Origins of turbulent mixing behind detonation propagation into reactive–inert gas interfaces

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1 Introduction

The interactions of mildly irregular detonation waves with sharp interfaces, separating combustible mixtures from inert gas, were modelled numerically. While detonation propagation into uniform mixtures has been studied extensively, detonation propagation into non-uniform mixtures has received much less attention. Specifically, situations where fuel concentration gradients lie perpendicular or oblique to the direction of the propagating detonation wave are not very well understood. Previous work on the topic include numerical simulations by Oran [1], and experiments and analysis by Tonello [2], in which detonation propagation into abrupt layers of reactive gas mixtures were considered. Furthermore, experimental work by Ishii and Kojima [3] considered the case of detonation propagation into diffuse mixing layers containing reactive and inert gases. Liebermann and Shepherd [4–6] also considered such arrangements, but isolating diffuse from sharp interfaces. More recently, detonation propagation in the presence concentration gradients and confinement has also been investigated [7,8]. While a curved detonation front and decoupling of the reaction zone from the leading shock wave were observed upon interaction with the mixing layer in all the previously cited studies, little focus was placed on experimentally examining the turbulent mixing zone (TMZ) and the source and influence of secondary combustion as the detonation propagated into the inert gas, except, perhaps, for the work of Liebermann [4]. Investigation of the source of turbulent mixing behind detonation waves upon interaction with gas interfaces requires further attention.

There have been several attempts to model detonation wave interactions with mixing layers, whose concentration gradients lie perpendicular to the initial wave flow direction [1, 9–13], however, all of these have been limited to regular mixtures with low activation energies using an inviscid formulation. None of these studies considered irregular detonations, nor addressed the affect of turbulent mixing on the wave structure as it passes through the reactive/inert interface. This work aims to address these shortcomings in order to gain further insight on the role of turbulent mixing on the observed wave structure for fuel rich ethylene-oxygen mixtures (i.e. mildly irregular detonations). For the purposes of this contribution, only interaction of detonation waves with sharp reactive–inert gas interfaces are considered. The objectives of this study are: (i) to validate the CLEM-LES approach [14] for detonation propagation into sharp interfaces following past experiments of Liebermann and Shepherd [4, 5]; (ii) to examine the source of instabilities in the resulting turbulent mixing zone that forms upon the interaction of a detonation wave with a sharp reactive–inert gas interface.

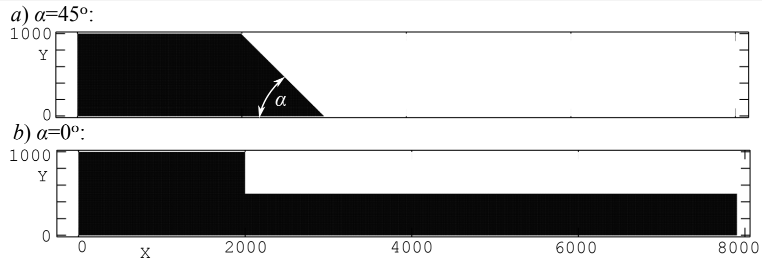

Figure 1: Initial profiles for reactive mixture and inert gas configuration. The dark regions represent the reactive fuel-oxidizer mixture, while the white regions represent the inert gas (or detonation products). A ZND detonation profile is initialized at $x = 0$.

2 Numerical Methodology

Two-dimensional simulations using the CLEM-LES approach were performed. The total domain size of each simulation was 8100 half reaction lengths ($\Delta_{1/2}$) long (x = 0.81 m) by 1000 $\Delta_{1/2}$ high (y = 100 mm); nearly to scale with the experiments of Liebermann and Shepherd [4, 5], which had a test section height of y = 150 mm. Several cases were considered as part of this investigation, here however, we focus on a sharp interface separating reactive mixture from inert gas at an angle of $\alpha = 45°$ and $\alpha = 0°$ (see Fig.1).

