Uncertainty on Predicted Detonation Cell Width

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1 Introduction

Detonation propagation relies on shock compression and auto-ignition and is characterized by a velocity of $\mathcal{O}$(1500-3000) m/s [1, 2]. The characterization of detonation related phenomena, i.e., propagation, initiation, transmission to open space, and limits, requires the knowledge of the wave structure. Lee [2] has defined the detonation cell width, the initiation energy, the critical, and limiting tube diameters, as the dynamic detonation parameters (DDP), by opposition to the Chapman-Jouguet (CJ) parameters, whose determination requires the knowledge of the thermodynamic equilibrium.
The quantitative knowledge of the DDP is relevant to accidental detonation risk assessment [2], and to design detonation-driven engines [3]. A number of theoretical models and semi-empirical correlations have been developed to predict the DDP [2,4–7] and in most cases, they rely on the induction zone length calculated using a detailed chemical kinetics model. While all the DDP models are developed with the goal of being as accurate as possible, the importance of the uncertainty on the parameters of the model is almost always neglected, in particular the uncertainty related to the thermo-chemical description of the chemical system. To the best of our knowledge, only Crane et al. [8] provided uncertainty on the predicted detonation cell width. However, they considered a constant proportionality factor between the induction zone and the cell width and ignored the uncertainty related to this parameter.
The goals of this study were to: (i) select and reduce an accurate reaction model to describe auto-ignition of hydrogen-air mixtures under detonation relevant conditions; (ii) determine the uncertainty on the predicted detonation cell width induced by the uncertainty on the rate constants; and (iii) determine the impact of the uncertainty of the induction length on simulated two-dimensional detonation waves.

2 Results and Discussion

2.1 Reaction model selection

Ng et al. [4] established an empirical model in predicting cell width (λ) by assuming a relationship between λ and induction length (Δ_i).

$$\lambda = A\Delta_i = \left(A_0 + \sum_{k=1}^{N} \frac{a_k}{\chi^k} + \sum_{k=1}^{N} b_k \chi^k \right) \Delta_i, \tag{1}$$

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where A_0, a_k, and b_k are fitting parameters; and χ is a stability parameter. Ignition delay-time (τ) is the the time-scale corresponding to induction zone length. Thus, according to Eq 1, the ability in predicting τ or Δ_i is essential in cell width prediction. To select an accurate reaction model, a comprehensive database of τ measured in shock tube was assembled from the literature. It includes 1039 data points for hydrogen-based mixtures and covers wide ranges of thermodynamic conditions, temperature T = 780-3134 K, pressure P = 233-15657 kPa, compositions Φ = 0.19-5.5 and mole fraction of diluent species X_{Diluent} = 0.074-0.698.

The model selection was made among 18 detailed reaction models from the literature for the H-O chemistry, and among 4 detailed reaction models for the chemistry of nitrogen-species, which led to 72 combinations. The method of Olm et al. [9] was employed to quantify the predictive capabilities of the models through a score of error, and determine the most accurate one. We found that the lowest score of error, E = 6.70, was achieved for the combination NUIGMech1.0-2020 [10] (for H/O kinetics)+Nakamura-2017 [11] (for H/O/N reactions). Figure 1 (a) illustrates the performances of the selected reaction model with respect to experimental delay-time from the literature [12].

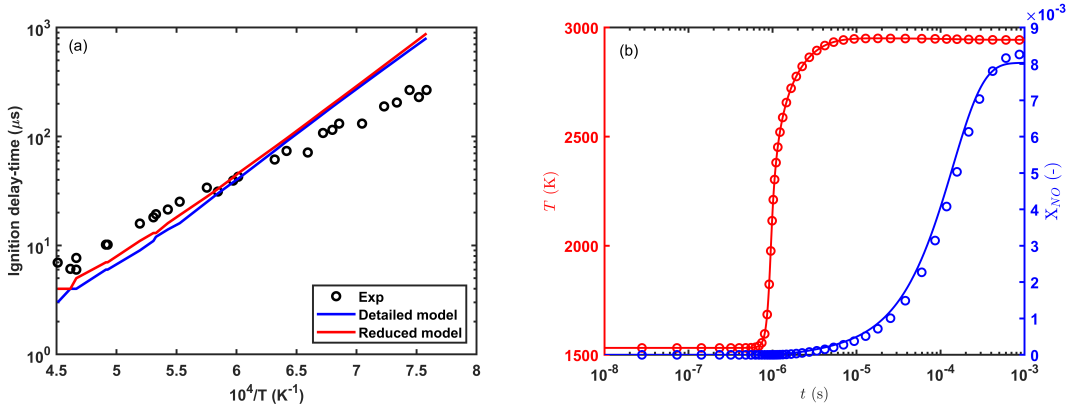


Figure 1: (a) Comparison between experimental ignition delay-time data (circle) [12] and simulation results of the selected detailed reaction model (blue line) and the reduced model (red line); (b) comparison of temperature (T) and mole fraction of NO (X_{NO}) profiles calculated with the full (solid line) and reduced mechanisms (circle).

