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Quenching limits and dynamics of multidimensional detonation waves confined by an inert layer

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Abstract: Two-dimensional inviscid simulations are conducted to assess the effect of chemistry modeling on the detonation structure and quenching dynamics of detonations propagating into a semiconfined medium. Two different simplified kinetic schemes are used to model the chemistry of stoichiometric H₂-O₂ mixtures: single-step and three-step chain-branching chemistry. Results show that the macroscopic characteristics of this type of detonations (e.g. detonation velocity and cell size irregularity) are very similar for both models tested. However, their instantaneous structures are very different before and upon interaction with an inert layer. Specifically, the minimum reactive layer height, h_{crit} , capable of sustaining detonation propagation is larger when a more realistic description of the chemistry is used. This outcome suggests that the quenching limits predicted numerically are dependent on the choice of chemical modeling used.

Keywords: *Detonation dynamics, simplified kinetics, quenching limits, numerical simulation*

1. Introduction

Understanding non-idealities and predicting detonation propagation limits in Rotating Detonation Engines (RDE) is of prime importance for realizing its practical implementation. The very complex, three-dimensional flow field present in real RDE can be approximated by an unrolled, planar projection in which the detonation front is propagating in a layer of reactive mixture bounded at the top by an inert layer. This canonical configuration has also profound implications for safety hazards.

Classical experiments by Dabora et al. [1] using this configuration revealed a velocity deficit due to the lateral expansions of the products and the curvature of the detonation front. Experimental diagnostics are limited due to the small length and time scales inherent to the phenomenon which renders it inaccessible for optical/flow visualization. Numerical simulations offer an alternative to gain insight into the dynamics of detonation waves in RDE-like configurations. Recent work [2, 3] showed an interesting, rather complex front structure near the interface between reactive mixture and inert gas.

Reynaud et al. [2] used single-step chemistry to mimic stable and unstable mixtures. They found that the inert confinement influences the detonation propagation differently depending on the mixture sensitivity. Unstable mixtures are essentially driven by the generation of transverse waves

whereas stable mixtures seem to be only more gradually affected by the front curvature caused by lateral flow expansion. These waves emanating from the reactive-inert interface induce the quenching of the detonation below a certain critical height, h_{crit} . While previous numerical findings using single-step chemistry report significantly larger h_{crit} for unstable than stable mixtures [2, 4], experimental studies on detonation undergoing lateral losses reported contradictory results [5].

To potentially gain some insight into the source of this discrepancy, the present work uses two different chemical models of increasing complexity (i.e. single-step and three-step chain-branching chemistry) to assess their effect on quenching limits predictions for detonation propagation in a semiconfined environment. The detonation front dynamics and the two-dimensional structure of the front during steady propagation and quenching are examined.

2. Computational methodology

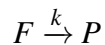
2.1 Governing equations and numerical techniques

The flow at hand is described by the compressible reactive Euler equations. Particulars about the numerical methods used, spatial and temporal discretizations as well as the parallelization methodology can be found in [2]. Briefly, we used a time-operator splitting to couple the hydrodynamics and the chemistry together with directional splitting, and a ninth order monotonicity preserving interpolation in space, and a third-order explicit Runge-Kutta integration in time. Simulations were run in the laboratory frame of reference using a sliding window technique to keep the propagating detonation within the computational domain at all times [2, 6]. Details of the simulation setup are described in subsection 2.3.

2.2 Chemistry modeling

The chemistry is modeled using two simplified kinetic schemes: single-step and three-step chain-branching to assess their effect on the detonation front structure and quenching dynamics. While one-step descriptions of the chemistry have been the standard in the detonation modeling community, three-step chain-branching models, although available in the literature for a long time [7] and used by some researchers [8–10], have not been widely adopted despite the fact that they offer additional physical insight with a rather negligible increase in computational cost (only one extra equation).

