Numerical study of detonation transmission and propagation through a gravity-driven layer of hydrogen-oxygen over an inert gas

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1 Introduction

An important aspect of explosion safety is predicting detonation propagation in a combustible cloud that forms following an accidental release. When buoyancy is important, as is the case with light or heavy fuels, such clouds take the form of a stratified layer bounded by a single solid wall. Partially confined reactive layers are also found in rotating detonation engines and has also generated research interests in layer detonation waves.

While there have been a number of numerical studies on detonation propagating in a combustible layer with a sharp interface [1, 2], there are less numeric studies on propagation in layers with a diffuse interface. Recently a numerical investigation was performed by Melguizo-Gavilanes *et al.* [3], simulating detonation propagation in a gravity-driven layer performed by Leiberman et al. [4]. They checked the applicability of the Bauwens and Dorofeev detonation failure criterion [5] that states there is a critical cell size gradient of $\mathrm{d}\lambda/\mathrm{d}x = 0.1$. They proposed a modified critical cell size gradient of $\mathrm{d}\lambda/\mathrm{d}x = 0.4$ from their simulations.

This study simulates experiments [6] carried out in a narrow channel where a detonation wave propagates through a gravity-driven stratified layer of hydrogen-oxygen above an inert gas with a diffuse interface. The objective of this study is to investigate detonation failure observed in the experiment that is not predicted by the Bauwens and Dorofeev [5] cell size gradient failure criteria and hypothesized to be because of insufficient number of cells needed for a detonation to propagate.

2 Model and numerical method

The 2D compressible, reactive flow is modelled using the Euler equations for a perfect gas. The chemical reaction is modelled with a single step Arrhenius rate law

$$\hat{\omega} = \hat{k}\hat{\rho}(1-Y)^{\nu}\exp\left(-\hat{E}_a/\hat{R}\hat{T}\right),$$

where k is the pre-exponential factor, $\nu = 1$ is the reaction order, E_a is the activation energy and R is the gas constant. The reaction progress variable Y has values between $Y = 0$, representing an unreacted

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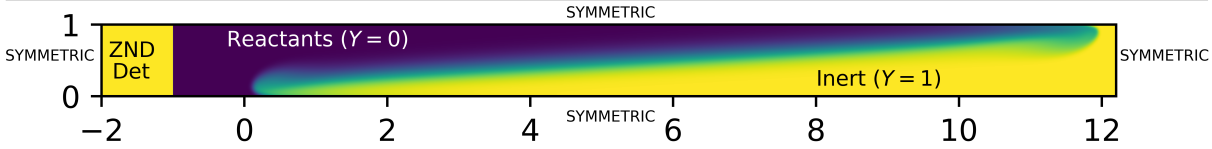

Figure 1: Initial reaction progress as mass fraction Y, consisting of argon in the gravity current and combustion products behind the detonation

mixture, and $Y = 1$ for a reacted mixture. Temperature T, pressure p and density ρ are related through the ideal gas equation of state.

The equations are non-dimensionalized, choosing initial density, pressure and temperature for their respective scales. Length is scaled by the channel height $\hat{h} = 63.5$ mm. The dimensionless variables are as follows

$$p = \frac{\hat{p}}{\hat{p}_0}, \qquad \rho = \frac{\hat{\rho}}{\hat{\rho}_0}, \qquad T = \frac{\hat{T}}{\hat{T}_0}, \qquad x = \frac{\hat{x}}{\hat{h}}, \qquad y = \frac{\hat{y}}{\hat{h}},$$

The heat release $Q/RT_0 = 23.15$ is determined using Chapman-Jouguet theory [7] to match the detonation Mach number in $2H_2 + O_2$. The von Neumann isentropic exponent $\gamma = 1.315$ was used throughout the domain. The pre-exponential factor k scales the reaction to give the correct non-dimensional ZND half-reaction length.

The activation energy E_a governs the reaction sensitivity to temperature and is quantified using the San Diego mechanism [8], reduced for hydrogen chemistry, for a constant volume reaction of the reactants at the von Neumann state. For $2H_2 + O_2$ at initial pressure $\hat{p}_0 = 101.325$ kPa and temperature and $\hat{T}_0 = 300$ K, an activation energy $E_a/RT_0 = 28.2$ is used. A non uniform distribution of temperature exists in the numerical domain as density and pressure were chosen to match the initial conditions of the physical study. The employed value of activation energy is lower than the typical values of activation energy ($E_a/RT_0 \sim 40$) of the reactant mixture at initial conditions as it allows ignition to seep further into the diffuse inert layer where there is a larger concentration of inert gas and temperature is lower since density was chosen to be true to the experiments. Figure 2 demonstrates the ignition time between these two activation energies. The increment of ignition time happens at larger inert concentrations for $E_a/RT_0 = 28.2$ as opposed to the larger E_a/RT_0. A study where adjusted values of E_a/RT_0 that accounts for the non uniformity of temperature in the numerical domain is currently underway.