2.2 Reaction model reduction

To reduce the computational cost, the selected reaction model was reduced through CHEMKIN-PRO [13]. A DRG method was applied by comparing equilibrium X_{NO} in 0-D contant-volume reactor with absolute tolerance of 1E-4. Thermodynamic conditions utilized for model reduction were T = 800-1700 K, P = 100-3200 kPa, Φ = 0.3-2.0, $X_{\text{O2}}/X_{\text{NO2}}$=1-10, and $X_{\text{N2}}/X_{\text{O2}}$=3.76 in $H_2/O_2/NO_2/N_2$ mixtures. Besides, the reduced model obtained after DRG reduction was further simplified by removing the following species NH, NH_3, HNO, NO_3, N_2O_4. Finally, the detailed model containing 223 reactions and 33 species was simplified to a reduced model including 75 reactions and 19 species. The reduced model was validated by calculating its score of error (E=6.86) against the ignition delay-time database and comparing the capability in predicting T and X_{NO} profiles in ZND simulations. Figure 1 compares the typical performances of the detailed and reduced reaction models in reproducing τ and the profiles of T and X_{NO} in the ZND simulation. The satisfactory performances of the reduced model are demonstrated.

2.3 Uncertainty quantification

To evaluate the reliability of the cell width predicted with the method of [4], we used the uncertainty quantification (UQ) method proposed by [14]. It relies on the following four steps: (i) determine the uncertainty on the model input (reaction rate parameters(A, n, E_a)); (ii) perturb randomly the model input with a Monte Carlo sampling approach; (iii) calculate the model output (cell width) with the perturbed model; and (iv) apply statistical tools to study the distribution of the model output. The uncertainty on reaction rate constant ($k = AT^n \exp(-E_a/RT)$) is described by the uncertainty factor (u) or the uncertainty parameter (f). The uncertainty factor is defined as $u = k_0/k_{min} = k_{max}/k_0$, with k_0 the nominal rate constant; k_{min} and k_{max} the minimal and maximal values of k_0. The uncertainty parameter corresponds to $f = \log_{10} u = 3\sigma/\ln 10$, with σ: the variance of $\ln k$ which obeys a joint normal distribution of ($\ln A$, n, E_a/R). For each reaction, k was sampled 10,000 times, while the resulting uncertainty on λ was quantified by the standard deviation (σ_λ). The values used for f for each reaction, as well as the resulting mean ($\bar{\lambda}$) cell width and its standard deviation, are given in Table 1.

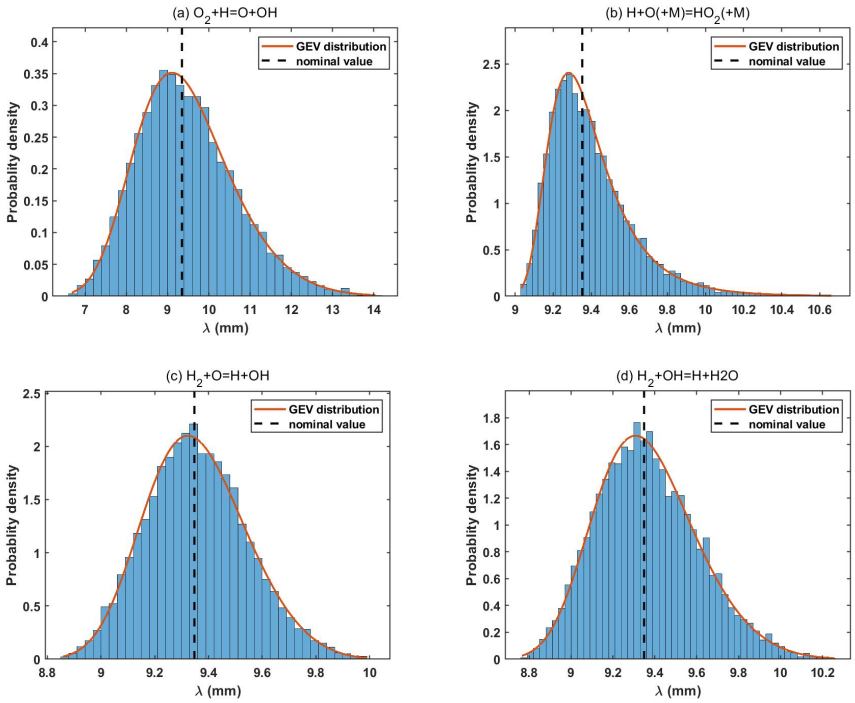


Figure 2: Probability distribution of predicted cell obtained when perturbing four reaction rates: (a) R_1: H+O_2=OH+O; (b) R_2: H+O_2(+M)=HO_2(+M); (c) R_3: H_2+O=H+OH; R_4: H_2+OH=H+H_2O. We considered a stoichiometric H_2-air mixture initially at T = 300 K and P = 101.325 kPa. The nominal value was obtained with the unperturbed reduced reaction model.