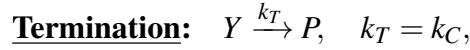
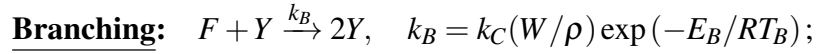
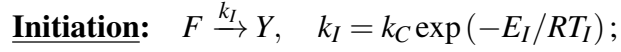
In the single-step model previously used in our group [2], the fuel, F , is directly converted into products following a single irreversible Arrhenius reaction:



The consumption of fuel is then given by:

$$\delta_t(\rho Y_F) + \nabla \cdot (\rho \mathbf{u} Y_F) = -\rho Y_F A_s \exp(-E_a/RT) \quad (1)$$

In the three-step chain-branching model, we account for initiation, branching and termination as follows:



part of the fuel, F , is initially decomposed to produce active radicals, Y , at rate k_I (initiation); the fuel subsequently reacts with them to increase their concentration significantly at rate k_B (branching); finally these radicals are converted into products, P , at constant rate k_T (termination). The local heat release is only associated with termination, i.e. $q = (1 - Y_F - Y_Y)Q$, where Y_F and Y_Y are the mass fractions of fuel and active radicals, respectively. The evolution described is representative of the combustion of hydrogen [7].

The species equations and net production/consumption rates based on the scheme above are:

$$\begin{aligned} \delta_t(\rho Y_F) + \nabla \cdot (\rho \mathbf{u} Y_F) &= -r_I - r_B \\ \delta_t(\rho Y_Y) + \nabla \cdot (\rho \mathbf{u} Y_Y) &= r_I + r_B - r_T \end{aligned}$$

where $r_I = Y_F \rho k_I \exp(E_I/RT)$, $r_B = Y_F Y_Y \rho^2 / W k_B \exp(E_B/RT)$, $r_T = Y_Y \rho k_C$

To model the behavior of a stoichiometric H₂-O₂ mixture the kinetic parameters were determined, for single-step chemistry, by tuning A_s and E_a/R to match the numerically determined cell size and steady detonation velocities with those reported experimentally [11]. For three-step chain branching chemistry, on the other hand, k_C , the activation temperatures (E_I/R , E_B/R) and cross-over temperatures (T_I , T_B) were found by tuning these parameters to match the constant volume ignition delay time, t_{ind} , obtained using the detailed mechanism of Mével et al. [12] which has been extensively validated against experimental databases available in the literature.

Figure 1 shows the results of the fitting together with the delay times obtained with single-step chemistry. The dashed and dotted lines are the percent error computed for single-step and three-step chain-branching chemistry using t_{ind} from detailed chemistry as a reference (black line). The parameters found are $A_s = 1.1 \times 10^9 \text{ s}^{-1}$, and $E_a/R = 11277 \text{ K}$, for single step; and $k_C = 2 \times 10^7 \text{ s}^{-1}$, $E_I/R = 25000 \text{ K}$, $E_B/R = 9300 \text{ K}$, $T_I = 2431 \text{ K}$, $T_B = 1430 \text{ K}$, for three-step chain-branching chemistry. The mixture properties are: molecular weight $W = 12 \text{ g/mol}$, ratio of specific heats $\gamma = 1.33$, and heat release $Q = 4.80 \times 10^6 \text{ J/Kg}$ and $4.99 \times 10^6 \text{ J/kg}$ for single-step and three-step chain-branching chemistry, respectively. Note that there is very good agreement between the delay times predicted by the three-step chain-branching and detailed chemistry. The low and high temperature regions are well captured by the simplified model.

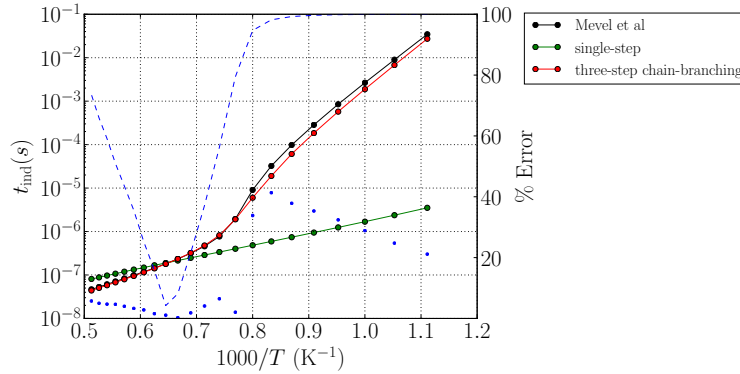


Figure 1: Constant volume induction times as a function of the inverse temperature. Initial conditions (von Neumann state) computed for a stoichiometric $\text{H}_2\text{-O}_2$ mixture at $p_o = 100$ kPa and $T_o = 295$ K.

