

**Detonation Prediction and Mitigation:
Some observations based on personal
experiences of process pipeline explosion safety
studies**

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Based on an outline of an invited plenary lecture(Geraint Thomas)
19th ICDERS Hakone Japan (2003)

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Introduction

- The number of reported detonation incidents within process plant and industry in general is thankfully low compared to other potential explosion hazards.
- However the extreme pressure generated in a detonation, ca. 1.8 Mpa for a hydrocarbon air mixture, increasing to 4.5 MPa during normal reflection poses a severe threat to industrial plant. The pressures and potential damage may however be greater in localized regions undergoing transition to detonation.
- Detonation is thus greatly feared by process safety engineers.
- Is this justified and, if so, how well can they be predicted/mitigated and what might the consequences be?

Evaluating explosion safety

- Basic recommended approaches
- The first stage in assessing any potential industrial explosion hazard is to conduct a thorough paper audit of all possible perceived hazards that could arise:
These are the familiar
 - HAZOP
 - HAZAN
- However, once a potential detonation hazard has been identified how does one quantify the probability of detonation developing?

The enigma of detonation

- Detonation is probably the most destructive accidental explosion event that could develop, especially within a confined process pipeline such as a vent header.
- The enigma of detonation is that from a theoretical standpoint our understanding of detonation in explosive mixtures is well advanced but our ability to predict if detonation will develop cannot be done using any proven scientific method
- A further complicating factor is that effective one dimensional theories are complicated in practice by complex three dimensional gasdynamic effects.
- Finally although detonation is a chemical phenomenon reliant on exothermic chemical reactions to sustain continued propagation, coupled to complex gasdynamic interactions, the development of conditions that lead to detonation is usually governed by turbulent deflagration phenomena at both macro-and micro-scopic scales

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How do detonations develop?

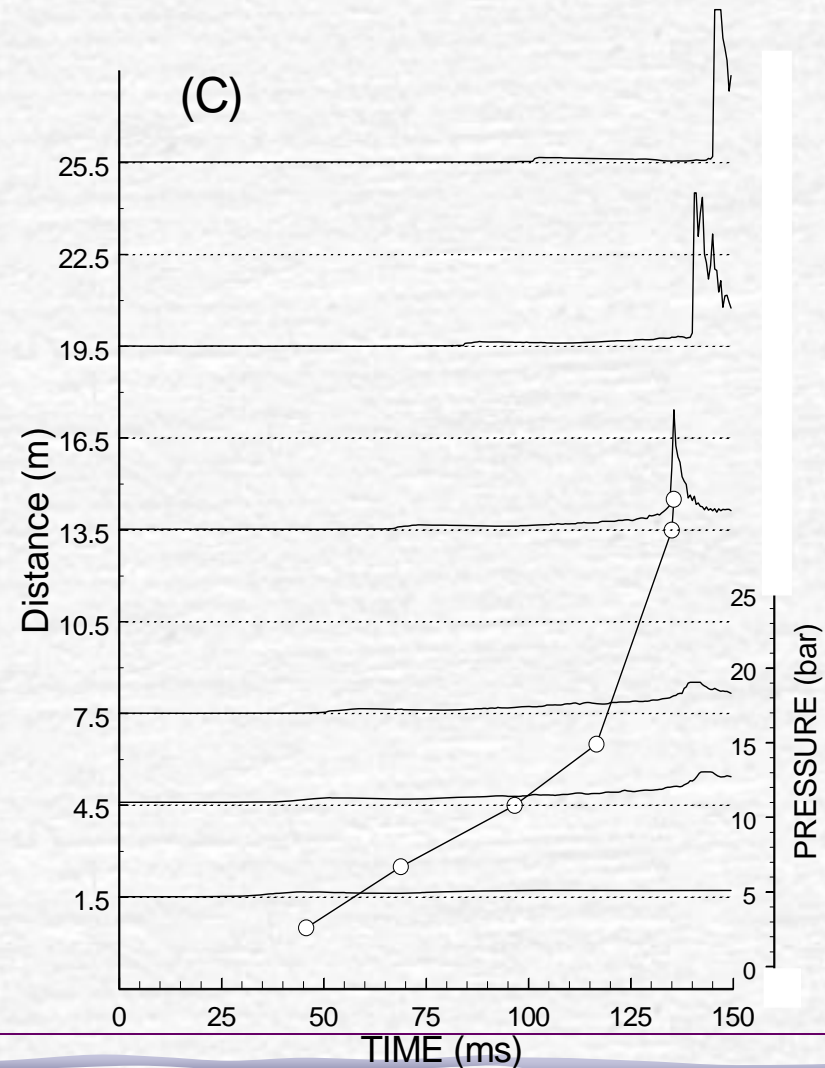
Pressure time history in an experiment to investigate DDT development in a 30 m long 150mm diameter pipe from a low energy source

Mixture: 6.9% ethylene in air at ambient atmospheric pressure.

the first feature is a weak acoustic pressure pulse

- this is then followed by a gradual increase in flame speed (O) but with little localised pressure increase

- there is now a rapid pressure increase leading to shock formation after 125ms and then a very localised DDT event



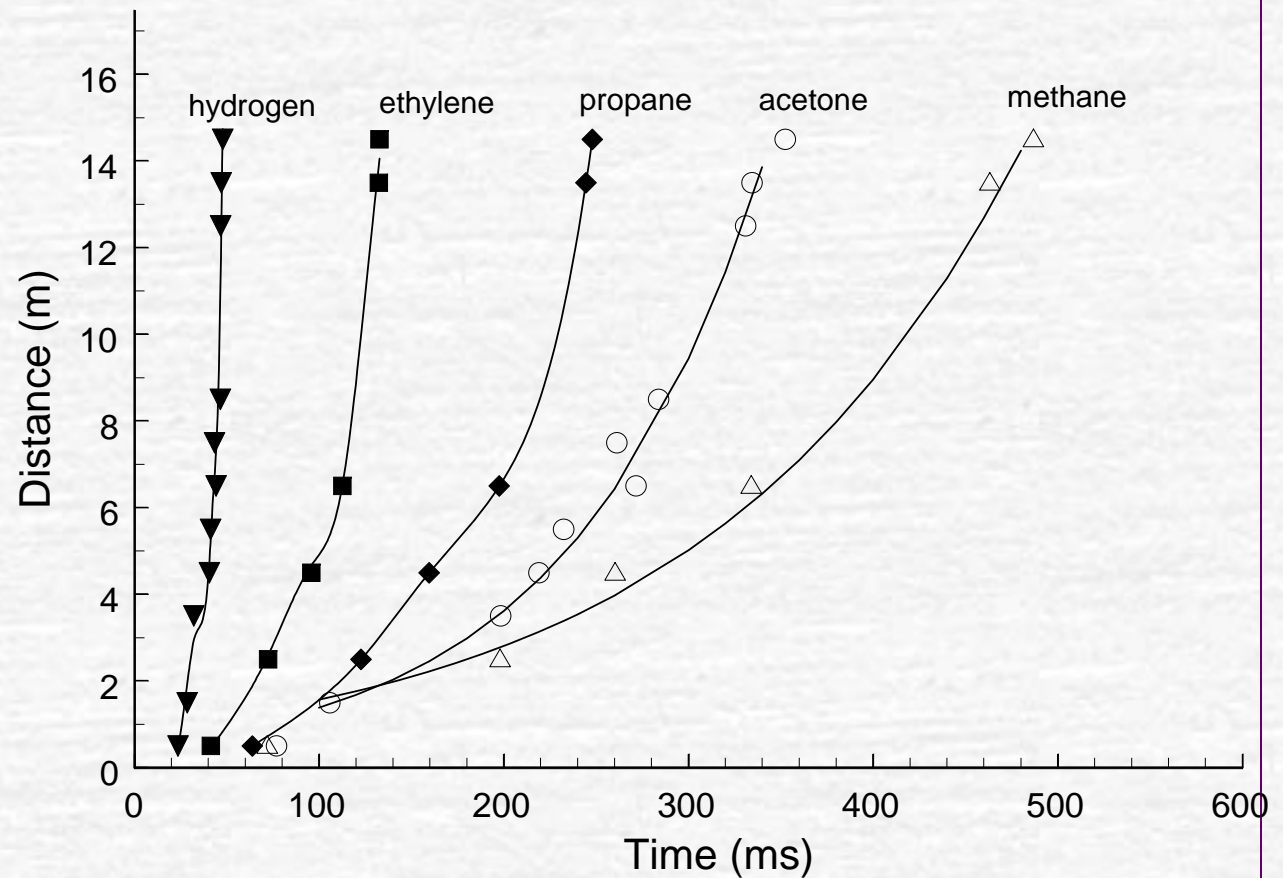
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Flame Acceleration Characteristics

Summary of flame acceleration characteristics for fuels in stoichiometric mixture with air. Ambient temperature and pressure. Only H_2 - and C_2H_4 -air detonated



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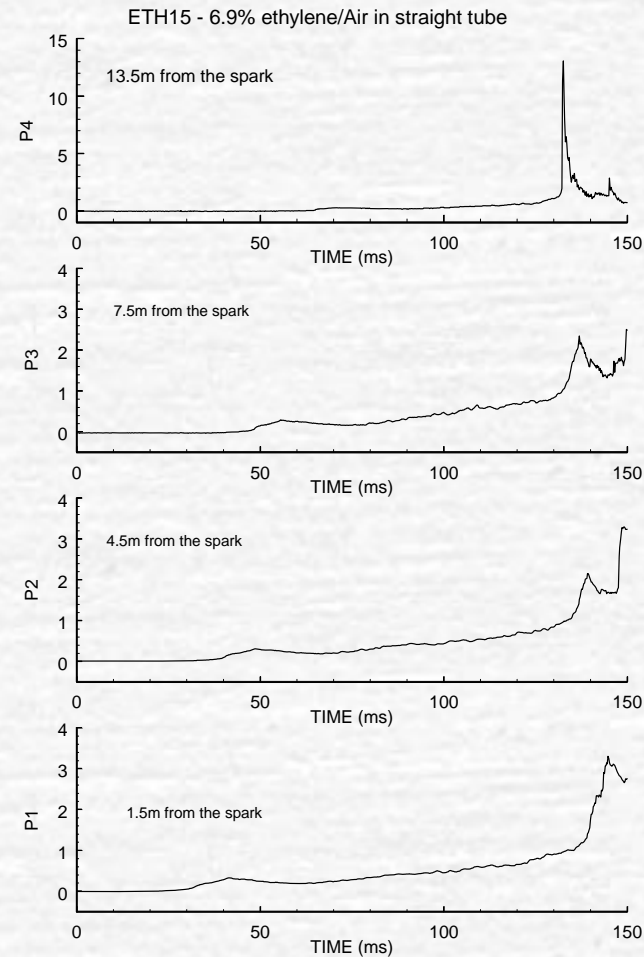
Phases of Pipe Explosion Development I

Pressure histories from gauges 1.5, 4.5, 7.5 and 13.5 m from the spark ignition source (0.6 J)

All gauges show a gradual, nearly homogeneous pressure increase as the flame first accelerates.

