Towards predictive simplified kinetics for detonation simulations

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1 Introduction

The integration of the chemistry is one of the main challenges in detonation modeling because characterizing most fuels using detailed kinetics remains prohibitively expensive [1]. The most common approach is to reduce existing detailed models to one- to five-step schemes developed with varying degrees of sophistication [2,3] seeking to retain the predictive capabilities of detailed kinetics but considerably lessen the computational cost.

Conventional fitting procedures for detonation modeling rely on using the laminar planar ZND structure as a target although the complex thermodynamic changes and associated chemical rates in the induction zone of multidimensional cellular detonations deviate significantly from the 1-D description of the wave. [4]. Recently, Veiga-López et al. [5] presented a methodology based on the fact that irrespective of the configuration considered (i.e., initiation, propagation, diffraction) detonation fronts are observed to be curved. The authors used the simplest extension to the ZND model, i.e., slightly-curved/quasi-steady detonation waves, and aimed to reproduce the $D - \kappa$ curves obtained with a reference detailed scheme with 1-step/3-step chain-branching kinetics.

The ability of the chemistry models using $D - \kappa$ curves to better reproduce the dynamics of multidimensional detonations compared to conventional fitting procedures is still an open question. The goal of this paper is thus to compare the results obtained using both approaches for detonations propagating in channels and confined by inert layers.

2 Chemistry modeling

Chemical schemes of increasing complexity (1-step, 3-step chain-branching and detailed kinetics) are used in this work. The chemical scheme of Mével et al. [6] is used to compute the reference $D - \kappa$ curves. It includes 9 species and 21 reactions and was previously used to simulate the propagation of detonations close to quenching providing sensible results [4]. It is worth noting that non-negligible differences exist among different detailed mechanisms; see [7] for a complete discussion. The predictive capabilities of the simplified schemes are thus limited by the reference mechanism chosen.

The simplified models are obtained via two different approaches: (i) using a conventional fitting procedure that aims to reproduce the constant volume induction time at the von Neumman state (vN) [4]; and (ii) following the methodology proposed by Veiga-López et al. [5], which entails capturing the critical curvature given by $D - \kappa$ curves obtained using a 1-D model that accounts for the curvature losses

Table 1: Detonation properties for a stoichiometric H_2-O_2 mixture for all chemical models used. Initial conditions: $p_0 = 100$ kPa and $T_0 = 300$ K.

	D_{CJ} [m/s]	T_{vN} [K]	l_{ind} [μm]	$E_{\text{a,eff}}/R_u T_0$
Mevel et al. [6]	2839.9	1768.7	41	28.78
CV 1-step [4]	2801.5	1674.8	87.9	33.93
$D\kappa$ 1-step [5]	2836.9	1769.5	36.2	36.16
CV 3-step [4]	2850.4	1723.7	46.8	30.84
$D\kappa$ 3-step [5]	2836.2	1768.7	21.4	30.48

present in the detonation front. For the remainder of this work, the simplified schemes will be referred as CV and $D\kappa$, respectively.

For completeness, detonation properties of interest to the discussion are included in Table 1. For details regarding the chemical schemes' kinetic and thermodynamic parameters, the reader is referred to the references provided above.

3   Ideal 2D propagation in channels

The predictive ability of the new simplified chemical schemes is assessed by simulating detonation propagation in a 2-D channel filled with a uniform stoichiometric H_2-O_2 mixture. The detonation front dynamics, the instantaneous flow fields and the numerical soot foils are analyzed once the detonation is propagating steadily at the ideal Chapmann-Jouguet speed, D_{CJ} ($\pm 2\%$). The numerical methodology, domain, mesh size and initial/boundary conditions used in the work of Taileb et al. [4] are adopted in this work to facilitate the comparison.

3.1   Detonation fields

Figure 1 shows the instantaneous temperature and normalized density gradient fields obtained with the reference (CV) and new ($D\kappa$) simplified schemes and the detailed mechanisms. The $D\kappa$ schemes provide much closer profiles to the detailed mechanism but with a lower final average temperature because of the discussed constant molecular weigth assumption [4]. The combined effect of (i) enhanced resilience to curvature, which allows the front to locally fold further without quenching, and (ii) the presence of stronger transverse waves that leads to a sharper density gradient behind the shock compared to the steady detonations calculated in [4], yields a more homogeneous detonation profile and reduces the amount of unburned pockets present in the flow field when the $D\kappa$ schemes are used. Furthermore, the more irregular detonation profile obtained with the 1-step may be directly related to its higher effective activation energy, $E_{a,\text{eff}}/R_u T_0$; see Table 1.