2.3 Simulation setup, domain, initial/boundary conditions

A schematic of the simulation setup is shown in Fig. 2. The simulations used 400 processors (~ 50 million cells were required for the largest computation) in rectangular domains of size $L_x \times L_y$, and were run in two steps: first, a detonation was initiated and allowed to propagate in a channel completely filled with reactive mixture until a quasi-steady structure was achieved ($\sim 100 \mu\text{s}$ of propagation); second, the resulting fields were then used as initial conditions for separate simulations in which the channel height was filled with a layer of inert mixture. Different reactive layer heights, h , were tested to find the minimum height, h_{crit} , capable of sustaining a detonation.

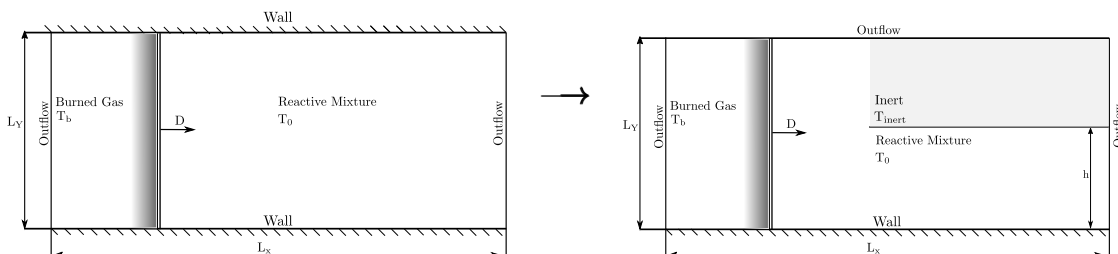


Figure 2: Simulation setup and computational strategy to determine the critical height.

4. Results and discussion

4.1 Uniform mixture: detonation front dynamics, instantaneous structure and soot foils

The simulations run in uniform mixture allowed to quantify differences in the quasi-steady detonation propagation between the two simplified chemical models tested. Figure 3 (left) shows instantaneous velocity profiles obtained by taking a spatial probe of the detonation front at the bottom wall, and Fig.3 (right) the probability density function (PDF) of the leading shock velocity. While the overall behavior is similar for both mechanisms, three-step chain-branching chemistry exhibits larger excursions in leading shock velocity than what single-step chemistry admits. Not surprisingly, the PDF also shows an increased range of velocity oscillations about D_{CJ} with the most likely

front velocity lying around $D/D_{CJ} \sim 1$. However, some differences are evident. For the three-step chain-branching model, the power-law dependence seems to break down for $D/D_{CJ} < 0.9$ and $D/D_{CJ} > 1.4$, exhibiting a rather flat region for $0.6 < D/D_{CJ} < 0.9$. For the lower values, this can be correlated to the low post-shock temperatures below the cross over temperature T_B for which the chemical times scale increases drastically (see Fig. 1). These time scales are thought to be too long when compared with characteristic detonation time scales, however, as will be shown later they change the nature of the flow field.

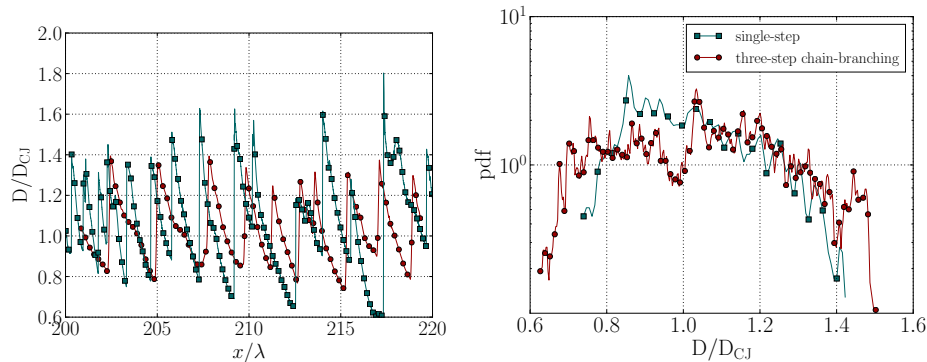


Figure 3: Normalized instantaneous ($t = 100 \mu\text{s}$) shock front velocity as a function of distance (left), and probability density function of the leading shock velocity (right) for single-step and three-step chain-branching chemistry – uniform mixture. Distance is normalized by the average cell size λ .