A sudden pressure increase is seen first at the gauge at 13.5 m, around the time the flame arrives

The pressure excursions seen by gauges closer to the spark are due to the pressure waves from the upstream transition



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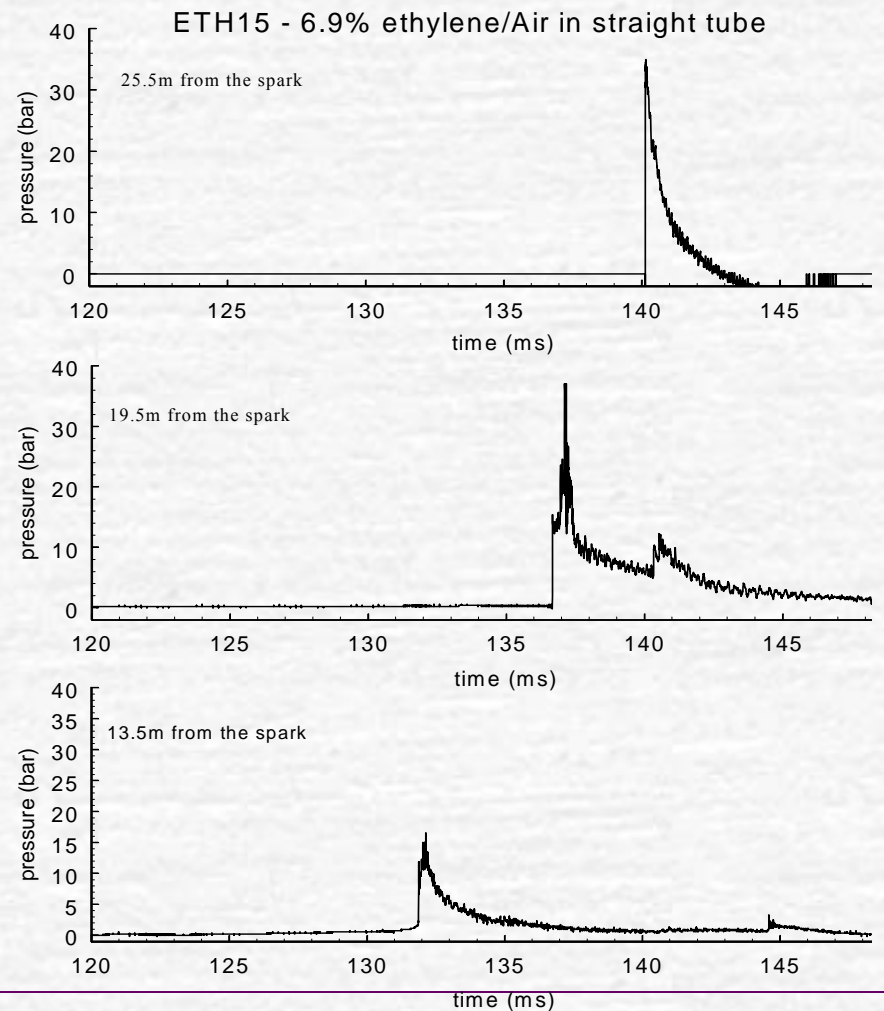
Phases of Explosion Development II

Pressure histories from gauges 13.5, 19.5 and 25.5 m from the spark source

A strong shock arrives at the first gauge(lower).

This has increase in strength by the time it reaches the gauge at 19.5 m, and is trailed by a flame and a further pressure increase(middle).

The last gauge(upper) shows a profile typical of a post-transition detonation. The blast from the transition can be seen on the middle gauge.

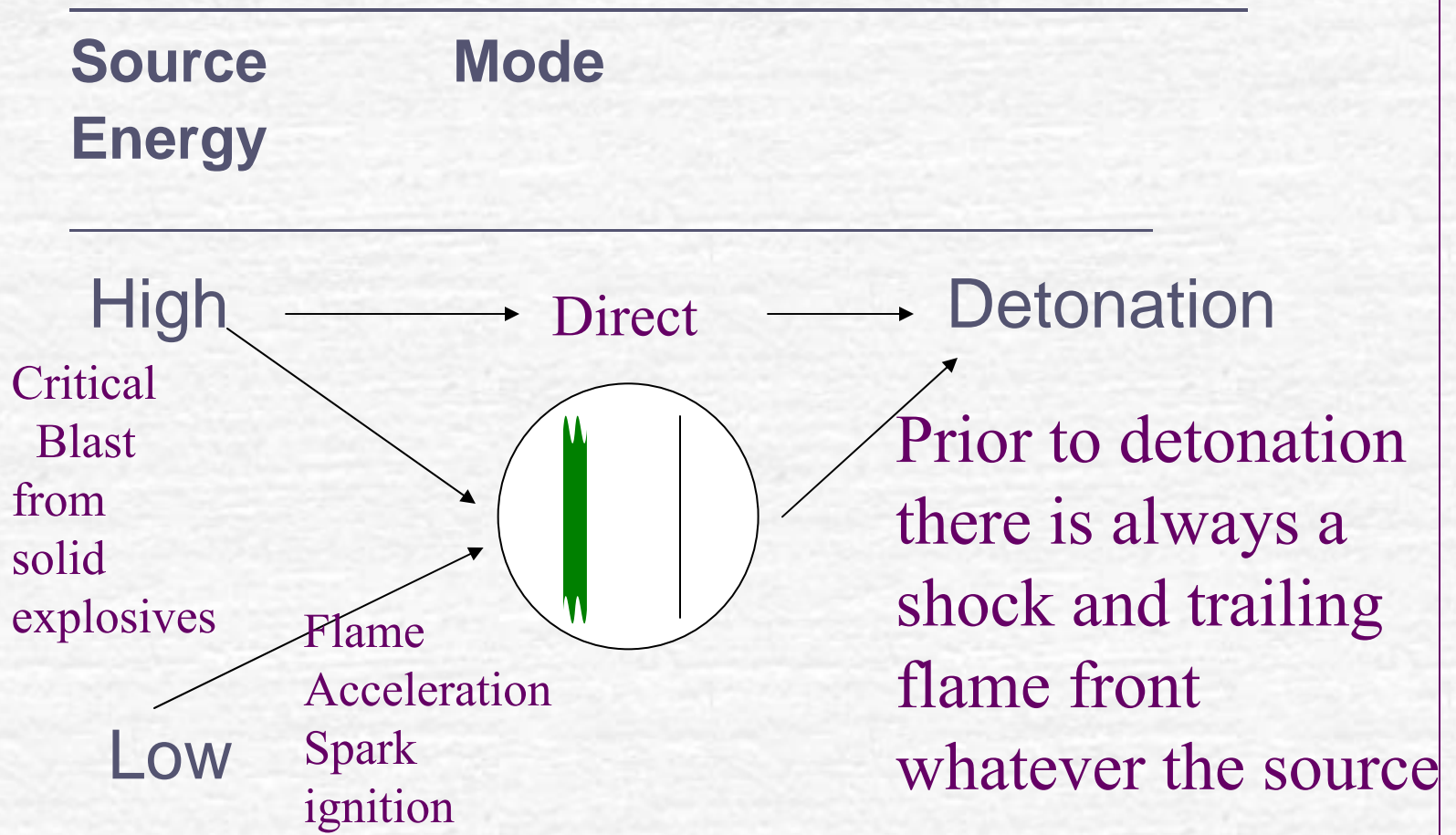


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Modes of Initiation of Detonation



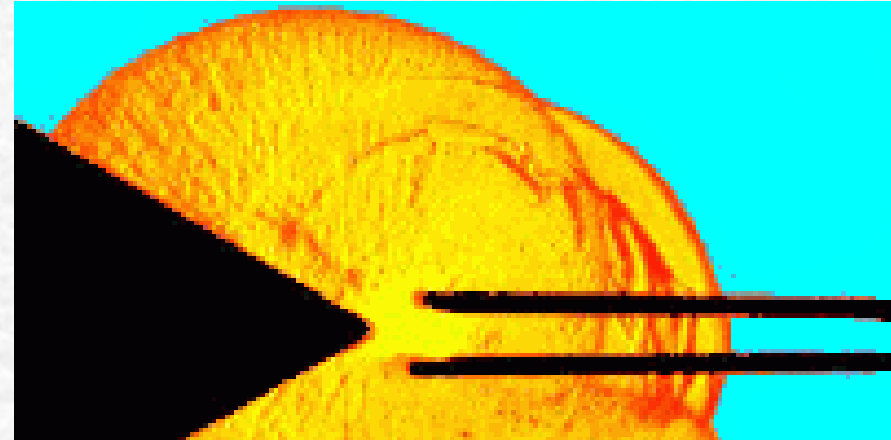
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direct initiation of detonation

- Smoked foil image of high energy spark initiation showing role of transverse cell structure left-cylindrical, right- spherical geometry $\text{C}_2\text{H}_2\text{-O}_2$



