Slow propagation dynamics of detonation in a non-uniform gas : a large activation-energy analysis

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1 Introduction

The determination of the conditions for self-sustained detonation propagation in a non-uniform gaseous mixture constitutes an important issue. The explosive composition formed with the oxygen of the air after the leak of a gaseous hydrocarbon from a duct or a tank necessarily involves a distribution in its temperature and composition. The state ahead the detonation front in a pulsed detonation engine or in a high-speed combustor is also non-uniform because of the injection and ignition techniques and of the repartition of the detonation products. A few laboratory experiments, where initial gradients are either parallel or normal to the propagation direction of the detonation, are reviewed in [3]. Our work is an attempt to model the conditions for detonation propagation in non-uniform compositions at constant pressure, a problem which, to our knowledge, has not yet received attention, contrary to the spontaneous onset of detonation in hot, non-uniform compositions, e.g., [5]. Our objective is not to interpret the experiments but rather to bring out the salient features and the magnitude orders of the phenomena by means of simplification of the physics and consideration of generic configurations.

2 Summary of calculations

We solve the classical eigenvalue problem for non-ideal self-sustained detonations starting from the compressible reactive Euler equations and the one-step Arrhenius reaction rate in the asymptotic limit of large reduced activation energies. We actually extend an approach used by He and Clavin [2] in their study of detonation initiation by an energy source in a constant initial state. The shock state then appears as a good representation of the induction state, and the mass, momentum and energy fluxes can be considered as conservative in the heat-release zone whereas their estimates in the induction zone must account for small corrections that are functions of the front acceleration $\delta D/\delta t$ and curvature κ and of the changes X_∞ in the initial temperature T_∞ and dilutant mass-fraction x_∞. Our calculations result in the compatibility relation

$$\frac{\delta D}{\delta t} = V^2\left(W - \kappa + X_\infty\right), \tag{1}$$

$$V^2(D) = \frac{2\gamma_b^2}{4\gamma_b^2+\gamma_f-3}D^2, \qquad W(D) = \frac{\gamma_f^2-1}{8\gamma_b^2}\left(\left(\frac{D_{CJ}}{D}\right)^2-1\right)\frac{1+\eta_\infty}{\ell_{st}},$$

$$X_\infty = \left(1+\frac{\gamma_f-1}{2\gamma_b^2}\right)\frac{1}{D}\frac{\delta \ln T_\infty}{\delta t}+\frac{\beta_\infty}{D}\frac{\delta x_\infty}{\delta t},$$

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where the index ∞ denotes the initial state, D is the detonation velocity, γ_f and γ_b are the heat-capacities ratios of the reactants (f) and products (b), ℓ_{st} is the planar steady-state induction length, β_∞ is a coefficient accounting for the contributions of the differences in the molar masses, in the enthalpies and in the heat-capacities ratios γ_{f1} and $\gamma_{f2}$of the non-diluted reactants and of the dilutant, and η_∞ is the $O(10^{-1})$ ratio $2M_\infty^{-2}/(\gamma_f - 1)$ with $M_\infty = D/c_\infty$ the shock Mach number and c_∞ the initial sound velocity. We thus observe that the detonation decelerates when the "loss term" $\kappa - X_\infty$ dominates the "production" term W. Using the identities $D = dR/dt$ and $dD/dt = (dD/dR)\,(dR/dt)$, we can substitute R^{-1} to t as independant variable and turn the hyperbolic evolution law (1) into an ordinary differential system of 2 separable equations.

