

Analysis of Hydrogen Detonation Diffraction

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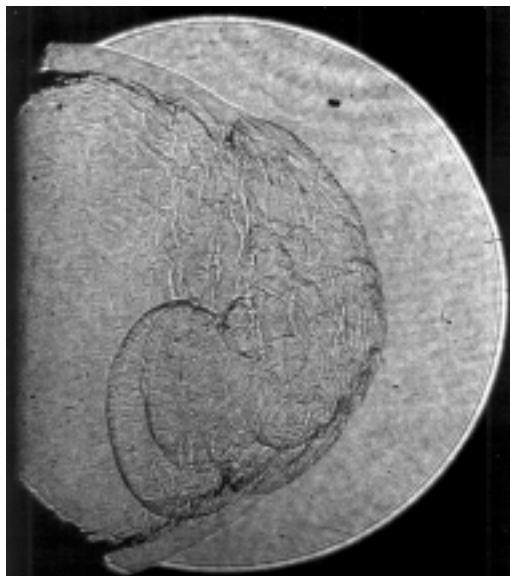
Abstract

Efforts are ongoing to develop a model which will permit a priori calculation of critical detonation diffraction conditions. A summary of initial experimental observations and computational results for hydrogen-oxygen-diluent detonations is provided, as well as an outline of the approach towards model construction.

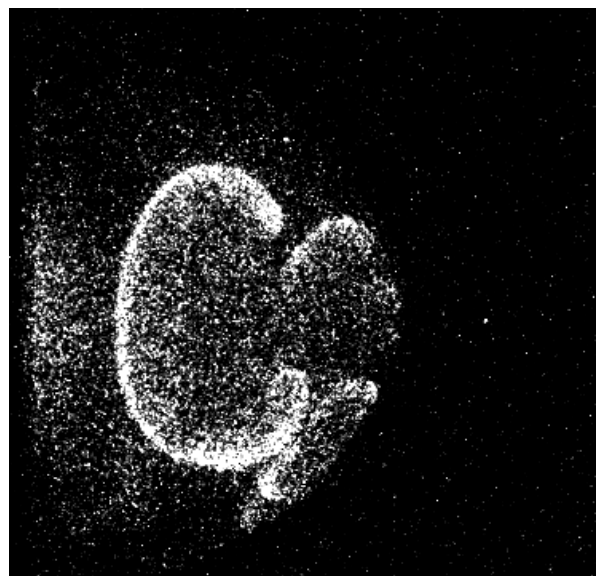
Introduction

Experiments and computational modeling are ongoing in an investigation of gaseous fuel-oxygen-diluent detonation diffraction. The outcome of a detonation wave propagating from a confined to an unconfined volume through an abrupt area change will fall into one of three regimes depending on initial and boundary conditions. The detonation is able to continuously transit the area change without failure in the super-critical regime. Sudden expansion from confinement results in shock wave separation from the reaction zone and complete failure of the detonation wave in the sub-critical regime. The critical regime is characterized by partial failure of the diffracting wave, followed by re-initiation leading to the detonation propagating throughout the unconfined volume (Fig. 1).

Detonation diffraction represents a fundamental process of interest to the scientific, safety, and propulsion communities. The critical tube diameter (d_c) from which a detonation diffracts is a characteristic length scale determined with much less ambiguity than the cell width. In addition, phenomena observed in the three regimes appear in all other detonation initiation, propagation, and failure processes. Although diffraction experiments and simulations have been previously conducted, the capability for a priori calculation of the critical conditions has not been achieved [1]. Experimental and computational results for hydrogen-oxygen-diluent mixtures are presented and analyzed to elucidate the dominant mechanisms involved and begin formulation of an analytical model. Future work will extend to ethylene and propane fuel based systems and continue the modeling effort towards the prediction of critical diffraction conditions.



(a) Ruby laser shadowgraph.



(b) Intensified CCD digital image.

Fig. 1 Detonation diffraction in $2H_2 + O_2$ at 62.5 kPa with re-initiation in progress.

Diffraction experiments were conducted with a 38 mm diameter, 1.5 m long tube coupled to a 152 mm square, 0.762 m long test section with optical access (Fig. 2). Detonations were initiated with a spark and turbulence-inducing spiral in the diffraction tube, and establishment of CJ conditions prior to diffraction was confirmed by piezoelectric pressure transducers. Diffraction into the test section was monitored with pressure transducers and flow visualization via ruby laser shadowgraph, ICCD digital imaging, and a framing camera shadowgraph system. Hydrogen-oxygen-diluent (argon, helium, carbon dioxide, nitrogen) mixtures provided variable initial conditions through the fill pressure, stoichiometry, and diluent type and concentration. The apparatus was evacuated to less than 10 Pa prior to filling with the partial pressure technique and recirculating the gases until uniformly mixed. A 280 mm diameter detonation tube was used to measure the cellular structure (cell width λ) of the mixtures by the soot foil technique.