Particulars of the CLEM-LES formulation are published elsewhere [14], here, we list those specific to the case at hand. The chemical parameters ($Q = 116$, $E_a = 27.8$, $A = 40.7$, and $C_\kappa = 1.5$) were chosen to reproduce the correct detonation velocity of $M_{CJ} = 8.0$ (2620 m/s), half reaction length ($\Delta_{1/2} = 0.1$ mm), post-shock laminar flame speed ($S_L = 6.64$ m/s at $M_D = 0.7M_{CJ}$), and cell size ($\lambda \approx 2$ mm) for a fuel rich ethylene-oxygen mixture (2.5C_2H_4+3O_2) at $p_o = 11$ kPa. A resolution of $\bar{\Delta} = \Delta_{1/2}/8$ with 16 subgrid elements within each LES cell, providing an effective resolution of $\bar{\Delta}_{\text{eff}} = \Delta_{1/2}/128$, was found sufficient to resolve both the post-shock laminar flame speed, and the experimentally observed cellular patterns (see Fig.2). Differences in molecular weight between the inert gas (N_2), reactive mixture (2.5C_2H_4+3O_2), and detonation products were neglected. As a result, we consider only the transport of a single reactant species (Y), whose value of $Y = 1$ represents the unburned reactive mixture (2.5C_2H_4+3O_2), while $Y = 0$ is used to denote the inert gas (N_2) and detonation products.

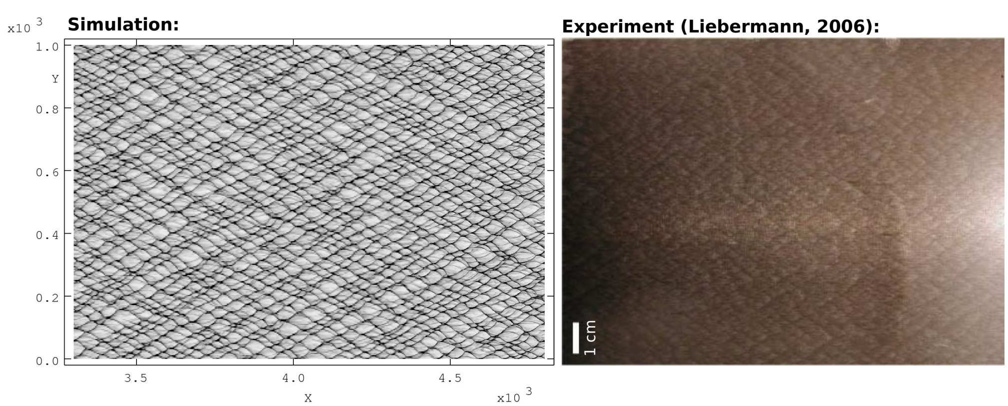

Figure 2: Comparison of numerical and experimental [4] sootfoil in 2.5C_2H_4+3O_2. Numerical cell size, 1.5 mm $\leq \lambda_{\text{sim}} \leq$ 4.5 mm; experimental average, λ_{exp} = 2 mm. (Scale: 1 cm = 100$\Delta_{1/2}$)