Next, extending to variable initial states our former results for constant initial states [6], we derive expression (2) for the actual induction time $\tau_{\rm det}$ and length $\ell_{\rm det}$ behind the shock of our self-sustained detonation. We then infer the shock-initiation criterion (3) where α is the iso-induction time parameter $\tau_{st}/\tau_{\rm det}$ and τ_{st} is the planar steady-state induction time. For example, setting $\alpha = 0$ or $\alpha = 1/2$ gives the constraints for $\tau_{\rm det}$ to be bounded or twice the steady-state induction time for the same value of D,

$$\frac{\tau_{\rm det}}{\tau_{st}} = \frac{1}{1 + nZ_0\Lambda_{\rm det}} \approxeq \frac{\ell_{\rm det}}{\ell_{st}}, \tag{2}$$

$$\Lambda_{\rm det} = 3\ell_{st}W - \frac{\gamma_f + 5}{\gamma_f + 1}\ell_{st}\kappa + \left(1 + \frac{\gamma_f}{\gamma_b^2}\right)\frac{\ell_{st}}{D}\frac{\delta \ln T_\infty}{\delta t} + \omega_\infty \frac{\ell_{st}}{D}\frac{\delta x_\infty}{\delta t} \geqslant \frac{\alpha - 1}{nZ_0}. \tag{3}$$

n is an $O(1)$ state function, Z_0 is the reduced activation energy $E_{act}/R_{gas}T_0$ relative to the shock temperature T_0 for a shock with velocity D and ω_∞ is a coefficient similar to β_∞ (1). We thus observe that all the self-sustained detonation shock dynamics are not compatible with bounded induction times which must remain small so detonation propagation be ensured.

3 Examples of results

We have chosen a sinusoidal function (Figure 1) to model the profiles of the initial temperature $T_\infty(r)$ and dilutant mass fraction $x_\infty(r)$. The quantities R_0 and $R(t)$ are the shock positions at times $t = 0$ and $t > 0$, and $R_{0T/x}$ and $R_{1T/x}$ are the abscissas where variations begin and finish (vertical bars in Figures 3 and 4). For simplicity, we have considered that the initial state before variation (subscript $\infty 1$) was nondiluted ($x_{\infty 1} = 0$) and x_∞ thus represents the relative dilutant mass fraction. The control parameters are the initial temperature $T_{\infty 1}$ before variation, the relative positions $\Delta R_{0T/x} = R_{0T/x}/R_0 - 1$ where variations begin, the variation lengths $\lambda_{T/x}$ and the relative variation amplitudes $\Delta_{T/x}$. The additional parameters $k_{T/x}$ are used for generating two cases of initial variations. Setting $k_{T/x} = 1$ simulates a dispersion of initial state, with monotonical variations of T_∞ and x_∞ from their initial values $(T_{\infty 1}, 0)$ at $R_{0T/x}$ to their final values $(T_{\infty 2}, x_{\infty 2})$ at $R_{1T/x}$. Setting $k_{T/x} = 2$ simulates a spatially-limited variation in initial state, such as a hot or a diluted layer of gas, for which T_∞ and x_∞ vary from their initial values $(T_{\infty 1}, 0)$ at $R_{0T/x}$, reach $(T_{\infty 2}, x_{\infty 2})$ in the middle of the variation interval and go back to their initial values at $R_{1T/x}$. We have chosen the initial state before variation identical to the reference thermodynamical state(index $*$, $p_* = 1.01325$ bar, $T_{\infty 1} = T_* = 298$ K, $x_{\infty 1} = x_* = 0$), and used the corresponding properties (density ρ_*, velocity D^*_{CJ} and induction length ℓ_* in the steady reaction zone of the planar detonation propagating at the reference velocity D^*_{CJ} in the constant initial state of reference p_∞, T_*, $x_* = 0$) to nondimensionalize the results.

Figure 2 shows the velocity D of a spherical sonic detonation as a function of its total curvature $\kappa = j/R$ for a constant initial state chosen as the reference state. The control parameter is the initial shock position R_0 at $D = D_{CJ}$. The largest values of R_0 are associated with the $D(\kappa)$ integral curves to (1) that always realize the planar CJ regime. Too small R_0's give integral curves that cannot reach the CJ point. A limiting initial radius $R^{\rm det}_{crit}$, here equal to 738.57 ℓ_*, generates a separatrix integral curve between the domain, on its left, for which the detonations continuously relax to the CJ point, and the domain, on

its right, for which the shock dynamics of the sonic detonation eventually fails to initiate combustion. The latter integral curves intersect the line $D(\kappa, \alpha = 0)$ representing the detonation criterion (3) for infinite induction. In this situation, the shock and the reaction zone (the flame) become decoupled. The integral curves, their bifurcation separatrix and the no-shock-initiation domain associated with the present high-activation energy analysis were first presented at an invited talk [7]. More recently, Kasimov and Stewart [4] have obtained similar integral curves with another integration approach.