A chemical equilibrium code was used to calculate the detonation velocity, post-shock conditions, and CJ conditions. Detonation reaction zone parameters were computed based on the ZND model to aid in the interpretation of experimental results and for use in developing a predictive analytical and computational modeling capability of the diffraction process. The one-dimensional reaction time/length (τ/Δ) is defined as the time/distance from the shock to the location of the maximum temperature gradient. Activation energies were calculated by varying the shock velocity off of V_{CJ} by $\pm 1\%$, essentially perturbing the post-shock temperature and determining the effect on induction time. Assuming the induction time for the overall chemical system is given by the Arrhenius expression $\tau = A \exp(E/RT)$, the activation energy (E) follows as $E/R = (\ln \tau_2 - \ln \tau_1) / (1/T_2 - 1/T_1)$, where R is the mixture gas constant, and states 1 and 2 refer to the perturbed conditions. The non-dimensional activation energy is defined by $\theta = E/RT_{VN}$, where T_{VN} is the post-shock temperature. The detailed reaction mechanism of Baulch et al. [2] was employed in all calculations, having been previously identified as the mechanism most suitable for hydrogen-oxygen-diluent detonation modeling through validation with shock tube induction time data [3]. Efforts continue on reaction mechanism validation for other fuels and to quantify uncertainties in calculated values.

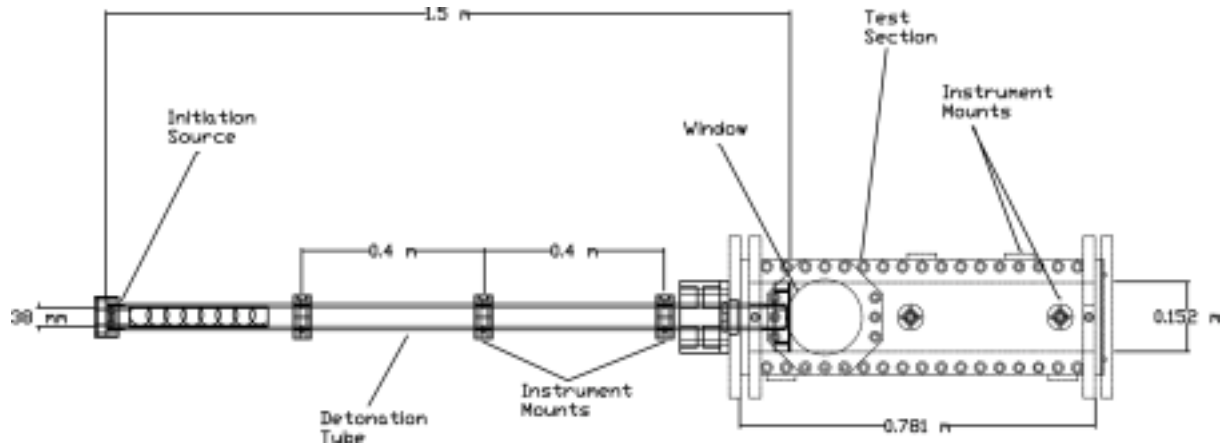


Fig. 2 Schematic of diffraction tube connected to test section.

Results

A summary of the critical diffractions conditions identified through the experiments and computations in this study are presented in Table 1. Tube diameter to average cell width ratios were found to lie between 10 and 25; cell width measurements for off-stoichiometric hydrogen-oxygen mixtures have not yet been obtained. There is no apparent correlation between the tube diameter and the reaction length, with the ratio of the two ranging from 400 to 700. Any correlation that may exist must be determined over a range of tube diameters, as has been investigated with regard to correlations between the tube diameter and cell width. Given the similar critical reaction lengths found in the present dilution series, this may lead to a $d_c - \Delta$ correlation which is not limited to fuel-oxygen-nitrogen systems as the $d_c - \lambda$ correlation is.

Table 1: Critical diffraction conditions with 38 mm tube.