2.1 Initial and boundary conditions

A 3D simulation of the gravity current of the physical experiment [6], where premixed stoichiometric hydrogen-oxygen stratifies over argon, is done in ANSYS Fluent. The composition distribution (mass fraction is provided in figure 1), pressure, density and velocity from the Fluent simulation are imported as initial conditions into `mg` [9], the compressible reactive gas dynamics code. In order to release heat at the diffuse interface, where there is a concentration gradient of the reactive mixture, the mass fraction of the inert gas (argon) from the gravity current simulation is initialised to be the reaction progress variable Y. In doing so, no heat is released where the inert gas concentration is 100% ($Y = 1$), the full theoretical heat is released where the reactant concentration is 100% ($Y = 0$), and a fractional value of the theoretical heat corresponding to the reactant concentration is released in the diffuse layer ($0 < Y < 1$).

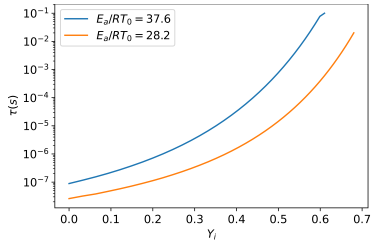

Figure 2: Ignition time vs inert mass fraction for a single-step perfect gas model

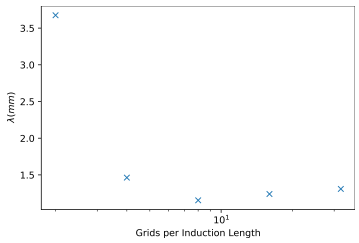

Figure 3: Detonation cell size measured for different grid resolution

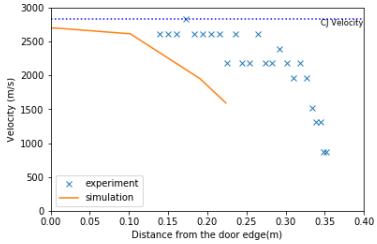

Figure 4: Detonation velocity along the top wall; $E_a/RT_0 = 28.2$, $\gamma = 1.315$

As shown in figure 1, a self-sustained ZND detonation was placed at $x = -1$ just before the argon layer that extends all the way to the end of the channel. Symmetric boundary conditions are specified on all the walls.

2.2 Resolution study

The 2D compressible Euler equations are solved using the computational package mg [9]. An exact Godunov [10] scheme with a van Leer flux limiter [11] is used to achieve a second-order solution in space, and a predictor-corrector scheme achieves a second-order solution in time. The numeric grid has a width of 18000 $\Delta_{1/2}$ (11.5 h) and a height of 1300 $\Delta_{1/2}$ (1 h). The equations are discretized over a 1128×84 Cartesian mesh. Adaptive mesh refinement [12] is used to increase the accuracy over the regions of interest. The resolution is doubled until seven levels of refinement are reached. This results in a maximum grid of 144384×10752, or 8 grids per half-reaction length.

In order to determine the resolution required for cell size convergence, a series of simulations with the channel filled with uniform premixed reactants were performed. The maximum pressure in each grid throughout the domain was recorded to generate a numerical soot foil. The cell size from the numeric soot foils was compared for different grid resolutions in figure 3.

For meshes with more than 8 grids per induction length, the measured cell size remained the same. The calculated numerical cell size was $\lambda_{\text{num}} = 1.15$ mm while the experimental cell size reported by Denisov and Troshin [13] was $\lambda_{\text{exp}} = 1.39$ mm.

3 Results and Discussion

The detonation in the simulation travels at the theoretical CJ velocity, measured along the top wall, for most of the channel but fails well before what was observed in the experiments [6] (see figure 4). This deviation could be a result of the single-step reaction model.

Simulations were run at different activation energies, while keeping all other thermodynamic parameters and the half reaction length constant. Increasing the activation energy resulted in the detonation failing earlier, see figure 5a), while decreasing the activation energy to account for the argon diffusion into the layer made the detonation propagate further along the layer. Although the constant E_a/RT_0 is a good approximation, it is not capable to fully replicate the detonation characteristics incurred in experiments. In order to better match with the physical experiments, the choice of E_a/RT_0 should be such that the detonation fails at the same location in the channel.