Consistent with the larger velocity oscillations admitted by the three-step model, the two-dimensional detonation structure obtained displays large variations in temperature behind the leading shock (see Fig. 4). Note however that these lower temperature regions behind the front are not necessarily associated with zones filled with fresh mixture or unreacted pockets (although some of them are) but are evidence of different burnt product equilibrium temperatures. It is also worth mentioning that single-step kinetics results in an almost flat detonation front, whereas three-step chain-branching kinetics shows a detonation front with larger bulbs and more pronounced cusps.

Despite the differences observed in the two-dimensional instantaneous fields described above, both chemical models yield roughly the same cell size and show very similar features in terms of the irregularity of the cells (see Fig. 5). The cell size was numerically predicted to lie in the range of $1.2 \text{ mm} \leq \lambda \leq 1.9 \text{ mm}$ whereas the average cell size reported experimentally is in the range of $1.4 \text{ mm} \leq \lambda_{\text{exp}} \leq 2.1 \text{ mm}$ [11]. This is reassuring evidence regarding the fitting of simplified models. Thus, using fundamental properties of the mixture (t_{ind}) may be a more sound approach to take instead of aiming to match experimental cell sizes.

4.2 Non-uniform mixture: instantaneous structure and quenching dynamics

To characterize and study the detonation structure and quenching dynamics, simulations with inert layers were conducted. The temperature of the inert layer was set such that the acoustic impedance

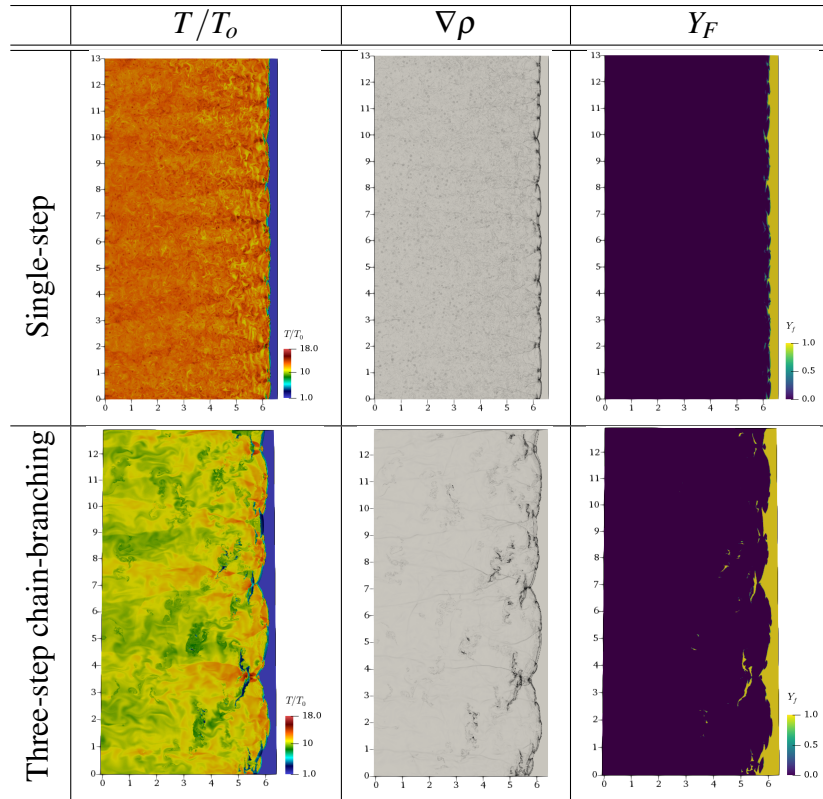


Figure 4: Instantaneous detonation structure for both simplified kinetic mechanisms after $100 \mu\text{s}$ of propagation into uniform mixture. Axes are normalized using the detonation cell size, λ .

