# **Propagation of Gaseous Detonations in Small Tubes**

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#### **1** Introduction

For a confined detonation in a tube, both the initial and boundary conditions play important roles on the propagation and of a detonation wave and on the limits where a detonation wave fails. For small tubes, boundaries introduce heat, momentum and mass losses that cause detonation velocity deficits; a detonation will fail to propagate when the tube diameter is below a critical value. Theories for detonation limits resulting from these losses have been developed in the past. Zeldovich included heat and momentum loss terms in the equations for the detonation structure and found that the detonation velocity decreases with increasing losses. At some critical value of the losses, no steady solution to the conservation equations is possible [1]. The Fay model treats heat and momentum losses as boundary layer effects [2]. The boundary layer behind a propagating detonation wave leads to flow divergence in the reaction zone, and the effect is similar to that of wave curvature that results in a velocity deficit. When the velocity deficit exceeds a certain maximum value (or there is a certain critical curvature of the front), no steady ZND solution can be obtained. This can be interpreted as the onset of a detonation limit. These theoretical considerations of limits are based on the ZND model for the detonation structure where the propagation mechanism relies on the shock-induced autoignition. Experimentally, it has been demonstrated that these theoretical limits only agree well with measured limits for special mixtures that have been highly diluted with argon. In these mixtures, a detonation is highly stable, and its propagation mechanism can be described by the ZND model [3].

However, for most gaseous combustible mixtures, detonations are unstable. Instabilities have been known to provide an essential mechanism for detonation propagation and are manifested by the characteristic cellular structure of a self-sustained detonation. The unstable mode is a function of the boundary conditions. In addition to heat and momentum losses, the existence of detonation limits can be a direct consequence of the interference of the boundary conditions with the inherent instability of the detonation front. When the boundary conditions do not permit even the lowest unstable mode to occur, the detonation fails.

The important problem of limits has not been clearly resolved. Although there have been attempts to correlate limits with instabilities (e.g. detonation-cell size with critical-tube diameter), none of these correlations is found to have any general validity. The near-limit propagation of the detonation is very complex. A spectrum of unstable phenomena can exist near the detonation limits (e.g. spinning and galloping detonations). Furthermore, the dual failure mechanisms of losses and instabilities make a unique operational criterion for the onset of detonation limits difficult to specify.

Because of the effect boundary conditions, the propagation limits should be governed by the tube dimension and geometry. With the importance of instability for near-limit conditions, the tube diameter should be correlated to the characteristic length scale of the detonation itself. The detonation limits in a tube or a channel can be estimated with knowledge of the cell size  $\lambda$ , which is a function of the chemical composition of the mixture and initial thermodynamic conditions. In round tubes, the minimum tube diameter  $d^*$ , in which a detonation with a cell size of  $\lambda$  can propagate, can be estimated

by  $d^* = \lambda/\pi$ . In this case, the criterion for the detonation limit in a given tube is defined by the propagation mode of a spinning detonation [4], which has been considered as the limiting criterion [5, 6]. It is interesting to note that Schott observed spinning detonations even in mixtures highly diluted with argon [7]; however, these detonations were not stable and failed when perturbed. Once failed, a spinning detonation cannot regenerate itself again.

In this study, detonation limits in very small capillary tubes are investigated to study the detonation propagation limit. Both stable mixtures with high-argon dilution and unstable mixtures without argon dilution are used in these experiments. For stable mixture highly diluted with argon (for which instabilities are not important and where failure is due to losses only), the limit obtained experimentally will be compared with a ZND theory using a flow divergence (or curvature) term to model boundary layer effects. For unstable detonations in undiluted mixtures, regimes for different near-limit propagation modes of the detonation are studied. Different modes of detonation propagation will be observed in detail to investigate an operational criterion for the propagation limits.

### 2 Experimental details

A 1.0 m long steel detonation tube section with an inner diameter of 64 mm was used to generate a CJ detonation. The detonation then propagated into a 2.0 m long transparent test section. Perfluoroalkoxy (PFA) tubing of different diameters were used for the test section (d = 1.8, 6.3 and 9.5 mm). A sketch of the experimental apparatus is shown in Fig. 1. Stoichiometric mixtures of acetylene-oxygen, methane-oxygen, and acetylene-oxygen with 70% argon dilution were tested. Each explosive mixture was prepared in separate gas bottles. The amount of each gas required to make each mixture was calculated using the method of partial pressure. Once the gases were mixed together, they were left for 24 hours to become homogeneous.