Mixture Class	Variation	Critical Value	λ (mm)	Δ (mm)	τ (usec)	θ
$2H_2 + O_2$	Pressure P_1	53.1 ± 3.1 kPa	3.8 ± 1	0.096	0.183	19.53
$(2\phi)H_2 + O_2$	ϕ Fuel Lean	0.38 ± 0.01		0.056	0.141	33.95
	ϕ Fuel Rich	1.7 ± 0.2		0.078	0.125	17.54
$2H_2 + O_2 + \#Ar$	% _{vol} Ar	$66.4 \pm 1.1\%$	2.6 ± 1	0.068	0.163	7.30
$2H_2 + O_2 + \#CO_2$	% _{vol} CO ₂	$4.8 \pm 1.5\%$	1.5 ± 1	0.065	0.134	35.73
$2H_2 + O_2 + \#He$	% _{vol} He	$47.8 \pm 2.2\%$	1.8 ± 1	0.079	0.105	8.80
$2H_2 + O_2 + \#N_2$	% _{vol} N ₂	$18.6 \pm 1.4\%$	2.2 ± 1	0.067	0.143	18.49

The order of diluent effect on diffraction from most to least sensitive is carbon dioxide, nitrogen, helium, and argon. This sequence generally follows the order of θ , with higher θ values corresponding to mixtures with greater reaction zone temperature sensitivity (and therefore greater sensitivity to perturbation of the detonation front) as a result of the exponential dependence of the induction time on the activation energy. The argon and helium dilution cases provide a significant point of comparison. For a given diluent concentration, reaction times, non-dimensional activation energies, and post-shock (v_N) and equilibrium (CJ) temperatures and pressures are identical. The reaction lengths and velocities (acoustic and fluid) within the wave are much greater for helium diluent. This is a direct consequence of the low molecular weight of helium; otherwise these two diluents exhibit identical thermodynamic behavior. Greater disturbance propagation rates in the reaction zone afforded by helium diluent is responsible for the 48% critical dilution level versus 66% for argon.

Image sequences from the framing camera reveal that the portion of the detonation not processed by the disturbance caused by the area change continues to propagate at V_{CJ} . In addition, the disturbance propagates transverse to the detonation within 15% of the chemical equilibrium acoustic velocity (a_{CJ}), resulting in approximate expressions for the spatial slope and time for the disturbance to reach the tube axis (t_c) of a_{CJ} / V_{CJ} and $d / 2a_{CJ}$, respectively. The distance from the tube exit to the location of the disturbance reaching the tube axis (x_c) is then given by $dV_{CJ} / 2a_{CJ}$. All re-initiations were localized events, resulted in overdriven detonations, and were observed to occur in the vicinity of x_c at the critical conditions. V_{CJ} / a_{CJ} does not exceed 1.85 for any mixtures considered in this investigation, and therefore the diffraction regime is determined within the first tube diameter of axial propagation. Depending upon the test section geometry and location of diagnostics, interaction of the diffracting wave with the boundaries can make determination of the diffraction regime impossible. Therefore, diffraction investigations conducted without the aid of flow visualization to image the re-initiation source should be approached with caution.

Analysis

At present the complex cellular structure of a detonation renders the derivation of an analytical diffraction model including such detail intractable, and so the simplifying assumption is made that the cellular detonation can be approximated with one described locally by the ZND model. Consideration must be given to the physical processes involved local to the interaction between the disturbance and the detonation wave which influence whether the diffraction regime is sub- or super-critical. The energy release acts to support the continued propagation of the detonation, while the wave curvature and unsteady expansion associated with the disturbance at the front tend to decouple the shock-reaction zone complex. In certain cases this localized region can be considered quasi-steady and competition occurs between the energy release and curvature, whereas other situations lead to a primary competition between energy release and unsteady expansion [4]. These notions will be explored analytically and experimentally to determine if a dominant balance type of simplification can be made.

Analytical expressions must then be developed which can describe the competing processes so that they can be evaluated against one another, such as in the form of characteristic rates/times. Given validated detailed reaction mechanisms, the ZND model provides the energy release rate. Relations providing the curvature and unsteady expansion rates at the interaction point will require careful consideration of existing analytic approximations, possibly the development of new tools, and certainly validation against experimental measurements.

Key to this portion of the effort is an understanding of the nature of the disturbance and its traversing of the detonation front. Note that the disturbance is not simply an expansion wave originating at the area change and propagating behind the detonation in a transverse fashion at the equilibrium acoustic speed a_{CJ} . Skews considered the interaction of a disturbance with a shock and presented a geometric expression for the angle of the disturbance propagation relative to the tube axis [5]. Application of the Skews construction to a CJ detonation leads one to conclude that the disturbance would never affect the core of the diffracting detonation. The disturbance could propagate into the core if the disturbance were to travel transverse to the front at the frozen acoustic speed, but the rate is too slow when compared with experimental observations. Therefore, in the context of the ZND model, the disturbance propagates through the reaction zone between the shock and the sonic plane.

Once the aforementioned pieces are in place, the model can be completed to solve for the critical diffraction conditions by requiring that the energy release rate is able to overcome the curvature and/or unsteady expansion effect of the disturbance just as it reaches the tube axis.

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