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Chemistry Modeling Effects on the Interaction of a Gaseous Detonation with an Inert Layer

S. Taileb, J. Melguizo-Gavilanes, A. Chinnayya
Institut Pprime, UPR 3346 CNRS, ISAE–ENSMA, University of Poitiers,
86961 Futuroscope-Chasseneuil Cedex, France

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 has also profound implications for safety hazards. Classical experiments by Dabora et al. [1] using the same setup revealed a velocity deficit due to the lateral expansions of the products and the curvature of the detonation front. Recent numerical simulations [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 affected by the front curvature caused by lateral flow expansion. 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 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 semi-confined environment. The detonation front dynamics and the two-dimensional structure of the front during steady propagation and quenching are examined.

2 Computational methodology

Governing equations and numerical techniques The flow 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. Special care was taken to ensure that the size of the window used did not influence the flow structure and quenching limits reported. Details of the simulation setup are described in subsection 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 [6] and used by some researchers [7, 8], have not been widely adopted despite the fact 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, $F \rightarrow P$, occurring at a rate $k = A_s \exp(-E_a/RT)$. In the three-step chain-branching model, we account for initiation, branching and termination as follows:

Initiation: $F \rightarrow Y$, $k_I = r_I \exp(-E_I/RT)$; **Branching:** $F+Y \rightarrow 2Y$, $k_B = r_B \exp(-E_B/RT)$;

Termination: $Y \rightarrow P$, $k_T = k_C$; $r_I = k_C \exp(E_I/RT_I)$; $r_B = k_C \exp(E_B/RT_B)$,

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 , releasing heat at constant rate k_T (termination). The evolution just described is representative of the combustion of H_2 - O_2 mixtures [6]. To model the behavior of a stoichiometric H_2 - O_2 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 [9]. 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 [10] 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. The parameters found are $A_s = 1.1 \times 10^9 s^{-1}$, and $E_a/R = 11277 K$, for single step; and $k_C = 2 \times 10^7 s^{-1}$, $E_I/R = 25000 K$, $E_B/R = 9300 K$, $T_I = 2431 K$, $T_B = 1430 K$, for three-step chain-branching chemistry. The mixture properties are $\gamma = 1.33$ with heat release $Q = 4.8 \times 10^6 J/kg$ and $4.996 \times 10^6 J/kg$ for single-step and three-step chain-branching chemistry, respectively.

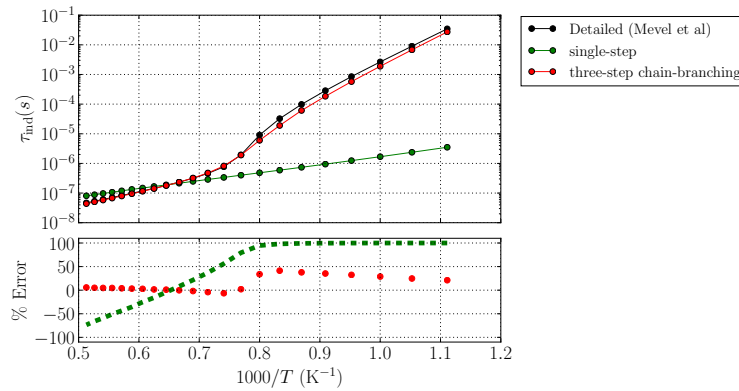


Figure 1: Constant volume induction times as a function of the inverse temperature. Initial conditions (von Neumann state) computed for a stoichiometric H_2 - O_2 mixture at $p_o = 1$ atm and $T_o = 295$ K.

Simulation setup, domain, initial/boundary conditions A schematic of the simulation setup is shown in Fig. 2. The simulations used 400 processors 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 ($\sim 100 \mu\text{s}$); 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.

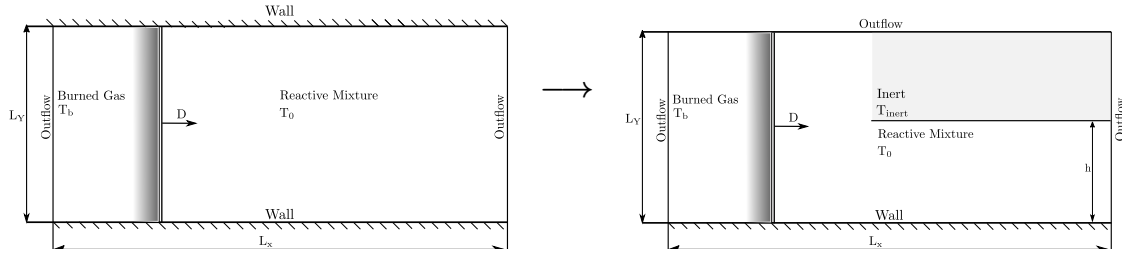


Figure 2: Simulation setup and computational strategy to determine the critical height.