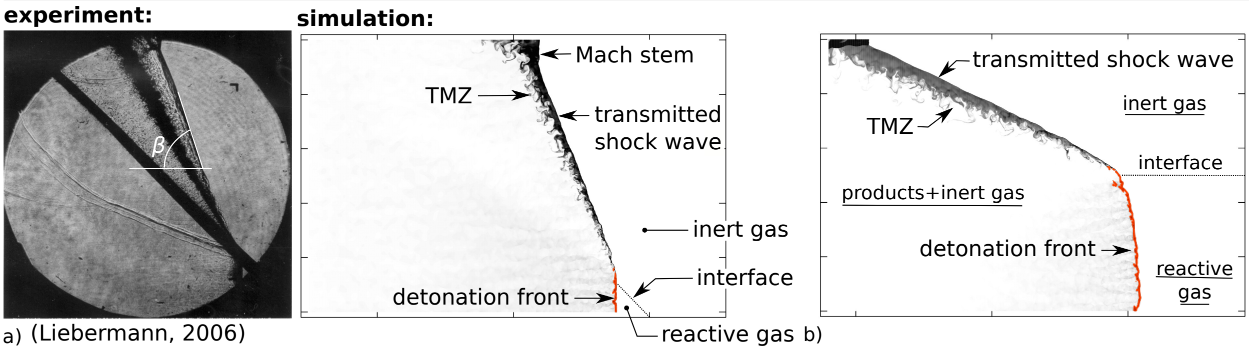

Figure 3: Resulting structure upon detonation interaction with a sharp interface at a) α = 45°; b) α = 0°. Experimental image [4]: Schlieren. Numerical images: density field with superimposed chemical reaction rate, $\bar{\dot{\omega}}$, in red. Experimental viewing window: 150 mm diameter; simulation height: 100 mm.

3 Results

In our first simulation, the detonation wave encountered a sharp interface with inert gas at α = 45° relative to the direction of wave propagation. An instantaneous snapshot of the resulting density field and a Schlieren image obtained from Liebermann [4] for the corresponding experiment are shown in Fig.3 a). A transmitted shock–TMZ complex formed as the wave travelled through the interface. Since there is no reactive gas present, the TMZ served only to mix detonation products with the inert gas. The transmitted shock waves from experiment and simulation were found to be in very good agreement, with angles of $\beta_{\text{exp}} = 70°$ and $\beta = 68.1°$, respectively. The numerical simulation also captured the experimentally observed formation of a Mach stem behind the transmitted shock reflection. Liebermann [4,5] found that by replacing the inert gas with oxygen, a much more pronounced Mach stem was observed. Liebermann attributed this observation to a postulated secondary combustion, where shock-heated oxygen was able to mix with the unbunred reactants present in the TMZ. However, this observation may also be attributed to changes in γ [15], which may result from the combustion process. In the limiting case of α = 0°, the lack of reactivity in the inert gas lead to a more pronounced decoupling of the transmitted shock wave and TMZ (see Fig. 3 b). The transmitted shock angle in this case was found to be $\beta = 25.7°$. Although less noticeable, the presence of a Mach stem was also observed in this case. Application of the CLEM-LES methodology was found to capture quite well the complex evolution of qualitative experimental features, these include the formation of a turbulent mixing zone (TMZ) separated by the incident shock by a gap of shocked gas.

To determine the growth of the TMZ evolution, flow fields from several dozen instances in time were superimposed and Favre-averaged, separately for each simulation, using the interaction point of the leading shockwave and reactive-inert gas interface as a reference. The density gradient fields for $\alpha = 0°$ and $45°$ are shown in Fig. 4. This averaging revealed smooth features of the transmitted shock, the TMZ thickness, and the gap separating the two. Owing to the self-similar nature of the wave dynamics obtained, various angles of interest were extracted accordingly for each simulation. These are reported in Table 1 where β is the transmitted shock angle; θ_{TMZ} and θ_{gap} are the angles associated with the TMZ size and gap size, as indicated in Figs. 3 and 4, respectively.

Note that while the measured β of simulation and experiment match within some margin of error, for $\alpha = 45°$, some discrepancies arise between the measured θ_{TMZ} and θ_{gap}. Each was numerically determined to be in the order of $\sim 2°$, Liebermann however, reported angles of $\theta_{\text{TMZ}} = \theta_{\text{gap}} = 7°$. There exists

Table 1: Wave and TMZ angles for detonation interaction with sharp interfaces.