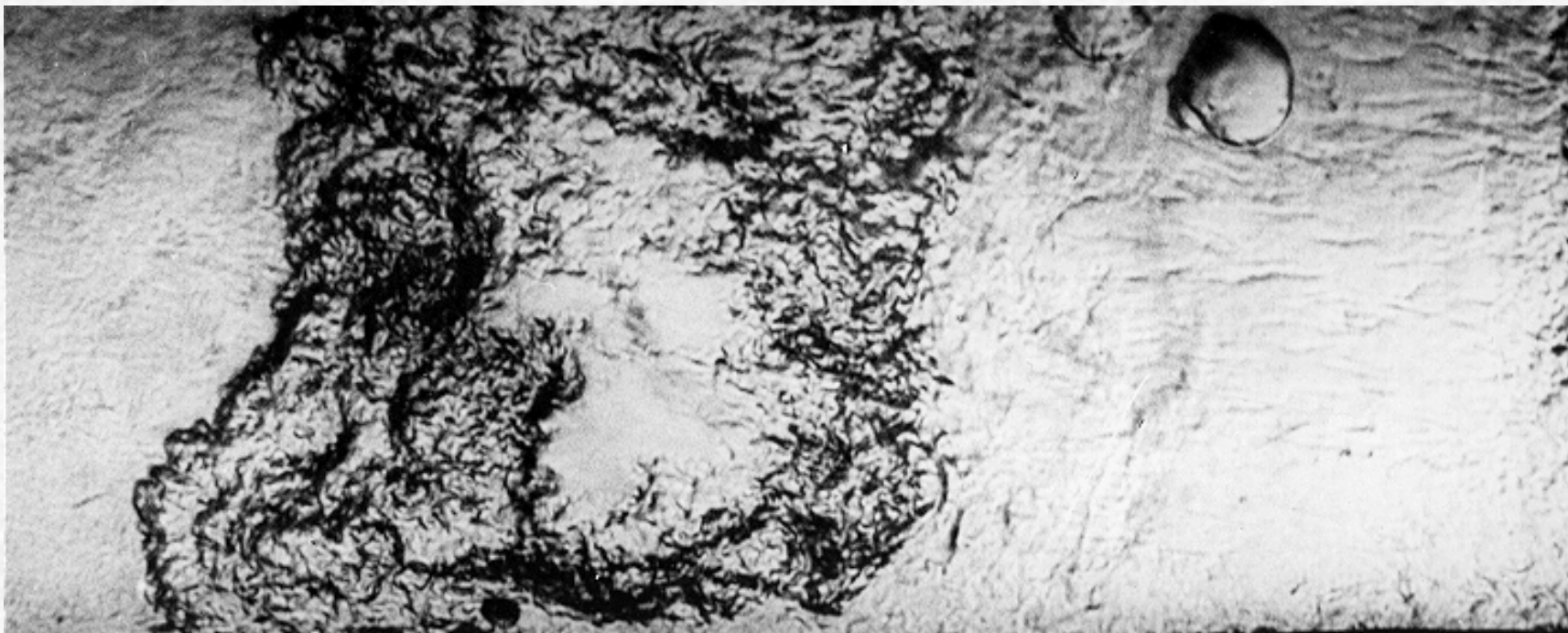
Note the visual evidence for initially unburned shocked gas between the lead shock front and trailing combustion within which evidence for a transverse detonation can be identified

Why/How does the final transition occur?

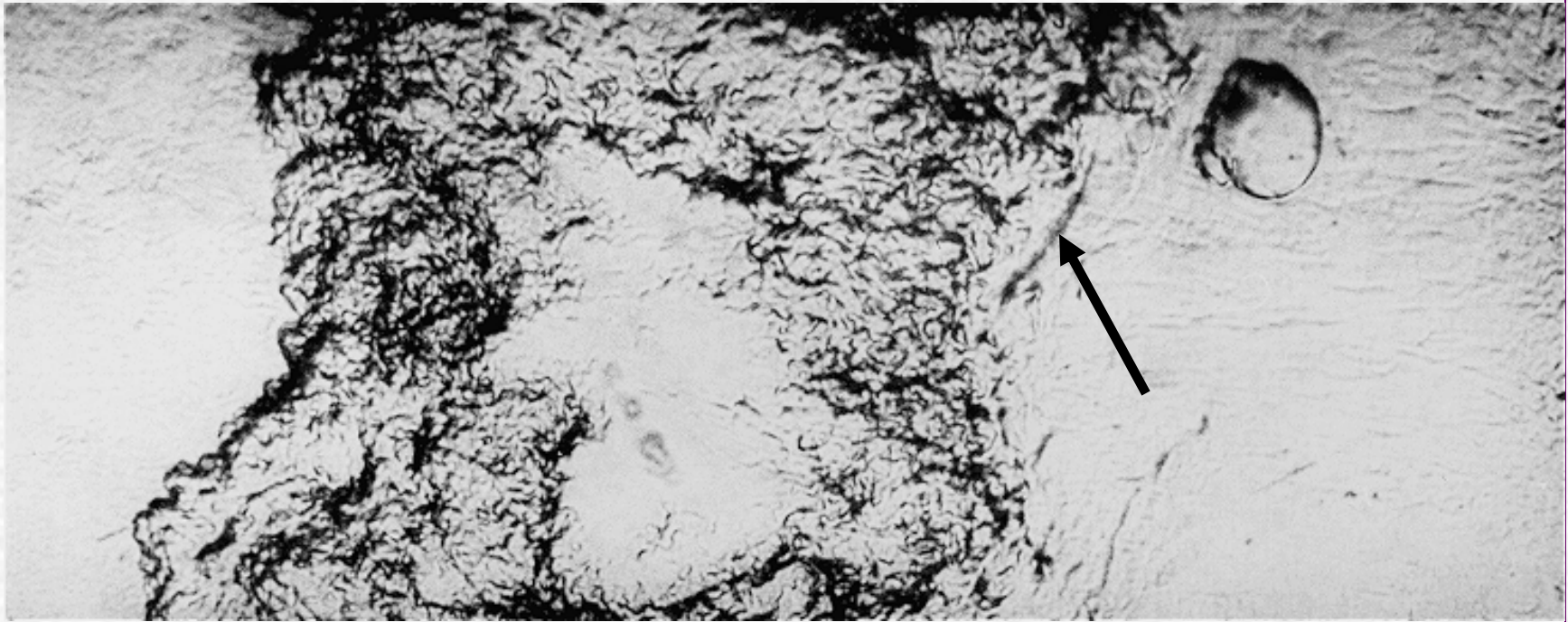
- Under field conditions it is impossible to study the onset of detonation in detail because of the stochastic nature of flame acceleration
- However we do know that the final deflagration to detonation transition (DDT) occurs in shock heated gas or mixtures compressed by other means- e.g. knock in internal combustion engines

We can therefore use laboratory reflected shock techniques to recreate the gas dynamic and thermodynamic conditions close to the transition conditions and watch how the flame develops

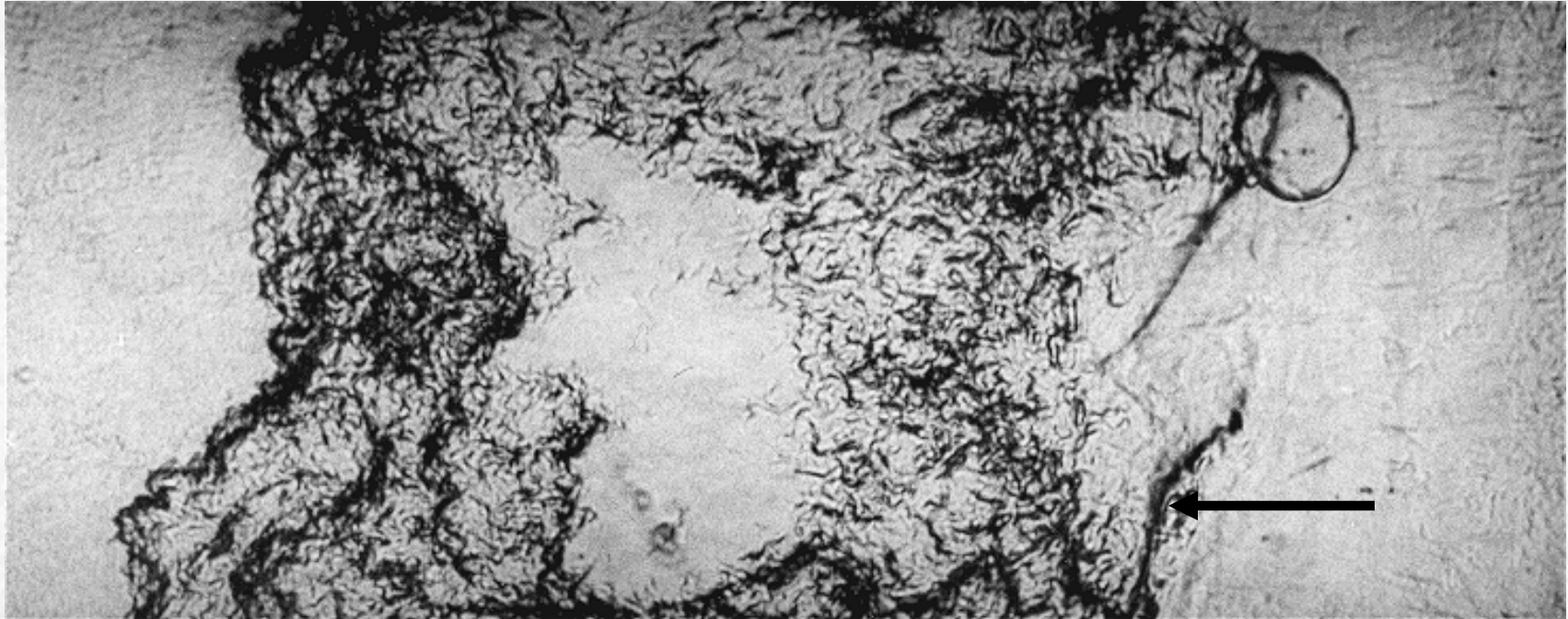
There is a rapid local acceleration of the 'flame' front



This example shows a flame front several 100's μs after a distributed auto-ignition. There is a 'turbulent like' flame front and one or two small spherical flame kernels



After $10 \mu\text{s}$ a compression front seems to be developing below the locally accelerating flame front, to the left of the spherical flame bubble