3.2   Numerical soot foils and cell size histogram

Figure 2 includes the numerical soot foils and the histograms of the cell sizes for all the chemical mechanisms tested. Note that the domain used for the new chemical schemes is smaller than that used in [4] since as it will be discussed below the critical heigths are smaller. The detonation cells obtained with the reference mechanisms are bigger and, therefore, a larger domain is required. The sample size is fixed to 90 and the size of the cells is measured manually from the soot foils, counting the number of
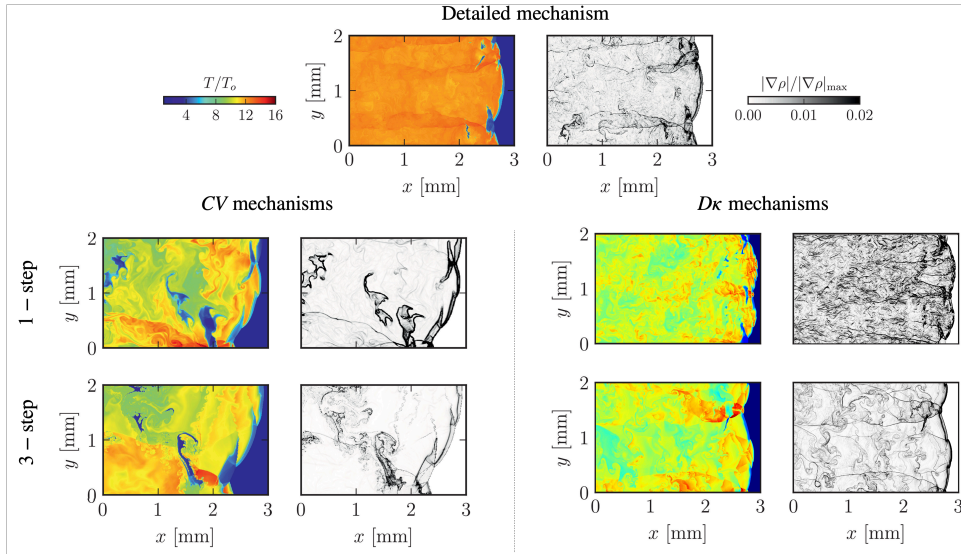
Figure 1: Instantaneous temperature and normalized density gradient fields obtained with the detailed, reference (CV) and modified ($D\kappa$) simplified chemical models.

times, i.e. *Frequency*, that a length scale appears. The histograms show that the cell size distributions are better predicted by the $D\kappa$ schemes. The latter yield smaller cells ($\lambda_{\max, D\kappa, \text{1-step}} = 1.8$ mm vs. $\lambda_{\max, CV, \text{1-step}} = 0.4$ mm ; $\lambda_{\max, D\kappa, \text{3-step}} = 1.2$ mm vs. $\lambda_{\max, CV, \text{3-step}} = 0.57$ mm), which are much closer to those estimated by the detail chemical mechanism ($\lambda_{\max, \text{detailed}} = 0.6$ mm). The reduction of the cell sizes may be directly related to the reduction of the induction length l_{ind}, which was left as a free parameter in the fitting procedure, as well as the stronger presence of transverse waves.

4   2D propagation confined by inert layers

The second analysis is carried out for 2-D detonations propagating in a channel confined by an inert layer at $T_{inert} = 130$ K to match the acoustic impedance of the physical case in which detailed thermochemistry is used (stoichiometric H_2-O_2 confined by N_2 at 300 K). Note that this canonical configuration is of interest to novel propulsion applications such as rotating detonation engines (RDEs) [8, 9]. Once a detonation at D_{CJ} is stabilized in an ideal channel, the upstream conditions are modified, including an inert layer to the domain. The size of the inert layer is progressively increased with a constant step ($\Delta h = 2$ mm), gradually obtaining a thinner layer of thickness h filled with reactive mixture. At a certain layer height (i.e., h_{crit}), the detonation quenches before reaching $x - x_{0,\,inert\,layer} = 200$ mm (150 mm) for the 1-step (3-step) simplified mechanism, where $x_{0,\,inert\,layer}$ is the axial position at which the ideal detonation meets the inert layer. A similar criterion to that used in [4] was selected to determine h_{crit} to facilitate the comparison. Once again, the reader is referred to [4] for further details about the initial and boundary conditions used.