α	β	$(\beta-\alpha)$	θ_{TMZ}	θ_{gap}
$0°$	$25.72 \pm 0.02°$	$25.72 \pm 0.02°$	$4.8 \pm 0.3°$	$2.7 \pm 0.1°$
$45°$	$68.1 \pm 0.1°$	$23.1 \pm 0.1°$	$2.0 \pm 1.3°$	$1.8 \pm 0.7°$
$45°$ (exp) [4]	$70 \pm 1°$	$25 \pm 1°$	$7 \pm 1°$	$7 \pm 1°$

several challenges in experimental measurement which contribute to this discrepancy: (i) the experimental measurement of θ_{TMZ} was taken directly from a single instantaneous Schlieren image. Locating the start and end points of the TMZ must be done subjectively to a flow field that is very turbulent, and difficulties arise in choosing satisfactory limits for θ_{TMZ}; (ii) ensuring the correct orientation of the detonation wave likely contributed to the largest source of error in the experiment; (iii) the presence of the diaphragm in the experiment may have influenced the growth rate of the TMZ. Despite the difference in θ_{TMZ} measured between simulation and experiment, of particular interest, is how the size of the TMZ at lower angles, namely $\alpha = 0°$, is much larger compared to the $\alpha = 45°$ case. Indeed, analysis performed by Liebermann indicated that as $\alpha \to 0°$, the shear layer growth in the TMZ resulting from Kelvin-Helmholtz instability, also approaches to zero [4]. Unfortunately, experiments were not conducted to verify this, nevertheless, the discrepancies found from our simulations warrant further analysis to determine the source of turbulent mixing in the observed TMZ, and to what extent shear due to a mismatch in velocity across the TMZ plays a role.

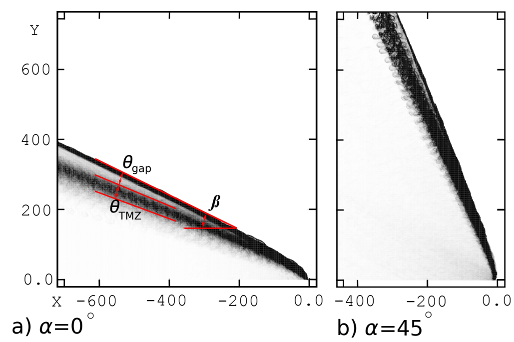

Figure 4: Numerical Schieren images super-imposed for each angle a) $\alpha = 0°$, and b) $\alpha = 45°$.

4 Discussion

Inert simulations in the frame of reference of the node were conducted using the CJ solution/states as initial conditions. Changing the of frame of reference has the benefit of removing the influence of the cellular structure from the flow field, allowing to isolate the contributions of Kelvin-Helmholtz instability to the TMZ growth.

Here, the same resolution and interface angles (α) as the lab-frame simulations were used but the domain size was reduced to a square of side $1000\Delta_{1/2}$ with the node centered at $(x, y) = (0, 0)$. The flow variables for the inert simulations are given by:

$$p(x,y) = p_{cj} = \frac{p_o + \rho_o D_{cj}^2}{\gamma + 1}; \quad u(x,y) = u_{cj} - D_{cj} = \frac{p_{cj} - p_o}{\rho_o D_{cj}} - D_{cj}$$

$$v(x,y) = D_{cj} \tan\alpha; \quad \rho(x,y) = \rho_{cj} = \frac{\rho_o D_{cj}}{D_{cj} - u_{cj}}, \tag{1}$$

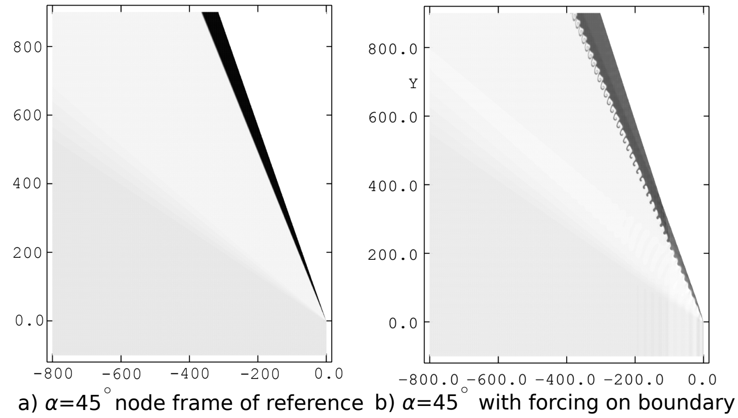

Figure 5: Instantaneous density fields of inert simulations in the frame of reference of the node.

