagation in a tube with a closed end (i.e. closed at x = 0).

CONCLUSIONS

The probability of occurrence of a detonation in fuel-air mixtures depends strongly upon the type of fuel. Very reactive fuels, such as hydrogen, acetylene or ethylene, may detonate in an accident situation. For accident situations involving such fuels, detonations should be regarded as a possible scenario.

Other fuels are less likely to detonate. Generally, however, in large gas clouds with a high degree of confinement and/or with a high density of obstructions, detonations cannot be ruled out.

Presently the most effective way of mitigating the occurrence of a detonation is to avoid situations where the deflagration can accelerate to a condition where transition from deflagration is possible, i.e. high pressure deflagrations.

Propagation and transmission of detonation waves depend mainly on the cell size (i.e. type of fuel and fuel concentration) and geometrical conditions. By operating with geometrical dimensions (d, w, h) smaller than the limits indicated it is very unlikely that a stable detonation will occur.

The cell size as a measure of detonability is not an exact number. In the literature a variation of a factor of two is often found. When using cell sizes for estimation of limiting conditions for successful propagation or
transmission, they should be regarded as approximate values. Hence safety factors should be used.

REFERENCES

Acton, M.R., Sutton, P and Wickens, M.J. (1990)
An investigation of mitigation of gas cloud explosions by water sprays, Piper Alpha: Lessons for Life Cycle Safety Management, Symposium Series No. 122, IChemE, Rugby, UK

Al-Hassan, T. and Johnson, D.M. (1998)
Gas explosions in large scale offshore module geometries: overpressures, mitigation and repeatability Paper presented during the 17th International confrence on Offshore Mechanics and Arctic Engineering, 6-9 July, Lisbon

Bartknecht, W. (1971)
"*Brenngas- und Staubexplosionen*".
Forschungsbericht F45 , Bundesinstitut für Arbeidsschutz (Bifa), Dortmund, W. Germany.

Berg, A.C. van den (1985)
"The multi-energy method. A framework for vapour cloud explosion blast prediction".
Journal of Hazardous Materials 12.

Bjørkhaug, M. and Hjertager, B.H. (1984)
"*The influence of obstacles on flame propagation and pressure development in a radial vessel of ten metre radius. Final Report*".
CMI Report No. 843403-9, Chr. Michelsen Institute, Bergen, Norway.

Engebretsen, T. (1991)
"*Propagation of gaseous detonations through regions of low reactivity*". PhD. Thesis, ITE, NTH, Trondheim, Norway.

Fickett, W. and Davis, W.C. (1979)
"*Detonation*".
University of California Press, Berkeley.

Hjertager, B.H., Fuhre, K., Parker, S. and Bakke, J.R. (1985)
"*Flame acceleration of propane-air in a large-scale obstructed tube*".
Progr. AIAA, Vol. 94, pp.504-522

Lee, J.H. (1984)
"*Dynamic parameters of gaseous detonations*".
Ann. Rev. Fluid Mech., 16.

Moen, I.O., Bjerketvedt, D., Jenssen, A. and Thibault, P.A. (1985)
"*Transition to detonation in a large fuel-air cloud*".
Combustion and Flame 61.

Moen, I.O., Bjerketvedt, D., Engebretsen, T., Jenssen, A., Hjertager, B.H. and Bakke, J.R. (1989)
"*Transition to detonation in a flame jet*".
Combustion and Flame 75.

Shepherd, J.E., Melhem, G.A. and Athens, P. (1991)
"*Unconfined Vapor Cloud Explosions: A New Perspective*",
International Conference and Workshop on Modelling and Mitigating the Consequences of Accidental Releases

Steen, H. and Schampel, K. (1983)
"*Experimental investigation of the run-up distance of gaseous detonations in large pipes*",
4th International Symposium on Loss Prevention and Safety Promotion in the Process Industries,
Pergamon Press, London, UK, pp. E23-E33.