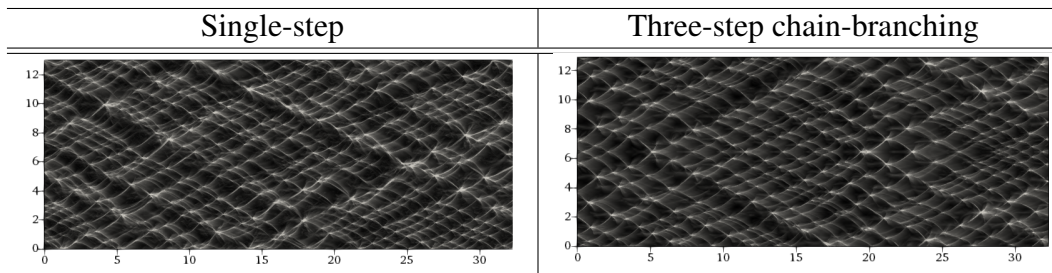


Figure 5: Numerical soot foils for both simplified kinetic mechanisms. Axes are normalized using the detonation cell size λ .

obtained was representative of a stoichiometric $\text{H}_2\text{-O}_2 / \text{Air}$ system ($Z = \sqrt{M_{\text{react}}T_{\text{react}}/M_{\text{inert}}T_{\text{inert}}} = 1.52$). The critical height for this system using single-step chemistry was found to be, $h_{\text{crit}} = 10.5\lambda$. Using a layer height slightly above this value ($h_{\text{crit}} = 11.5\lambda$), simulations using the three-step chain-branching model were run.

Figure 6 shows a comparison of the structure obtained after $20 \mu\text{s}$ of propagation. In both cases, characteristic features of non-ideal detonations are recovered, namely a curved front, an oblique transmitted shock and a shear layer separating shocked inert gas from detonation products. However, significant differences are evident in the instantaneous fields. While the detonation seems to propagate comfortably with uniform burning in the single-step results, the structure obtained for

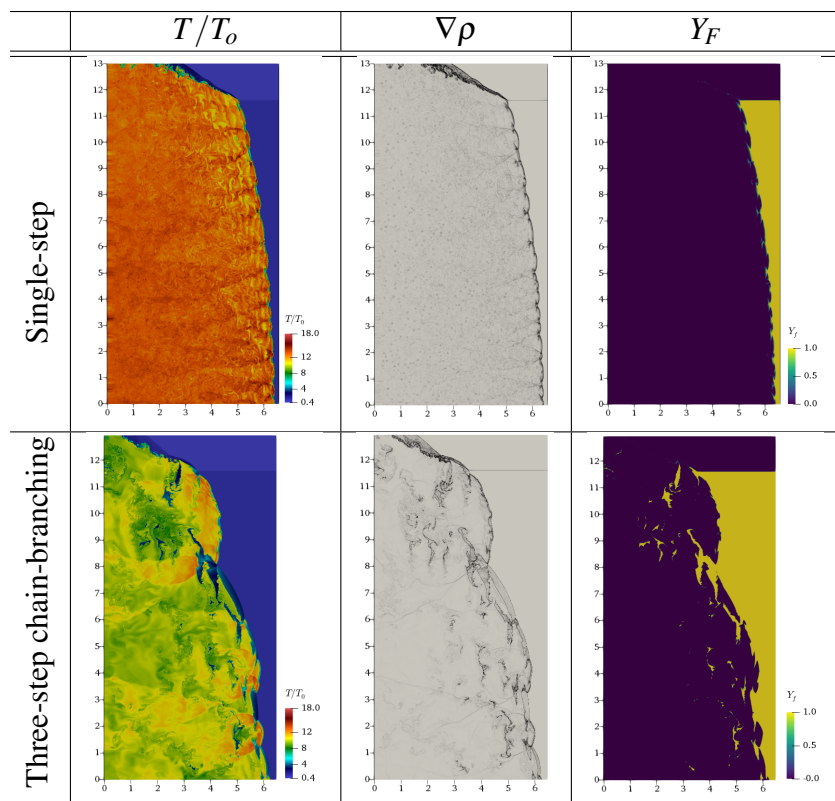


Figure 6: Instantaneous detonation structure for both simplified kinetic mechanisms after $20 \mu\text{s}$ of propagation into the inert layer. The height of the reactive layer is $h = 11.5\lambda$. Axes are normalized using the detonation cell size, λ .

three-step chain-branching chemistry exhibits a more irregular behavior with sizable pockets of unburnt gas distributed over the flow field, as well as larger distances between the leading shock and the start of chemical reaction in the vicinity of the interface.