where $\rho_o = 1$, $p_o = 1/\gamma$, and $D_{cj} = 8$. The right boundary, at $x = 0$, was prescribed to have the following conditions:

$$\rho(0,y) = \begin{cases} \rho_o & \text{if } y > 0 \\ \rho_{cj} & \text{otherwise} \end{cases} \quad ; \quad u(0,y) = \begin{cases} -D & \text{if } y > 0 \\ u_{cj} - D_{cj} & \text{otherwise} \end{cases}$$

$$v(0,y) = \ D_{cj} \tan\alpha \quad \text{for all } y \ ; \quad p(0,y) = \begin{cases} p_o & \text{if } y > 0 \\ p_{cj} & \text{otherwise} \end{cases} \tag{2}$$

The remaining boundaries were set to Von-Neumann type. The resulting unsteady flow was allowed to evolve naturally up to $t = 500$ (150 µs), sufficiently long to reach a steady structure.

An instantaneous density field for $\alpha = 45°$ is presented in Fig. 5a. Upon measuring the various state properties and wave angles, we found that the inert computation matched closely the gasdynamic solution for a perfect gas [4]. Additionally, very little shear was found to occur. Remarkably, by removing the cellular instabilities at the detonation front, the TMZ growth was nearly imperceptible.

To further investigate the influence of instabilities originating at the detonation front on the TMZ evolution, we considered the same inert setup but imposed controlled sinusoidal perturbations to the CJ-inflow boundary condition, such that the pressure in Eq. (2) is replaced with

$$p(0,y) = \begin{cases} p_o & \text{if } y > 0 \\ p_{cj} + 15\sin(2\pi t/2.5) & \text{otherwise} \end{cases}$$

The amplitude for p was chosen to be representative of the pressure pulses associated with changes in the detonation velocity up to 25% the CJ value, which may be expected owing to the true unsteady nature of detonations. The period of the forcing was chosen to roughly reflect the time it takes for a detonation wave to pass over a characteristic cell size.

In Fig. 5b the density field obtained for $\alpha = 45°$ resulting from the sinusoidal forcing is shown at a time in which a quasi-steady regime of the TMZ was established. Notably, the pressure fluctuations imposed seem to have a much larger influence on the TMZ evolution and growth compared to velocity shear alone. Upon time-averaging the flow fields obtained from the latter simulation and measuring the TMZ growth, $\theta_{\text{TMZ}} = 0.98 \pm 0.18°$ which is comparable to the lab-frame results for $\alpha = 45°$, where $\theta_{\text{TMZ}} = 2.0 \pm 1.3°$

and much larger than the value obtained for the simulation without forcing, $\theta_{\mathrm{TMZ}} = 0.28 \pm 0.05°$. Based on the previous results, it appears that pressure pulses originating from the unsteady cellular detonation front are largely responsible for the observed TMZ growth. To what extent, however, remains to be determined. We do anticipate that pressure pulses, including transverse waves, from the real unsteady detonation front to have a much higher impact on the shear layer growth in the TMZ.

5 Conclusions

Detonation propagation into sharp interfaces of reactive and inert gas was investigated using the CLEM-LES framework, and validated with previous experiments [5, 6]. The full-scale simulations were found to do a reasonable job at recovering experimental flow features, which consisted of a transmitted shock wave–TMZ complex, and a Mach stem. Upon re-casting the simulations in the frame of reference of the node, and by removing instabilities at the detonation front, shear growth rates were found to be insignificant when perceived from the node. Upon perturbing the detonation front pressure, in the latter simulations, it was found that the observed shear growth is heavily influenced by instabilities at the front.

This research was enabled in part by high performance computing resources provided by the Core Facility for Advanced Research Computing at Case Western Reserve University.

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