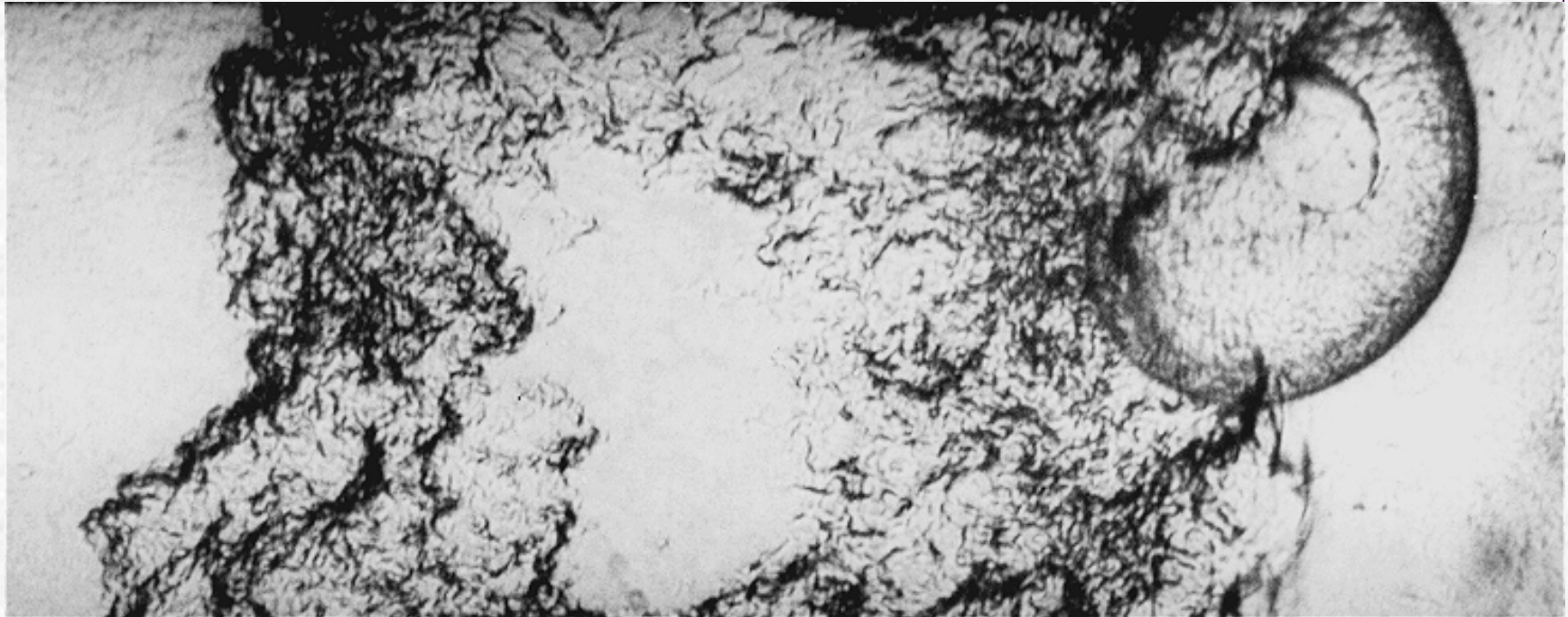
After a further $10 \mu\text{s}$ a second compression front develops closer to the lower wall. The original combustion front-pressure wave continues to evolve.

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Finally a detonation emerges



Detonation has formed 10 μ s later, centred near to the small flame bubble.

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Pressure during transition

The most significant pressures developed during a transition to detonation occur as shock heated mixture supports a local detonation

Lead shock velocity	post shock pressure	shocked gas CJ pressure
m/s	bar	bar
640	4.52	50.9
1000	9.92	77
2593	18.92	102

Data for undiluted ethylene-air, CJ pressure ca. 18.4 bar

What predictive tools do we have?

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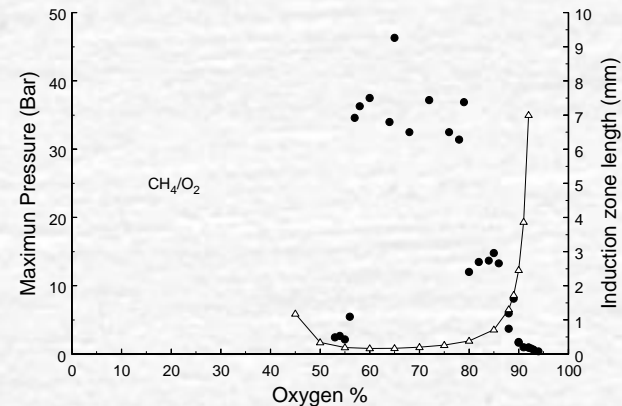
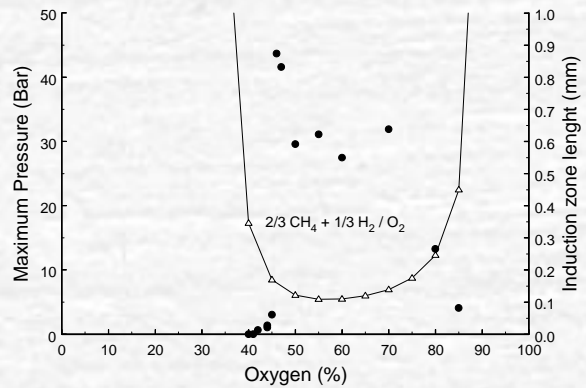
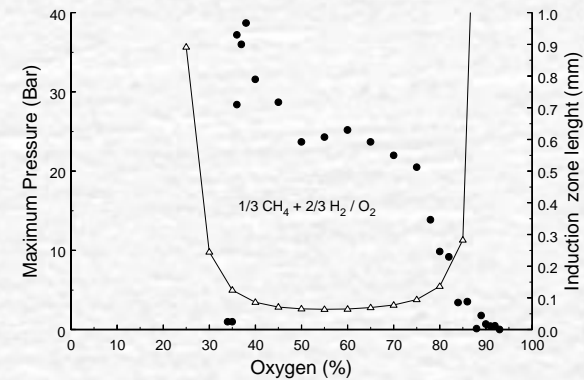
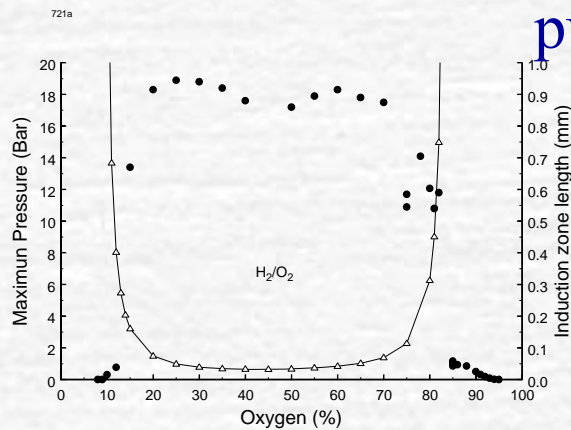
- For process pipe explosions
- cell size theories
- Studies at McGill suggest that detonations cannot develop if the detonation cell size(λ) is greater than some multiple of the pipe diameter(D), e.g λ must be greater than πD for detonation to develop

Studies in a 7mm tube at elevated T&P

- Experimental tests have been performed in a 7 mm tube with initial pressures and temperatures as great as 7 bar and 540K respectively: mixtures tested include C₂H₄-oxygen as well as H₂+CH₄ with oxygen.
- Cell widths were predicted as a multiple of the auto-ignition delay time in the theoretical von-neuman zone

Studies in a 7mm tube at elevated T&P

The limits for severe pressure events correlated well with predicted cell widths for four h₂/CH₄/O₂ mixes ranging from pure h₂ to pure CH₄



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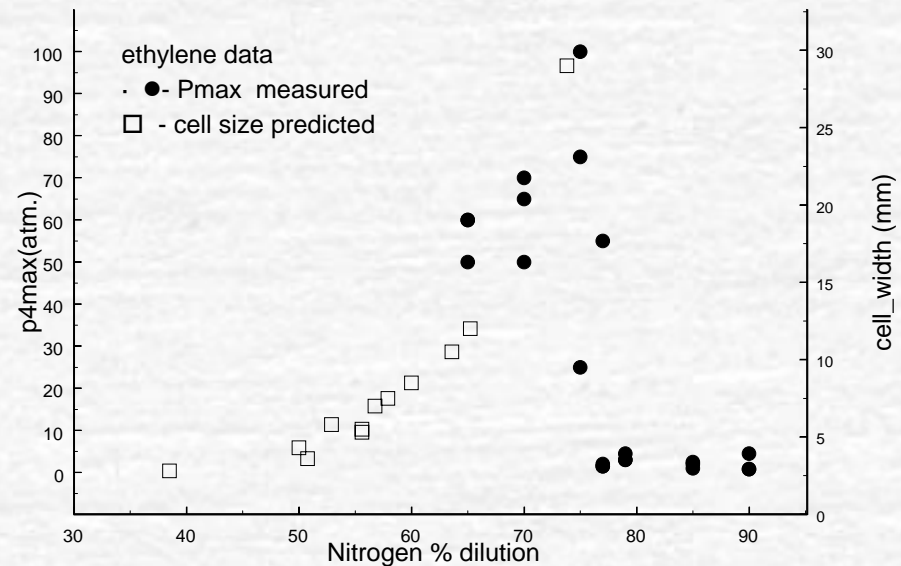
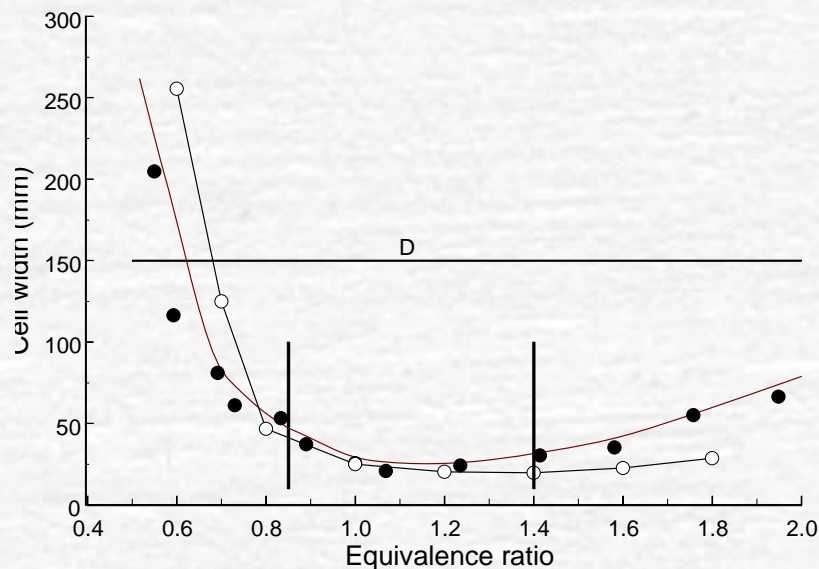
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Ethylene air in 150 and 50 mm pipes

Predicted(\circ) and published measured(\bullet) cell widths are close but measured detonation limits (150 mm tests) correspond to a much smaller cell width than anticipated

During tests in a 50 mm pipe the limit for overpressure development(\bullet) again correlates with published cell widths(\square) but the critical cell width is not as anticipated