Further examination of the flow field at longer times (Fig. 7), specifically after $\sim 100 \mu\text{s}$ of interaction with the interface, reveals that while the detonation continues to propagate without any issues for single-step chemistry, three-step chain-branching chemistry does not allow a detonation to propagate at this layer height. A probe of the instantaneous shock front velocity as a function of distance provides quantitative evidence of the quenching of the detonation (see Fig. 8 – left). The leading shock ceases to oscillate for $x/\lambda > 505$ indicating its decoupling with the detonation reaction zone. The PDF taken over the entire interaction with the inert layer reveals that the most likely front velocity is around $D/D_{CJ} = 0.7$, significantly below the expected value for quasi-steady propagation (see Fig. 8 – right).

This outcome suggests that the quenching limits, characterized here using h_{crit} , are dependent on the choice of chemical modeling used. The magnitude of this dependency, however, remains to be determined. Additional simulations are currently underway to find h_{crit} for three-step chain-branching and detailed chemistry to quantify the aforementioned deviation.

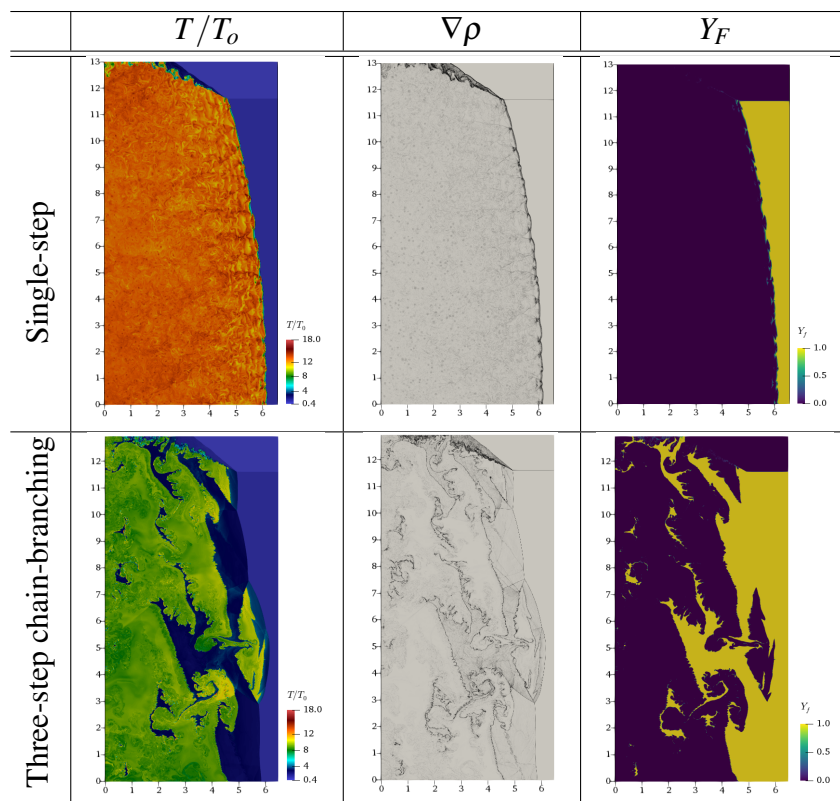


Figure 7: Instantaneous detonation structure for both simplified kinetic mechanisms after $100 \mu\text{s}$ of propagation into the inert layer. The height of the reactive layer is $h = 11.5\lambda$. Axes are normalized using the detonation cell size, λ .