3 Results and discussion

Front dynamics 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 tracking the detonation front during the simulations, 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} . Numerical soot foils are shown in Fig. 4. Notably, both chemical

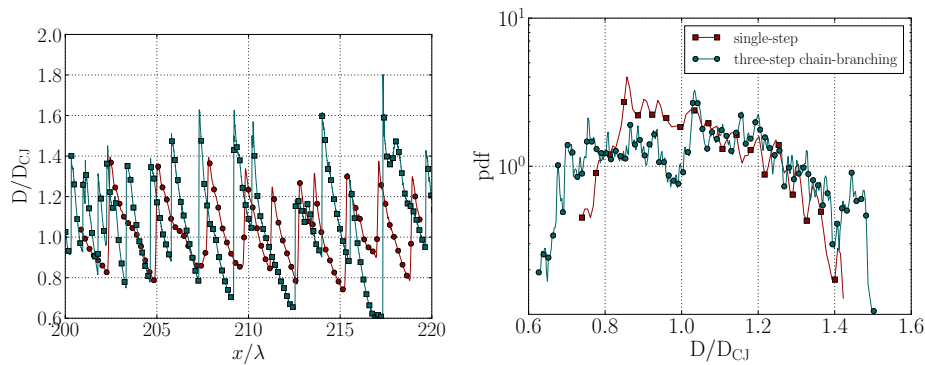


Figure 3: Normalized instantaneous shock front velocity a function of the distance (left), and probability density function of the leading shock velocity (right) for single-step and three-step chain-branching chemistry. Distance is normalized using the average numerical detonation cell size $\lambda = 1.55 \text{ mm}$.

models yield roughly the same cell size and show very similar features in terms of the irregularity of the cells. The cell size was numerically predicted to lie in the range of $1.2 \text{ mm} \leq \lambda_{\text{num}} \leq 1.9 \text{ mm}$. The cell

size reported experimentally is in the range of $1.4 \text{ mm} \leq \lambda_{\text{exp}} \leq 2.1 \text{ mm}$ [9]. This is reassuring evidence regarding the fitting of simplified models. Using fundamental properties of the mixture (t_{ind}) may be a more sound approach to take instead of aiming to match experimental cell sizes.

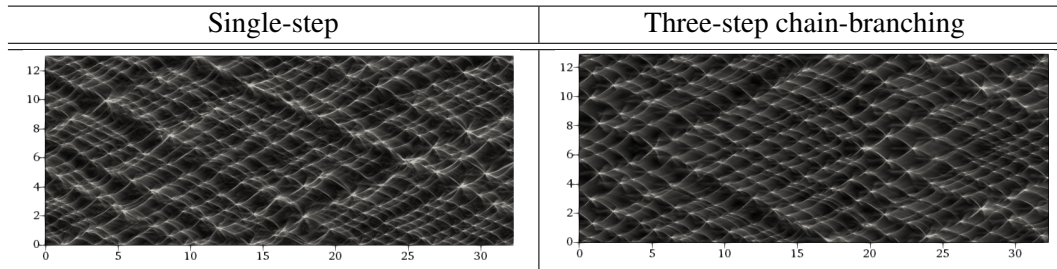


Figure 4: Numerical soot foils for both simplified kinetic mechanisms. Axes are normalized using the average numerical detonation cell size $\lambda = 1.55 \text{ mm}$.

Detonation 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 obtained was representative of a stoichiometric $\text{H}_2\text{-O}_2$ - Air system ($Z = \sqrt{M_{w,\text{react}}T_{\text{react}}/M_{w,\text{inert}}T_{\text{inert}}} = 1.52$). 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 5 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 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. 6), 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. This outcome suggests that the quenching limits, characterized here using h_{crit} , are dependent on the choice of chemical modeling used; three-step chain-branching chemistry yielded a critical height of $h_{\text{crit}} = 16\lambda$. Additional simulations are currently underway to find h_{crit} for detailed chemistry.