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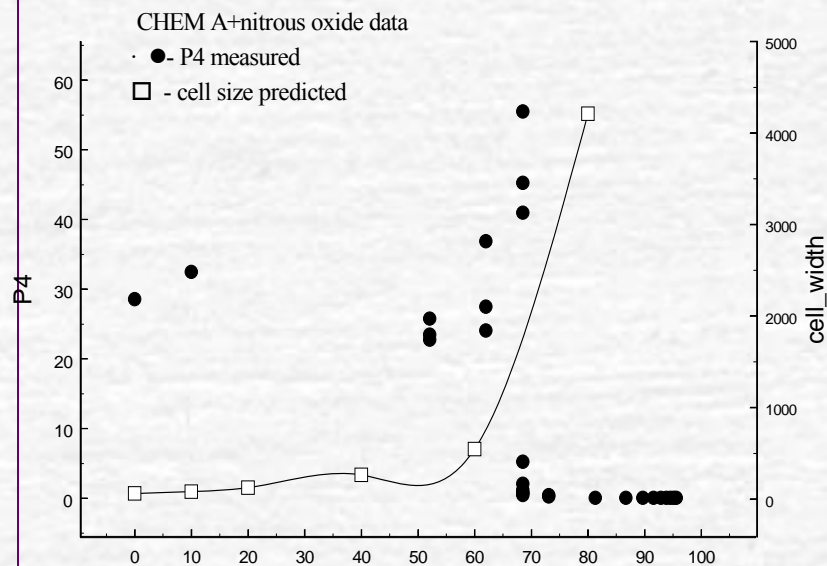
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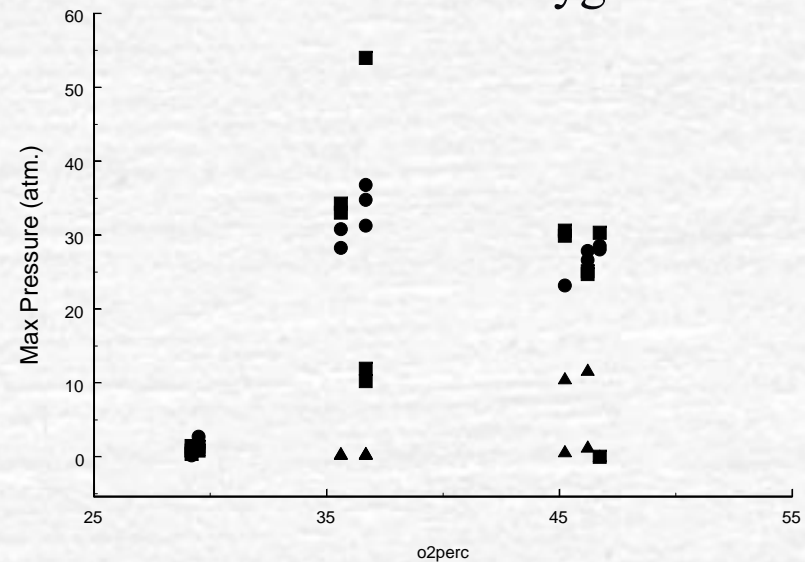
Recent results with non-standard fuel-oxidisers

- No cell size data is available for the mixtures tested and limited supporting kinetic data for cell size prediction calculations.
- However pressure measurements identify distinct limits of detonation

CHEM A+Nitrous Oxide



CHEM B+Oxygen



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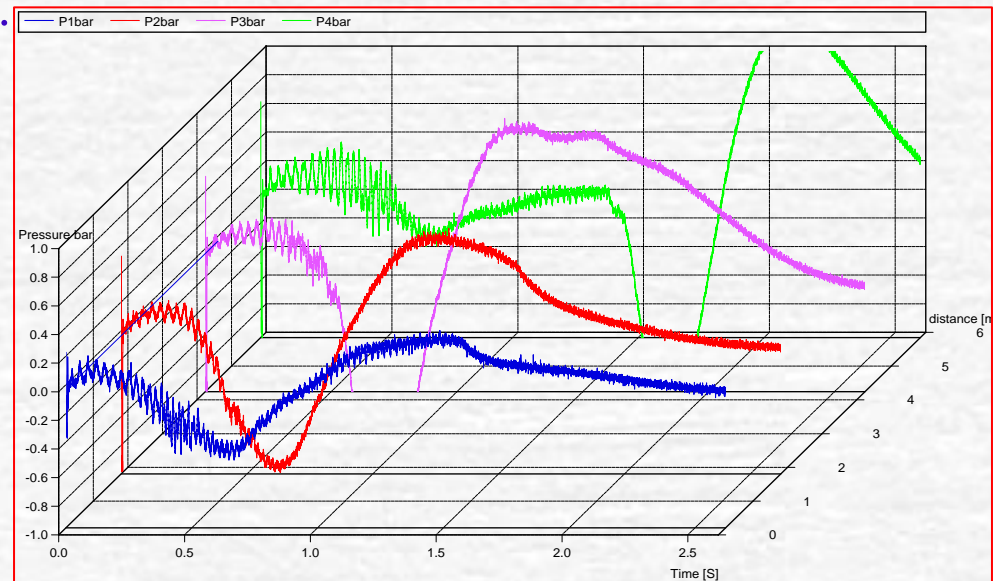
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Preliminary tests with standard unleaded fuel

As in the previous tests Chemical B was a liquid at room temperature the fuel delivery apparatus was also used for some preliminary observations of flame propagation with a standard commercial (Murco) unleaded automotive fuel, again in a 50 mm diameter 6m long steel pipe.

Note: the testing dates were in early September so the fuel was probably a low vapour fraction summer blend.

Initial tube wall temperature
140°C, Fuel:air ratio ~14:1
Spark ignition
Max press. ca. 1 barg
Flame speeds 9.8→1.7 ms⁻¹



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What predictive tools do we have



CFD capabilities are in general limited in their usefulness when it comes to detonation.

Because of the need to model accurately the early turbulent deflagration phases most explosion codes excel in this area and unfortunately the solution techniques used cannot then capture the critical shock development phase.

Recent code developments at Tel Tek Norway have however provided a code that does capture most of the operative physics and gas-dynamics

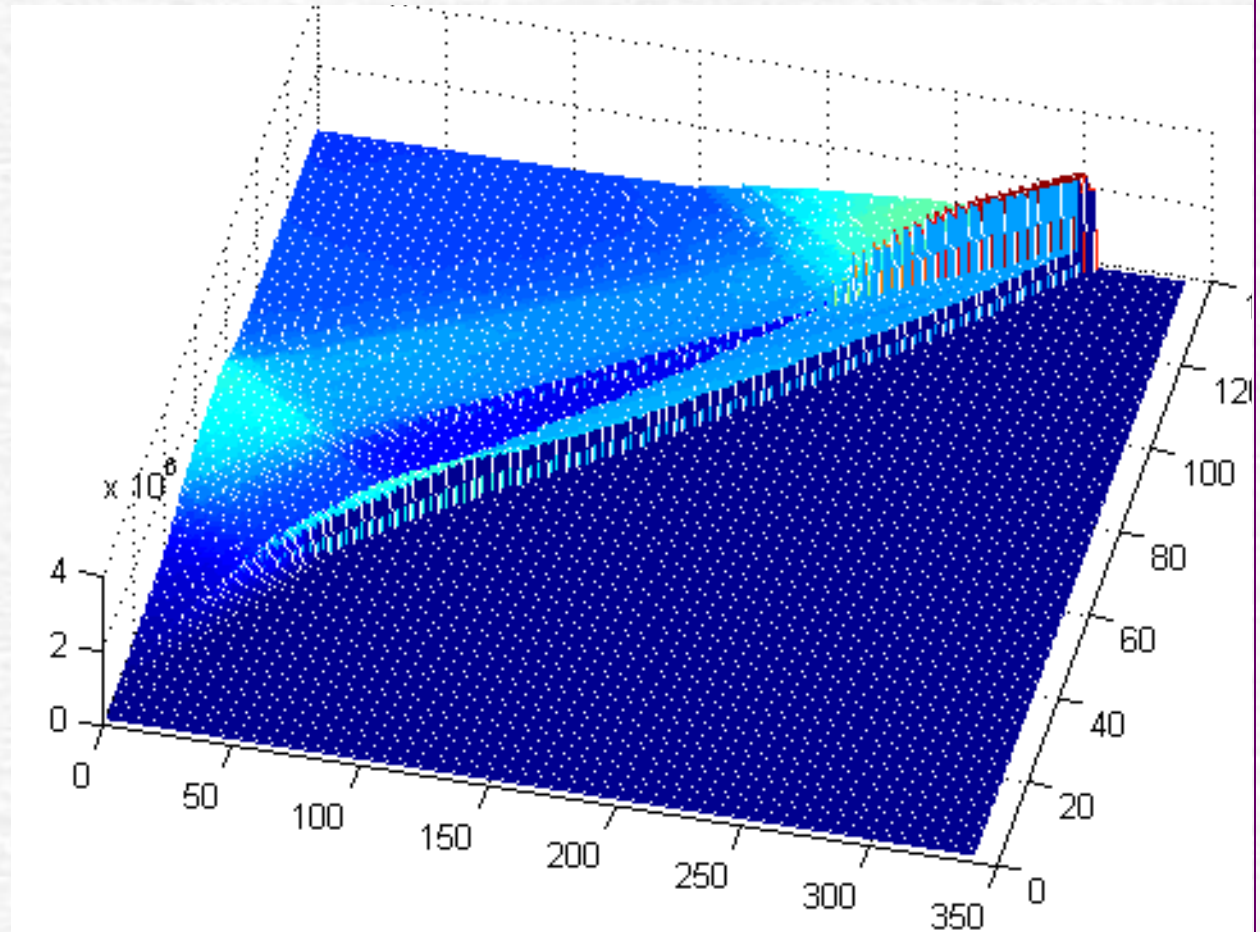
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Recent CFD Modelling Activity

Initial results of flame acceleration and transition to detonation obtained using a MATLAB based RCM code with a turbulent energy release model.



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RCM Deflagration Solution

- The new combustion model for RCM is based on the Rankine-Hugoniot relations. The burning velocity, S_t , is directly related to the states either side of the of the combustion wave
- From the conservation of mass and energy we can calculate the Hugoniot curve.
- When the turbulent burning velocity S_t is specified the state of the combustion products can be found at the intersection of the Hugoniot curve with the Rayleigh line, also known as the weak deflagration solution
- The new combustion model used in RCM, which is illustrated in Figure 2, treats the combustion wave as a discontinuity.
- If S_t and heat release q is known we can treat the flame propagation in the domain between two grid points as a reactive Riemann problem.