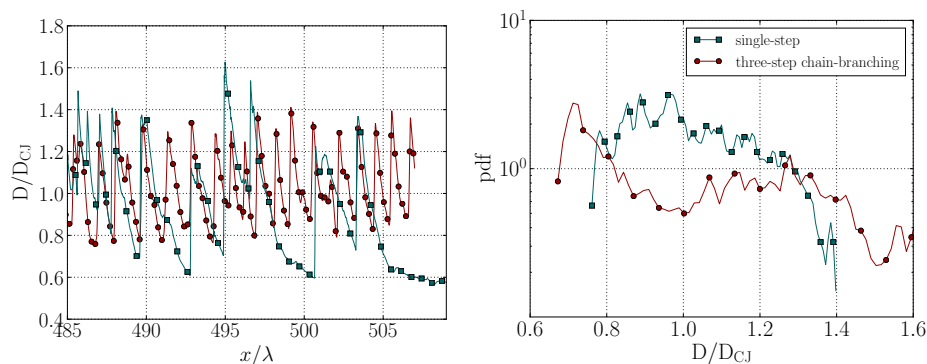


Figure 8: Normalized instantaneous ($t = 100 \mu\text{s}$) shock front velocity as a function of distance (left), and probability density function of the leading shock velocity (right) for single-step and three-step chain-branching chemistry – interaction with inert layer. Distance is normalized by the average cell size λ .

5. Conclusion

Two-dimensional simulations were conducted to assess the effect of chemistry modeling on the detonation structure and quenching dynamics of detonations propagating into a semiconfined medium.

Two different simplified kinetic schemes were used to model the chemistry of stoichiometric H₂-O₂ mixtures: single-step and three-step chain-branching chemistry. Although the macroscopic characteristics of this type of detonations (e.g. detonation velocity and cell size irregularity) were very similar for both models tested, their instantaneous structure was found to be very different before and upon interaction with an inert layer. The minimum reactive layer height, h_{crit} , capable of sustaining detonation propagation is larger when a more realistic description of the chemistry is used. The magnitude of this deviation, however, remains to be determined. This outcome suggests that the quenching limits predicted numerically are dependent on the choice of chemical modeling used. Determination of upper/lower bounds on reported quenching limits as a function of chemistry modeling strategy are thus required to provide a more meaningful metric.

6. Acknowledgements

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References

- [1] E. K. Dabora, The influence of a compressible boundary on the propagation of gaseous detonations, tech. rep. Report No. 3559-E, NASA, 1963.
- [2] M. Reynaud, F. Viot, and A. Chinnayya, A computational study of the interaction of gaseous detonations with a compressible layer, *Physics of Fluids* 29 (2017) 056101.
- [3] R. W. Houim and R. T. Fievisohn, The influence of acoustic impedance on gaseous layered detonations bounded by an inert gas, *Combustion and Flame* 179 (2017) 185–198.
- [4] K. Mazaheri, Y. Mahmoudi, M. Sabzpooshani, and M. I. Radulescu, Experimental and numerical investigation of propagation mechanism of gaseous detonations in channels with porous walls, *Combustion and Flame* 162 (2015) 2638–2659.
- [5] M. I. Radulescu, A detonation paradox: Why inviscid detonation simulations predict the incorrect trend for the role of instability in gaseous cellular detonations?, *Combustion and Flame* (2018).
- [6] A. Sow, A. Chinnayya, and A. Hadjadj, On the viscous boundary layer of weakly unstable detonations in narrow channels, *Computers & Fluids* 179 (2019) 449–458.
- [7] M. A. Birkan and D. R. Kassoy, The unified theory for chain branching thermal explosions with dissociation-recombination and confinement effects, *Combustion science and technology* 44 (1986) 223–256.
- [8] G. J. Sharpe and N. Maflahi, Homogeneous explosion and shock initiation for a three-step chain-branching reaction model, *Journal of Fluid Mechanics* 566 (2006) 163–194.
- [9] M. Short and J. J. Quirk, On the nonlinear stability and detonability limit of a detonation wave for a model three-step chain-branching reaction, *Journal of Fluid Mechanics* 339 (1997) 89–119.

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- [10] J. Melguizo-Gavilanes and L. Bauwens, A comparison between constant volume induction times and results from spatially resolved simulation of ignition behind reflected shocks: implications for shock tube experiments, *Shock Waves* 23 (2013) 221–231.
- [11] M. Kaneshige and J. E. Shepherd, *Detonation database*, (1997).
- [12] R. Mével, J. Sabard, J. Lei, and N. Chaumeix, Fundamental combustion properties of oxygen enriched hydrogen/air mixtures relevant to safety analysis: Experimental and simulation study, *international journal of hydrogen energy* 41 (2016) 6905–6916.