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 $\text{H}_2\text{-O}_2$ 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 upon interaction with an inert layer. The minimum reactive layer height, h_{crit} , capable of sustaining detonation propagation is larger ($h_{\text{crit}} = 16\lambda$) when a more realistic description of the chemistry is used. This outcome suggests that the quenching limits predicted

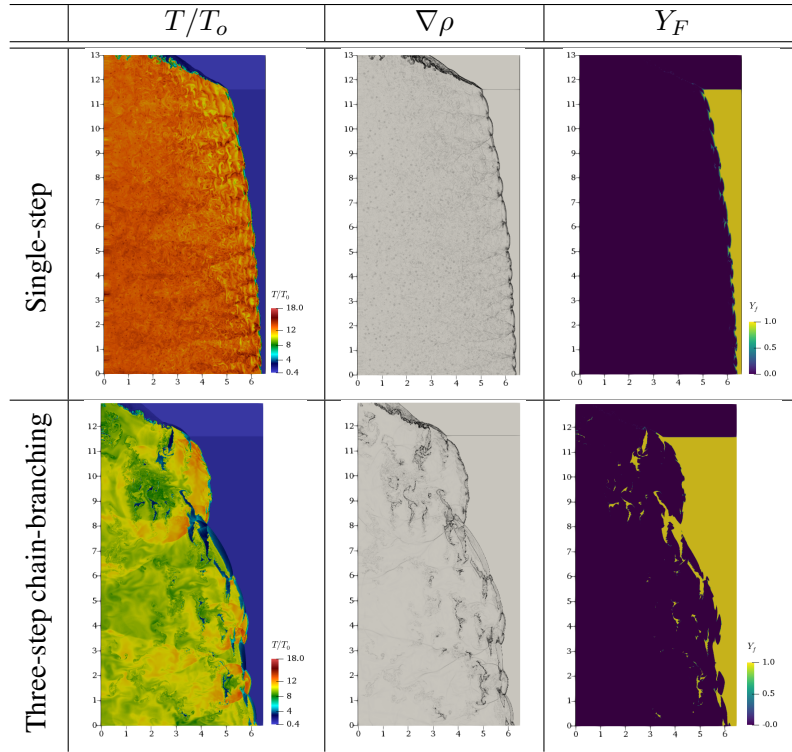


Figure 5: Instantaneous detonation structure for both simplified kinetic mechanisms after $20 \mu\text{s}$ of propagation into the inert layer. The height of the reactive layer is $h = 11.5\lambda$. Axes are normalized using the average numerical detonation cell size $\lambda = 1.55 \text{ mm}$.

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.

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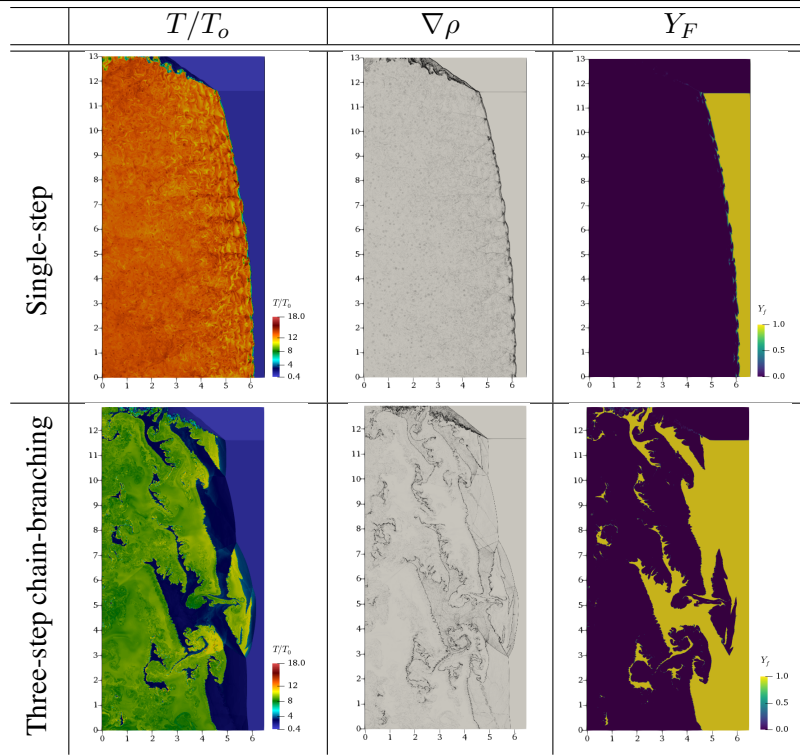


Figure 6: Instantaneous detonation structure for both simplified kinetic mechanisms after $100 \mu\text{s}$ of propagation into the inert layer. The height of the reactive layer is $h = 11.5\lambda$. Axes are normalized using the average numerical detonation cell size $\lambda = 1.55 \text{ mm}$.

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