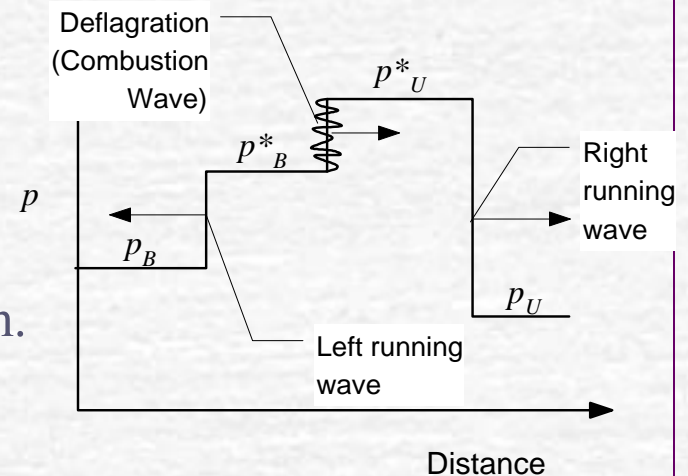


Fig. 2 : RCM combustion model

Quasi-1D Model for Pipe Explosions

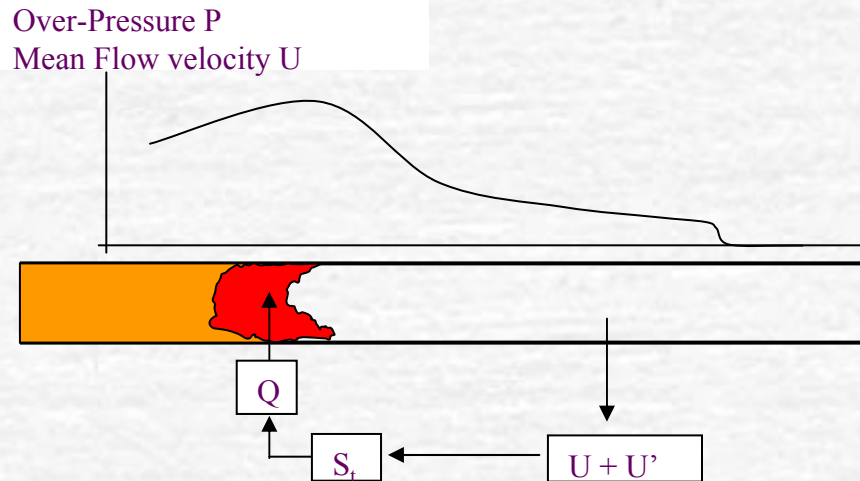
- Although 1-D in macroscopic terms, local flame front structure will be multi-dimensional
- We therefore confine locally a complex flame front interface to a single mesh point
- We represent the correct mass burning rate and corresponding energy release by an effective turbulent burning velocity S_t
- if A is the cross sectional area of the pipe.
- $$dQ/dt = S_t \rho A q$$
- We must now introduce a model for the turbulent burning, based initially on turbulence intensity u' in the unburned gas
- Unfortunately, little data exists on u' dependence on mean gas flow u even for steady flows, and none for transient pipe flows
- Initially use correlation due to Lawn; $u' = 0.168 u Re^{-0.119}$

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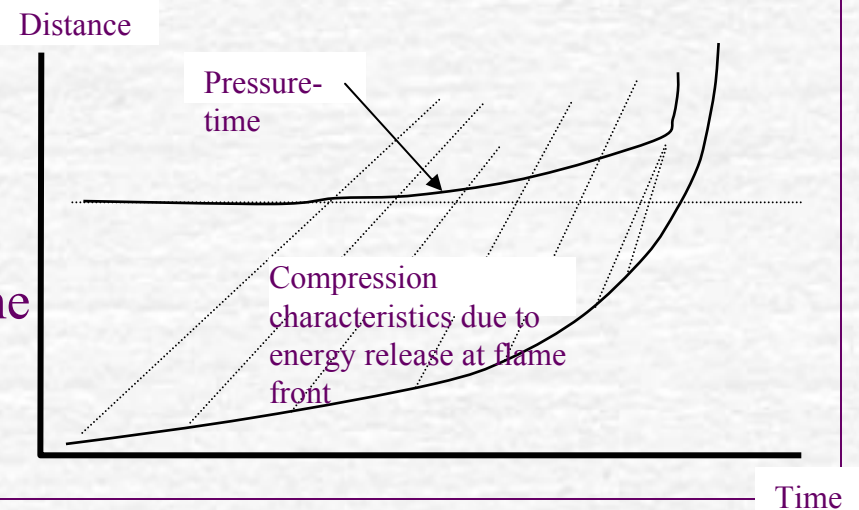
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Development of Pipe Explosions



The extent of flame acceleration is controlled by the degree of turbulent combustion feedback generated due to viscous interaction with the tube walls

As the flame accelerates, pressure and waves propagate forward into the unburned mixture along characteristics. The unburned gas velocity is no longer zero. As the flame velocity and local flame pressure increase, the characteristics converge and a shock forms



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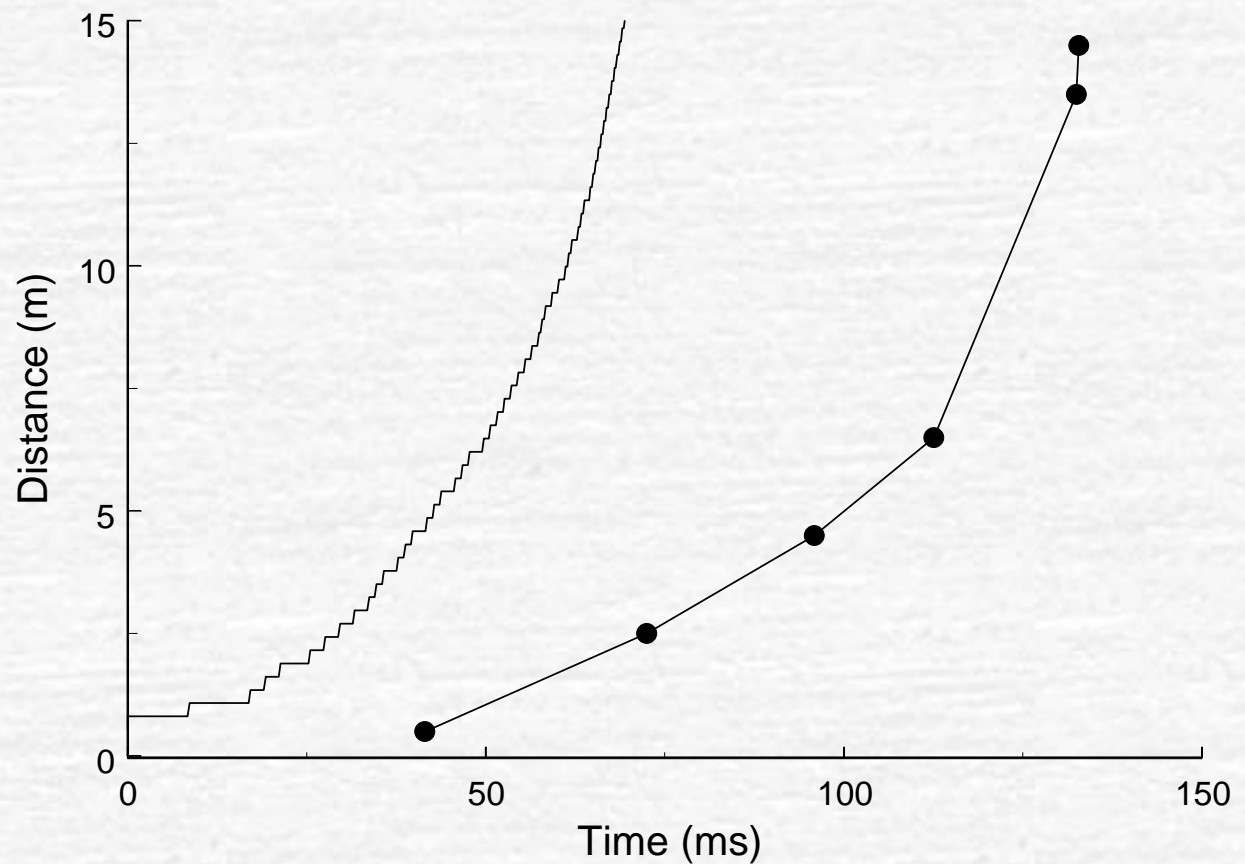
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Preliminary RCM Simulations of Pipe Explosions

Flame front position with time

Initial acceleration is over-predicted

Need a better description of the initial laminar to wrinkled flame transition phase



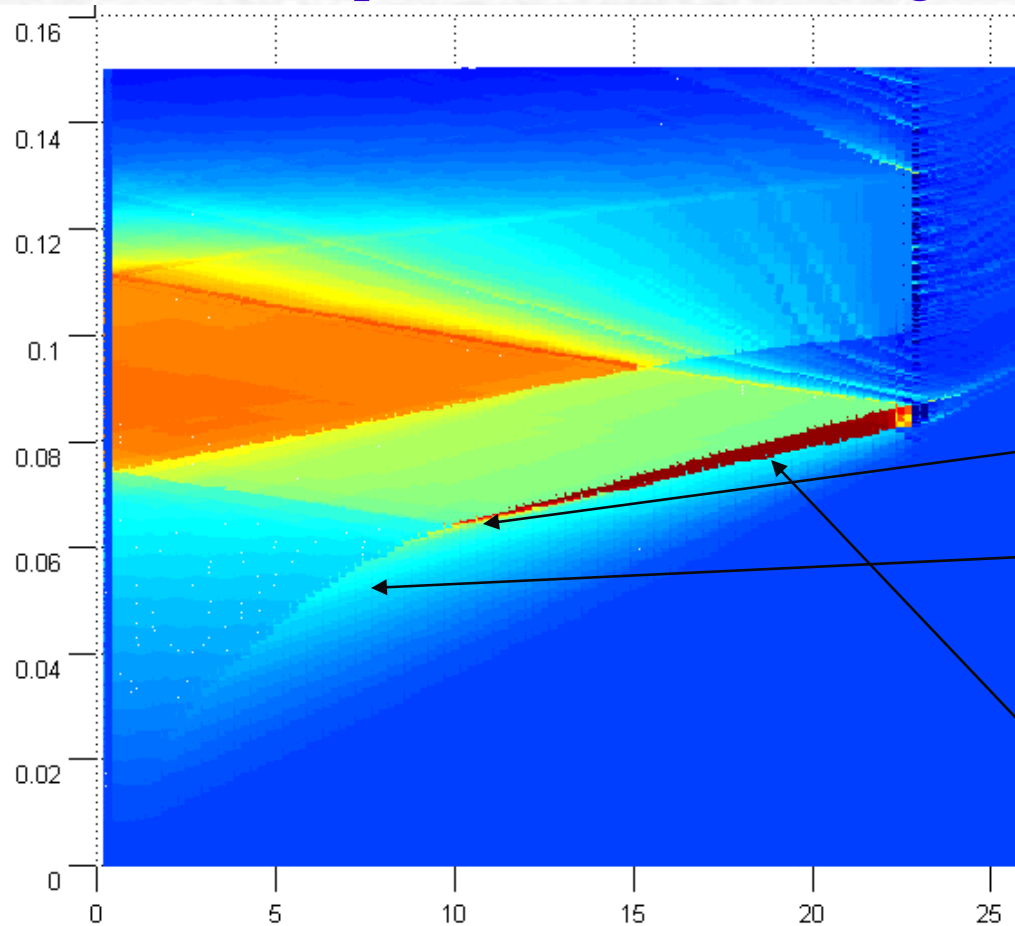
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Preliminary RCM Simulations of Pipe Explosions

Flame front position with time as given by the pressure field



General features are reproduced but the absolute times and pressures are incorrect

Shock formation following convergence of compression waves from the accelerating flame front is caught but we need a further transition to detonation criterion based on ignition delay data.