Figures 3 and 4 show the velocity D of a spherical sonic detonation ($j = 2$) as a function of its position R for a localized increase in the dilutant mass fraction (Fig. 3) and for a combined localized increase in the dilutant mass fraction and in the initial temperature (Fig. 4) ($k_{T/x} \equiv k = 2$). The detonation initial radius R_0 at $D = D_{CJ}$ is chosen larger (840 ℓ_*) than the minimal value $R_{crit}^{\rm det} = 738.57\ \ell_*$ for continuous propagation of a spherical detonation on the constant initial state before variations (Fig. 2). We observe a complicated dynamical behavior with first a wave reacceleration and then a deceleration. Reacceleration occurs if the detonation initial radius is larger than the value $R_{crit}^{\rm det}$ for constant initial state. The larger Δ_x, the larger the effect on the detonation velocity and too large Δ_x lead to bifurcation towards the no-shock-initiation domain (Fig. 3). A very small temperature increase is then enough to obtain bifurcation to a continuous propagation of detonation (Fig. 4). The dotted line N is the zero-acceleration curve which, for constant initial state, reduces to the well-known "curvature-celerity relation", e.g., [2], [4]. The dashed line is the local (instantaneous) CJ velocity.

Many other examples can be generated. All expected dynamical behaviors draw on the same physics with either continuous relaxation to the final CJ regime or shock-flame decoupling. In this case, the process can no longer be described by the sonic detonation dynamics (1), which is only valid for induction lengths small compared to the shock position. What happends is that the flame propagates by itself, acting as a piston on the shock ahead. Reinitiation can occur at larger distances in the shocked domain between the flame and the shock if, depending on the initial conditions, the adiabatic cooling due to the flow divergence becomes again small enough, compared with the energy release [6], [7]. Small hemispherical detonations then appear at one or several points close to the flame front, overcome the shock and rapidly propagate transversally in the shocked domain between the flame and the shock. Once these transverse processes are achieved, the self-sustained regime of spherical detonation is obtained (see the review in [1] and the references therein). The detail of these transients is beyond the reach of our model. However the model identifies subcritical and supercritical limits which, respectively, give necessary and sufficient conditions for detonation. Below the subcritical limit, the combustion front cannot be coupled to the shock front because the volumetric expansion rate behind the shock is too large. Above the supercritical limit, the relaxation from an overdriven regime to the self-sustaining regime or from one self-sustaining regime to another self-sustaining regime is a continuous process, without decoupling and recoupling of the combustion and shock fronts. We interpret the domain between these limits as the parametric zone in which experiments show successions of decouplings and transverse recouplings of the combustion and shock fronts before the final self-sustaining CJ regime. Also, the model yields characteristic critical lengths larger than the CJ characteristic chemical length of reference by several orders of magnitude, a well-established experimental feature of gaseous detonations.

Numerical simulations now catch the experimental dynamical behaviors of gaseous detonations such as cellular structures, transverses reinitiations after shock-flame decoupling or bifurcation from a multi-cells front to a spinning front. However, their predictive ability is constrained by the difficulty to implement precise chemical kinetics and by very long computing times. Much work remains to be done not only to numerically handle large chemical schemes but also to experimentally determine high-pressure chemical kinetics. The type of analysis presented in this paper is limited to slow detonation dynamics and thus has a short reach compared to numerical simulations. However, it is helpful for determining orders of magnitude, for bringing out the salient features of complicated phenomena in generic configurations and for assessing the predictive ability of numerical simulations.