The detonation tube was evacuated to at least 80 Pa. In order to ensure a uniform distribution of the explosive mixture in the test section, the detonation tube was overfilled from one end and evacuated from the other end to the desired test pressure. In all experiments, the sensitivity of the explosive mixture was varied by changing the initial pressure,  $p_0$ . A high-energy discharge spark of 800 J was used to directly initiatiate the explosive mixture. For the cases of very insensitive mixtures, a driver section was used. It was separated from the upstream steel section with a thin mylar diaphragm and filled with stoichiometric acetylene-oxygen at 30kPa. A manifold equipped with an Omega pressure transducer (PX02-I) and a Newport digital meter (IDP) was used to monitor the pressures in the detonation tube at any stage of the experiment.

Pressure transducers were used in the upstream detonation tube section to ensure that a CJ detonation was obtained prior to entering the transparent test section. A rotating-drum streak camera with a constant film speed of about 87 m/s was used to obtain self-luminous trajectories of the detonation wave propagating in the transparent test section. Near the failure limit, the spinning and galloping modes were expected to be observed. Four 1000µm fiber-optic probes were used in the the PFA transparent test section to obtain time of arrival measurements as the detonation propagated through the test section.



Figure 1. Schematic of the experimental apparatus

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## 3 Quasi-steady ZND theoretical analysis

To compare the experimental results and elucidate the failure mechanism, the velocity deficits and limits are calculated theoretically by solving the quasi-one-dimensional ZND structure equations with a curvature term and detailed chemical kinetics for the reactions. In the quasi-steady ZND formulation, the wall effect is modelled by the negative displacement thickness of the boundary layer behind the leading shock front following the pioneering work of Fay [2, 3, 8]. The effect of the viscous boundary layer tends to remove mass from the free stream flow and is accounted for by the flow of an inviscid fluid through an expanding nozzle where the cross-sectional area change is related to the displacement thickness of the boundary layer developed behind the shock front. The effective cross-sectional area of the tube at any point is given by  $A = \pi ((d + 2\delta^*)/2)^2$ . The area change and the mass displacement thickness  $\delta^*$  are given as:

$$\xi(x) = \frac{1}{A} \frac{dA}{dx} = \frac{4}{d + 2\delta^*} \frac{d\delta^*}{dx} \qquad \delta^* = 0.22 \cdot x^{0.8} \left(\frac{\mu}{\rho_0 D}\right)^{0.2}$$

The ZND model equations [9] with the flow divergence term in the conservation of mass equation and together with the chosen detailed chemistry model are solved numerically to seek the eigenvalue solution satisfying the generalized CJ criterion in order to achieve a continuous transition through the sonic plane (i.e. when the flow is choked in the frame of reference of the leading shock, the rate of chemical energy release must balance the rate of mass divergence). The system of equations was numerically integrated using the CHEMKIN II package. Following the methodology discussed in [9, 10], different detonation velocities were iterated to determine numerically the eigenvalue solution when the flow condition attained M = 1 in a continuous regular transition. The limit is achieve when the velocity deficits exceeds a certain maximum values (or a certain critical curvature of the front) and no steady ZND solution can be obtained. For both the acetylene-oxygen-argon and methane-oxygen mixtures, the UC San Diego reaction kinetic mechanism was used.

#### **3** Results and discussion

Results of the velocities found in the different capillary tubes are summarized and shown in comparison to the theoretical quasi-steady analysis in Figs. 2a to c for acetylene-oxygen with 70% argon dilution, acetylene-oxygen, and methane-oxygen, respectively. Typical self-luminous streak photographs are also shown to illustrate near-limit propagation phenomena that were observed (i.e. galloping and spinning modes). It was found that for the case of high-argon-diluted acetylene-oxygen mixtures, the detonability limits can be readily determined unambiguously from the velocity deficit plot. No unstable near-limit phenomena was observed. The agreement between the theoretical model and the experimental results is quite good, and hence, these results suggest that boundary conditions influence the propagation of stable detonation waves. Therefore, the failure of a stable detonation occurs mainly through the effect of boundary conditions on the ZND structure [3].

Although the ZND theoretical prediction gives a fair estimate of the limit for acetylene-oxygen without argon dilution, velocity fluctuations appear near the critical pressure at the limit where velocities measured from the streak photographs and light probes vary over a large range of velocity deficits. For the case of methane-oxygen, a spectrum of near-limit behaviors can be seen where the ZND curvature model fails to predict the limit. The ZND model predicts a larger critical pressure at the limit than those observed experimentally. It appears that the inherent instability of the detonation front tends to support the front from failure and allow the detonation to propagate at lower pressure, however, resulting from large fluctuation in velocities as shown in Fig. 2c.



Figure 2: Experimental results and comparison of theoretical model for (a)  $C_2H_2$ - $O_2$ -70%Ar; (b)  $C_2H_2$ - $O_2$ ; and (c)  $CH_4$ - $O_2$  mixtures.

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