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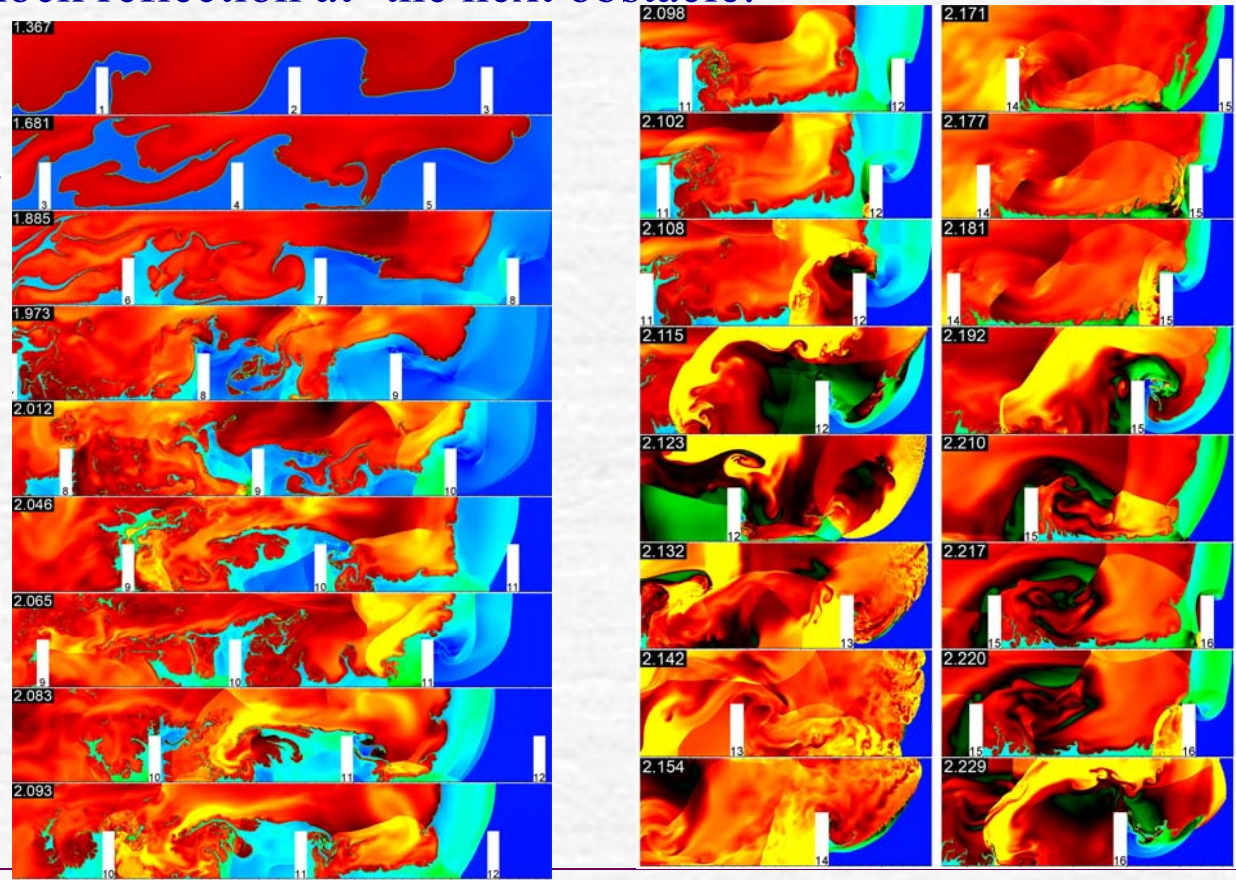
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Unconfined detonation

- Flame acceleration is now probably dominated by flow interaction with obstacles,, which continues up to the point where compressions again combine to give a shock. The final transition (not shown) follows initiation by shock reflection at the next obstacle:

images
courtesy of
Gamezo,
Takanobu,
and Oran



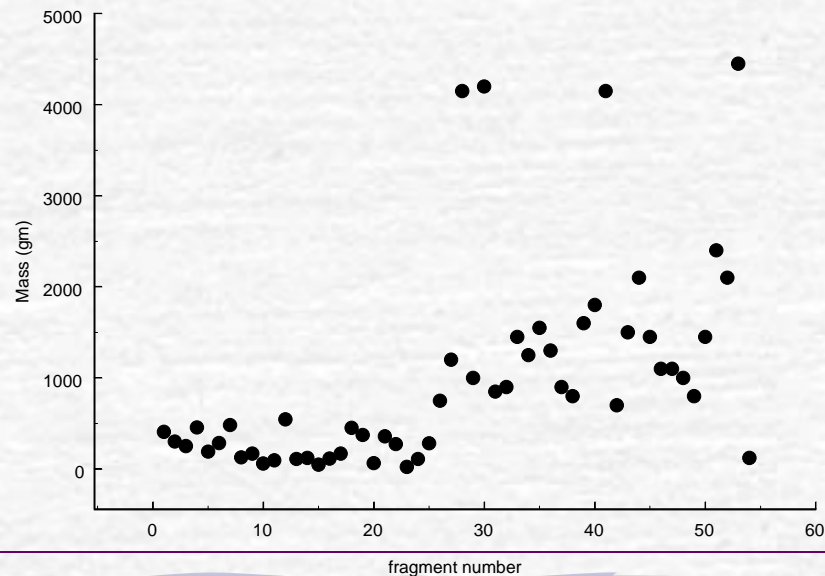
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Pipeline detonations: Possible consequences

- mechanical failure!, as with this HDPE pipe.
- Original 4 sections of 300mm diameter, these were reduced to 54 pieces after the passage of an ethylene-air detonation

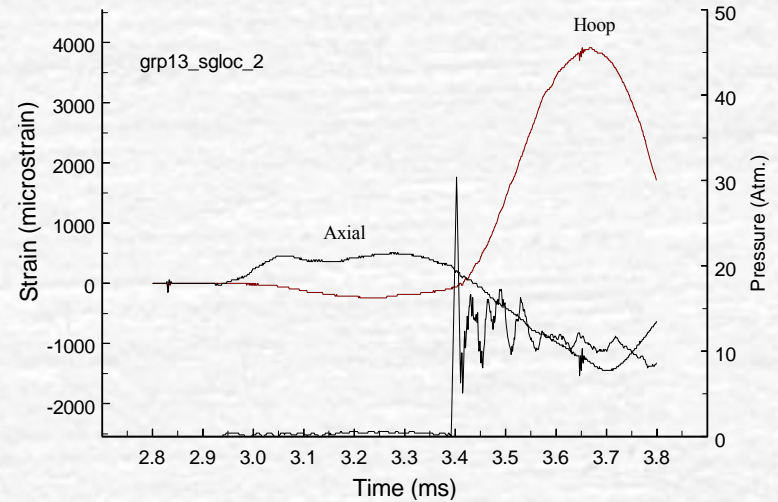
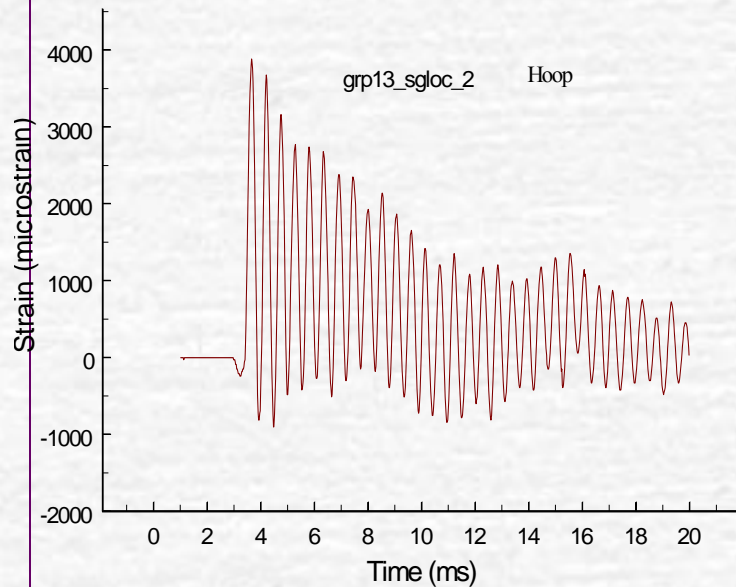