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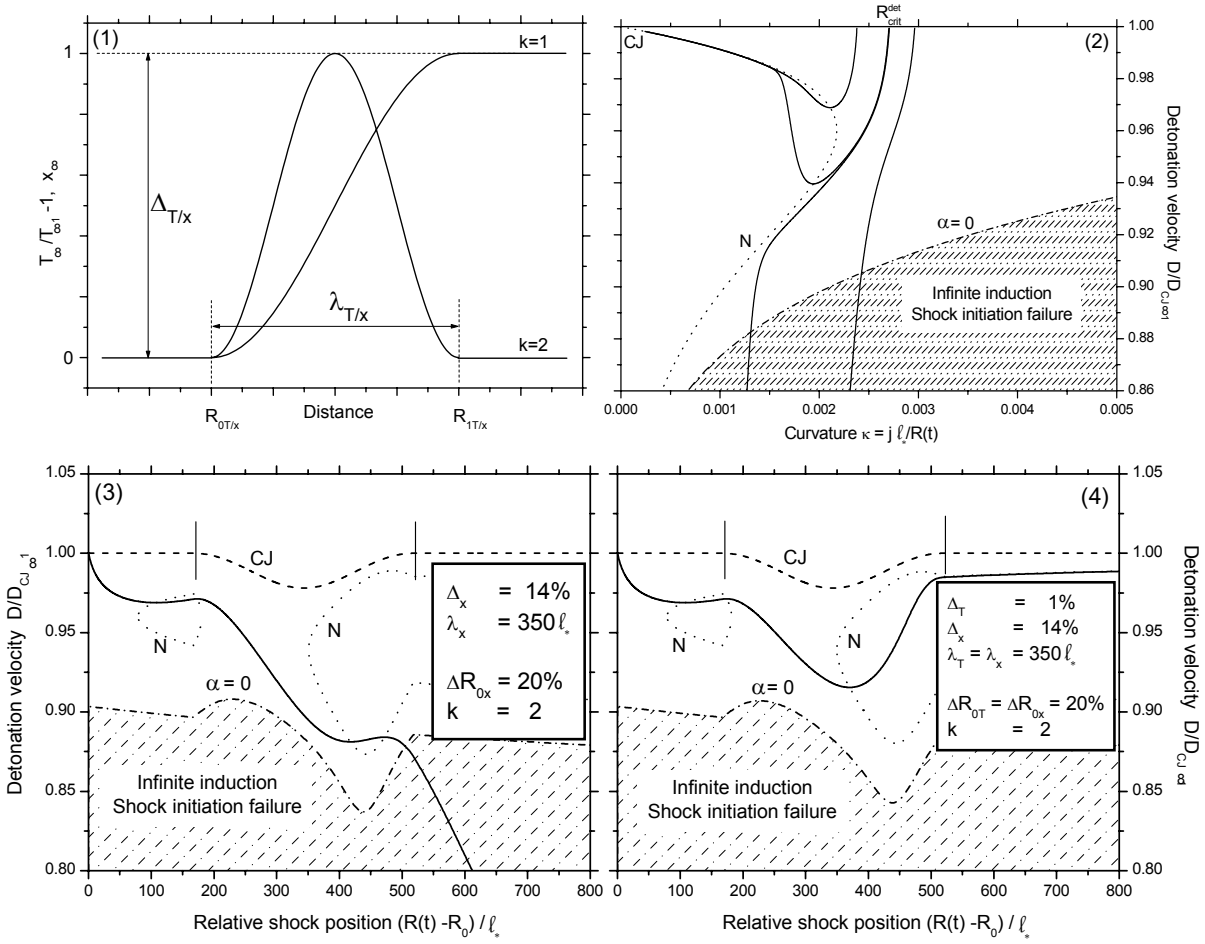

Figures : (1) Notations. (2) Spherical detonation in a constant initial state.
(3)-(4) Spherical detonation coming across a locally-variable initial state.

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