4.1   Critical heights

The ability of the $D\kappa$ mechanisms to predict the critical height, h_{crit} is assessed next. Table 2 includes the results of our simulations. The prediction of the $D\kappa$ models are better than those of the CV mechanisms, yielding a reduction in h_{crit} from 20 mm (24 mm) to 8 mm (12 mm) for the 3-step (1-step) model. The results are much closer to those obtained with the detailed mechanism as well as to the experimental
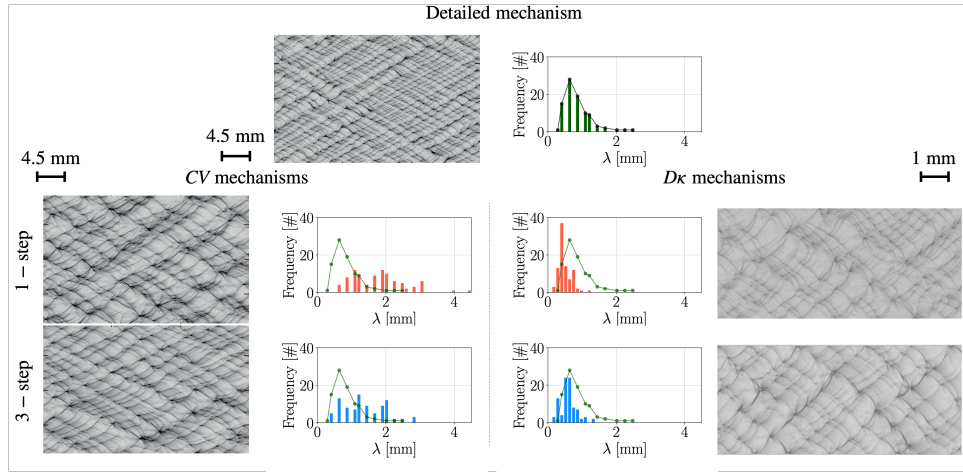
Figure 2: Numerical soot-foils and cell-size histograms obtained with the detailed, reference (CV) and modified ($D\kappa$) simplified chemical models.
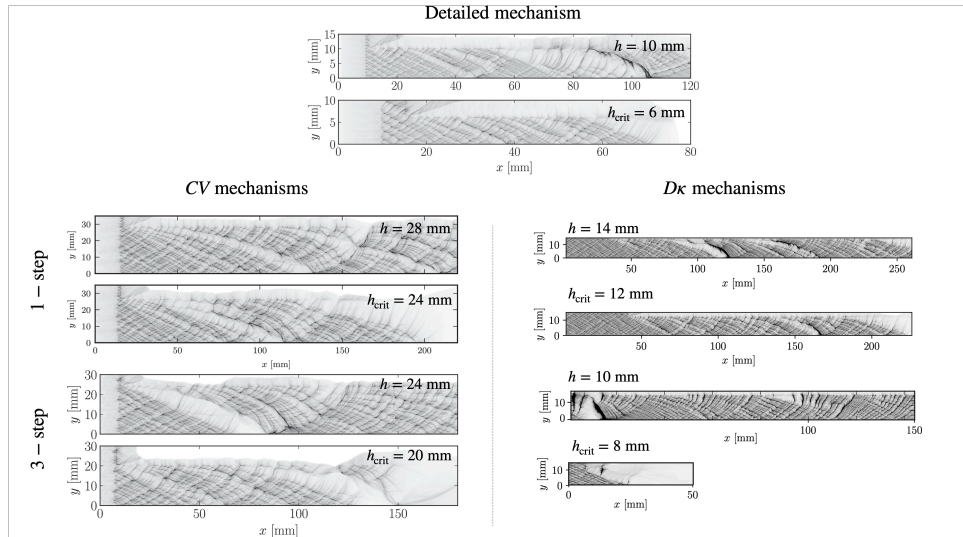

Figure 3: Numerical soot-foils for detonation waves propagating through channels of size $h = h_{\mathrm{crit}} + \Delta h$ and $h = h_{\mathrm{crit}}$ with all the studied mechanisms.

measurements. Therefore, it can be concluded that using the critical curvature from $D - \kappa$ curves obtained with the 1-D model including curvature losses seems to be a valid fitting target to develop simplified schemes with predictive capabilities. Adding the physics expected to play a role as part of the fitting procedure helps to properly capture important detonation features and seems to improve the predictive capabilities in simulations of multidimensional detonations.

The numerical soot-foils are included in Fig. 3. These show the complex dynamics of the interaction between the detonation and the inert layer prior and during quenching. The presence of strong expansions partially quench and curve the detonation close to the interface; transverse waves and their reflections at the lower wall re-initiates the detonation.