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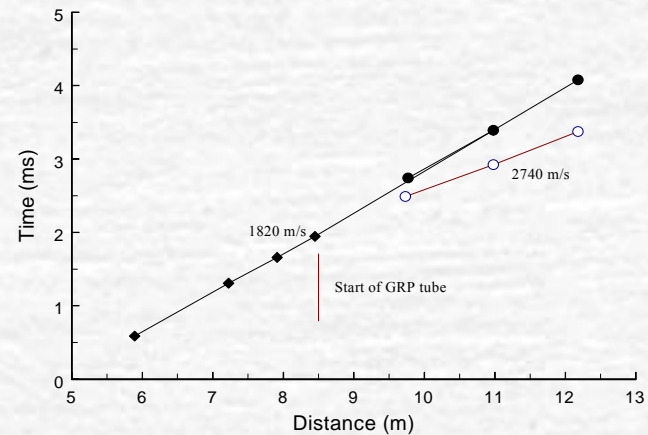
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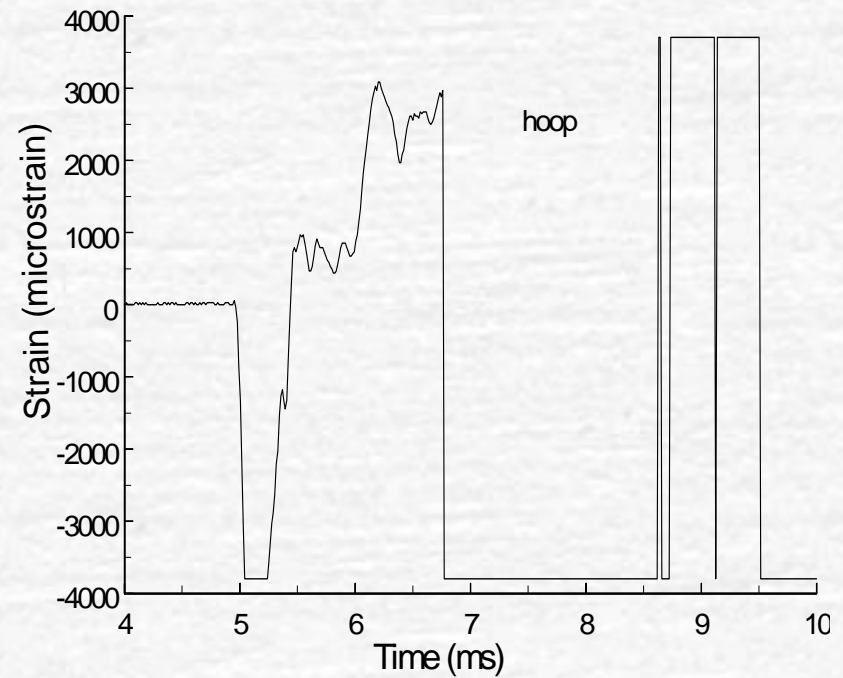
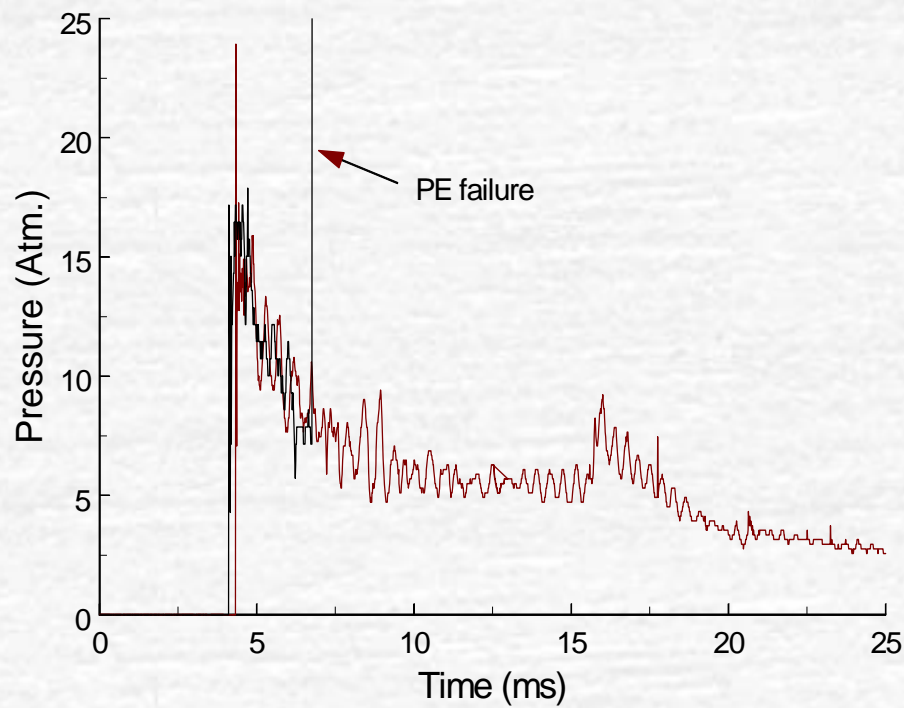
Passage of a detonation leads to axial and hoop strains in the pipe wall



The Propagation velocity of the axial wave is greater than that of the hoop strain, which is close to the detonation velocity



Until perhaps there is local mechanical failure

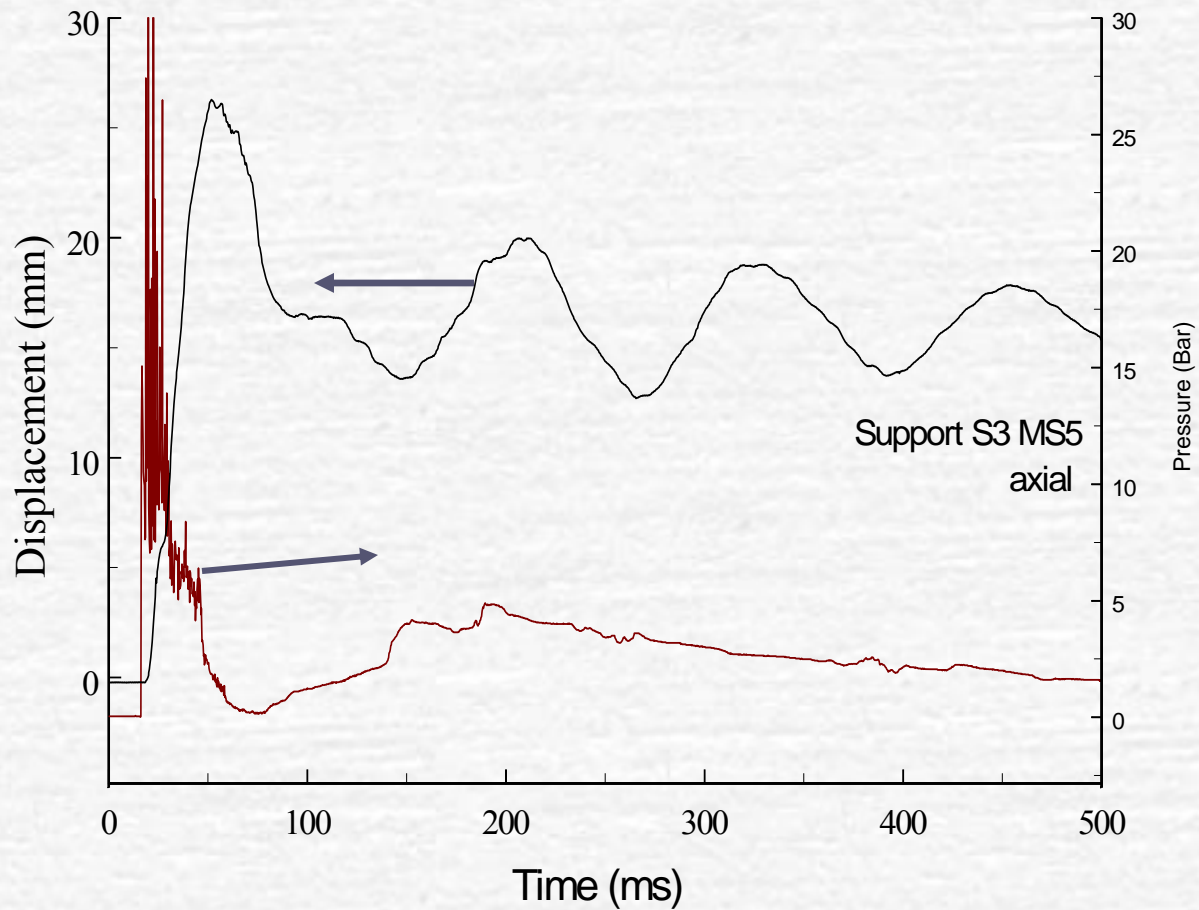


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However one must not forget the impulse imparted to the pipe supports



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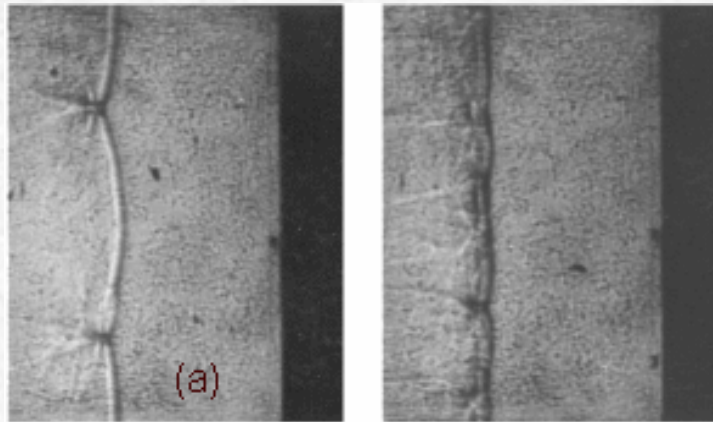
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Mitigation

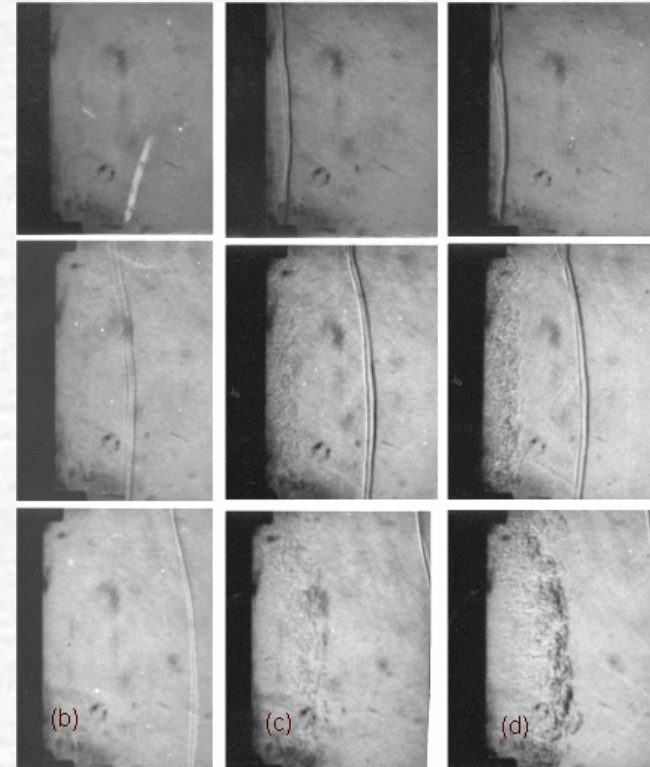
several approaches are possible:

- a) Dilution with an inert, usually nitrogen, to reduce intrinsic reactivity and detonability.
- b) For fuel- oxygen systems- robust controls on oxygen content
- c) Water sprays have been shown to work but have attendant problems as part of an active explosion barrier
- d) Passive explosion arrester devices

Detonation arresters



The exact mechanisms by which these work are not known precisely. Most are *assumed* to work by destroying the transverse wave structure and then abstracting heat energy and momentum from the detonation products.



Schlieren images of detonation waves incident on and hot gases emerging from a simulated crimped ribbon explosion arrester

Current capabilities and deficiencies

- We do not know how to characterize or rank the relative hazards of mixtures other than the widely studied hydrocarbons and hydrogen. Often the only recourse available is direct experimental testing using the final geometry and mixtures.
- There is a distinct lack of CFD capabilities that can predict accurately the generation of the compressed heated gas that undergoes the final onset of detonation process