Another limitation of the model is that it only uses a single value of the isentropic constant γ, independent of Y. Simulations where a compensated value of the isentropic constant $\gamma = 1.49$, which

incorporated the isentropic constant of argon resulted in detonation propagation further along the layer than when $\gamma = 1.315$, see figure 5b). Note, to keep E_a/RT_{vN} the same while increasing γ to 1.49 requires increasing E_a/RT_0 from 28.2 to 32.21.

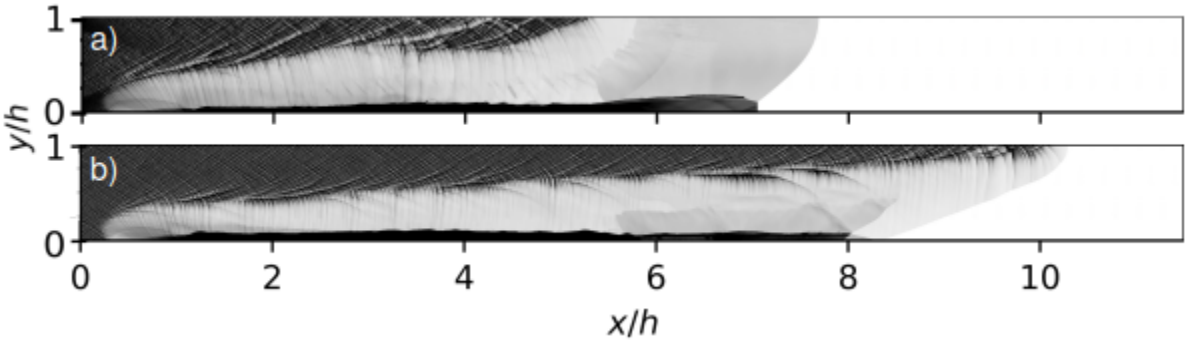

Figure 5: Numerical soot foils for a) $E_a/RT_0 = 45$, $\gamma = 1.315$; b) $E_a/RT_0 = 32.21$, $\gamma = 1.49$

The use of constant properties in the perfect gas law can also cause a deviation from experiments. The ZND half-reaction length calculated from the perfect gas assumption grows faster in argon dilution. The difference in γ between the reactive and inert layer results in a higher acoustic impedance and offers more confinement. However, this is not replicated in the perfect gas simulations, since only one value of γ is be used. A larger ZND half-reaction length would mean a larger cell size which would result in the detonation decoupling earlier. A better reaction model should be developed when using the perfect gas assumption for the simulations and is left for future studies.

3.1 Failure Criteria

The ZND half-reaction length of a stiochiometeric composition of $H_2 - O_2$ increases rapidly for argon dilution mole fraction greater than 70% by mole (88% by mass). Lieberman [4] used this as a detonation failure criterion. The simulations shows good agreement with Lieberman et al.'s [4] failure criterion along the bottom layer interface, where the reactant and argon gases meet to create a stratified layer. Figure 6 shows an overlay of the argon concentration distribution and the numerical soot foil. The cells enlarge at the bottom boundary of the layer (where the argon concentration is roughly 70%, denoted in green). At $x \approx 9.5$, the detonation fails, producing scattered triple-point trajectories, typical of a decoupled detonation wave.

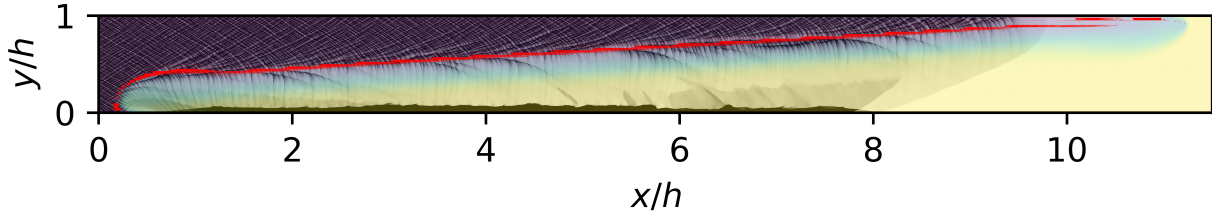

Figure 6: Numerical soot foil with initial argon concentration and $\mathrm{d}\lambda/\mathrm{d}x = 0.1$ contour overlay; $E_a/RT_0 = 28.2$, $\gamma = 1.315$

The Bauwens and Dorofeev [5] failure criterion indicates that a detonation fails to propagate in a nonuniform mixture where the spatial gradient in the cell size is greater than $\mathrm{d}\lambda/\mathrm{d}x > 0.1$. Using the argon mass fraction distribution from the gravity current simulation, the appropriate heat released throughout

the layer is calculated and the ZND half-reaction length is determined throughout the domain. Assuming a linear relationship between the cell size and the ZND half-reaction length in the undiluted reactant ($Y = 0$), a scaling factor is determined. The cell size for all points in the domain is then calculated by multiplying the scaling factor with the ZND half-reaction length. The gradient in cell size over the domain is then calculated and the contour corresponding to $\mathrm{d}\lambda/\mathrm{d}x = 0.1$ is shown in figure 6.