Table 2: Summary of critical heights predicted by the different chemical models.

Chemistry modeling	h_{crit} [mm]	x_Q [mm]
CV 1-step	24	200
$D\kappa$ 1-step	12	176
CV 3-step	20	140
$D\kappa$ 3-step	8	12
Detailed	6	60
Experiments [10]	4.6	-

4.2 Front curvature

Due to the interaction with the inert layer and the lateral expansion of burnt gases, the leading shock curves. The curvature increases for decreasing reactive layer height, h. The detonation wave slows down and eventually quenches for a significantly thin channel. This effect amplifies close to the inert layer as shown in Fig. 4 for a detonation wave propagating through a reactive layer height near $h = h_{\text{crit}}$. These fields provide means to assess to which extent the 2-D front curvature could be compared with the maximum critical curvature predicted by the $D - \kappa$ model (i.e., 1-D quasi-steady curved detonations). To that end, the absolute value of the instantaneous local and average curvature of the propagating fronts are computed from the simulations. Note that the quantitative values of the local curvature will depend on the smoothing (high-enough to avoid noisy signals) and (ii) degree (fifth order) of the curve fitting of the detonation front. Results show that, expectedly, the local curvatures can be very high ($\kappa_{\text{loc, 2D}} \sim 500$ m^{-1}), five times larger than the curvature predicted by the 1-D model for a detonation propagating at $D \sim 0.95 D_{CJ}$ (deficit obtained from the 2D simulations), that is, $\kappa_{\text{1D}} \sim 100$ m^{-1}. On the other hand, the average curvatures ($\kappa_{\text{avg, 2D}} \sim 70$ m^{-1}) are consistent with κ_{1D} and conjectured to be representative of the assumption of weak curvature used to derive the 1-D model. Results thus far are encouraging and seem to suggest that the predictive capabilities of the simplified kinetic schemes can be improved by including the dominant physics in the fitting procedure. Furthermore, the critical curvatures predicted by the 1-D model may serve as fast and inexpensive estimates to characterize the limiting behaviors of hydrogen detonations.
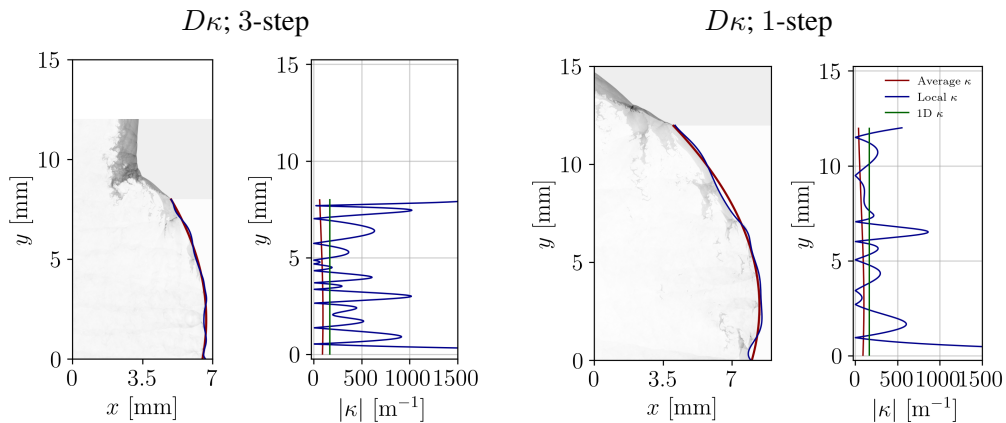

Figure 4: Density fields obtained for detonations propagating through layers with $h = h_{\text{crit}}$ and curvature measured from the instantaneous front profiles.

4.3 Conclusion

Reduced chemical schemes obtained using two different approaches were used to compute detonation propagation in 2-D channels, and determine the critical reactive layer height for quenching, h_{crit} using the configuration of Taileb et al. [4]. Results show that the $D\kappa$ mechanism yields more similar front structures when compared to the detailed scheme (i.e., smaller cell sizes and lower critical layer heights) than what conventional simplified kinetics yields, thus providing better agreement with experimental data. Including the physics expected to play a role in the quenching process as part of the fitting procedure of simplified kinetics, results in an overall improvement in the prediction of limiting behaviors in multidimensional simulations when compared to conventional fitting methods such as matching the constant volume induction time. Furthermore, since the average curvatures obtained from the 2-D simulations are of the same order of magnitude as those predicted by the 1-D model, these may serve as fast, conservative and inexpensive estimates to characterize the limiting behaviors of hydrogen detonations.

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