While 70% argon and the $\mathrm{d}\lambda/\mathrm{d}x = 0.1$ failure criteria hold true for the bottom layer interface it still does not predict the detonation failure before the leading edge of the layer ($x > 9.5$, $y > 0.75$), where the reactant mixture is still present and meets both criteria.

The Bauwens and Dorofeev [5] failure criterion also states that the detonation needs 5-10 cells across the layer height in order to avoid decoupling. In order to test this criterion and confirm that the cell size gradient is not the reason causing the detonation to fail, the inert argon layer is modified by eliminating the axial gradient and extending the layer from different axial positions (while keeping the vertical gradient constant). In doing so, a critical layer thickness can be found, independent of the axial gradient that was removed.

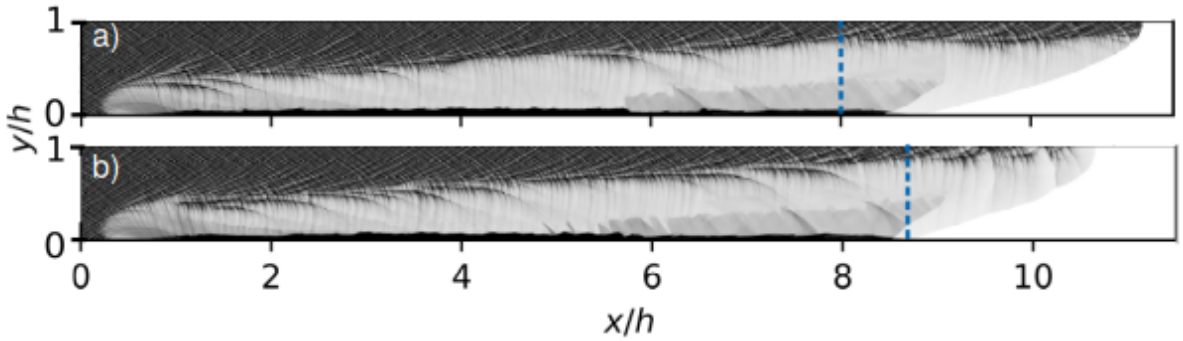

Figure 7: Numerical foil for the layers a) extended at 5-7 cells across the channel, starting $x = 8$; b) extended at 3-5 cells across the channel, starting at $x = 8.75$; vertical lines indicate beginning of layer extension; $E_a/RT_0 = 28.2$, $\gamma = 1.315$

The numerical soot foil for a layer that was extended starting at $x = 8$, where there are 5-7 cells across the layer, is provided in figure 7a). The detonation propagates the full length of the channel. For the case where the layer is extended from where there are only 3-4 cells across the layer, the detonation fails soon after. The numerical soot foil in figure 7b) shows the cell structure fades away as the triple points do not regenerate.

In both the modified layer cases, Lieberman *et al.* [4] and the $\mathrm{d}\lambda/\mathrm{d}x = 0.1$ failure criterion hold true for the bottom layer. The above findings support Bauwens and Dorofeev criterion [5] that 5-10 cells across the layer are required for a detonation to propagate.

4 Conclusion

Numerical simulations of detonation propagation through a layer of stoichiometric hydrogen-oxygen over argon were performed and compared to experimental results [6]. The detonation wave failed before the end of the layer, just as in the experiment. The exact decoupling location did not match perfectly with the experiment, this is believed to be a consequence of the approximations associated with a single-step reaction model, the non uniform distribution of temperature, and the perfect gas limitation of a constant γ. Further work varying activation energy with mixture composition is being conducted.

The numeric simulations confirmed the failure criterion proposed by Bauwens and Dorofeev [5]; specifically the $\mathrm{d}\lambda/\mathrm{d}x = 0.1$ propagation limit applied along the bottom layer interface, and the 5-10 cell requirement applied at the layer leading edge, where the detonation failed well before the $\mathrm{d}\lambda/\mathrm{d}x = 0.1$ limit.

An investigation on varying activation energy spatially to account for the non uniform distribution of temperature and better replicate the detonation failure under the limitations of a single step perfect gas model are currently underway.

5 Acknowledgements

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