We performed a number of sensitivity analyses to determine which reactions control the value of the induction zone length. In most conditions, the two most sensitive reactions were the chain branching reaction R_1: H+O_2=OH+O, and the termination reaction R_2: H+O_2(+M)=HO_2(+M). Other sensitive reactions include R_3: H_2+O=H+OH, R_4: H_2+OH=H+H_2O and the other 6 reactions. For the UQ analysis, we focused on the impact brought out by perturbing the reaction rate of the most sensitive reactions. Figure 2 shows the probability distribution of cell with for perturbed R_{1-4} under stoichiometric H_2-air mixture initially at 300 K and 101.325 kPa. Probability distribution of cell width was determined to follow a generalized extreme value (GEV) distribution through Lilliefors test. Under such conditions, the uncertainty of cell width induced by perturbing the rate of R_1 is much larger than those induced by

perturbing the rates of R_2 to R_4, which is consistent with the sensitivity analysis.

Table 1: Parameters' values for the UQ analysis and resulting predicted cell width with uncertainty. $\bar{\lambda}$: average cell width. σ_λ: Uncertainty on cell width. HPL/LPL: High/low pressure limit.

N°	Reaction	f	Source	$\bar{\lambda}$ (mm)	σ_λ (mm)
R1	$H+O_2=OH+O$	0.208-0.321	[14]	9.46	1.184
R2(HPL)	$H+O_2(+M)=HO_2(+M)$	0.079	[15]	9.40	0.220
R2(LPL)	$H+O_2(+M)=HO_2(+M)$	0.180-0.393	[14]		
R3	$H_2+O=H+OH$	0.2	[16]	9.36	0.188
R4	$H_2+OH=H+H_2O$	0.103-0.308	[14]	9.37	0.243

Figure 3 illustrates the probability density function of cell width for H_2-air mixtures over a range of equivalence ratios. Initial conditions are T = 298 K and P = 101.325 kPa. Only the rates of R_1 and R_2 were perturbed. When perturbing the rate of R_1, the uncertainties are similar over the full range of ϕ studied. On the contrary, uncertainties around Φ=1 are much smaller than those of rich mixtures when the rate of R_2 is perturbed.

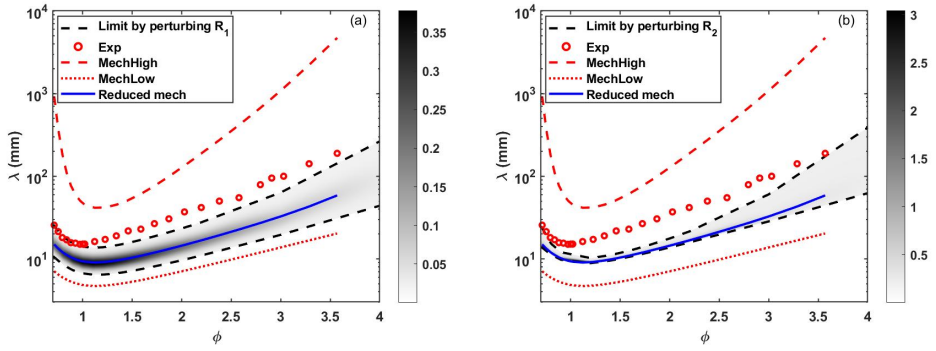
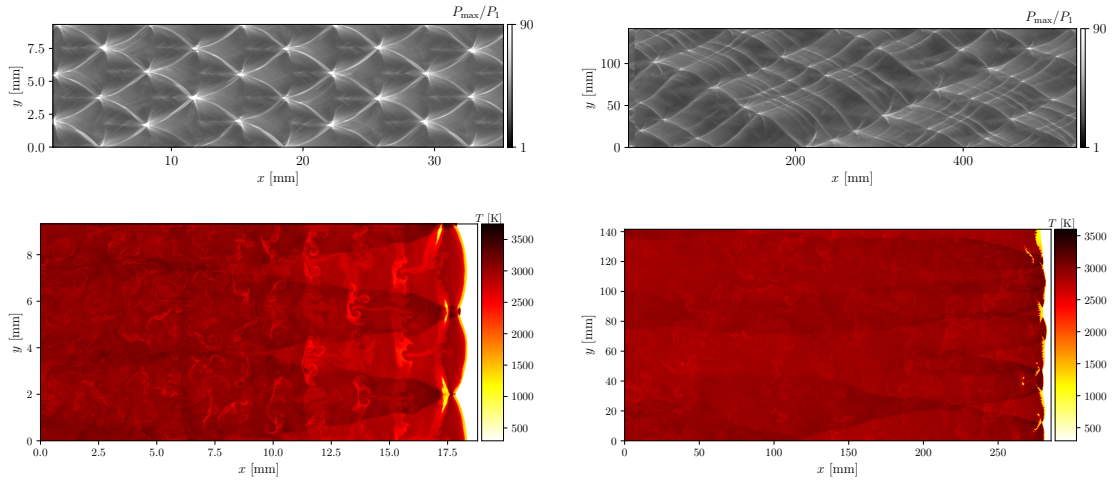


Figure 3: Probability density function of cell width over a range of equivalence ratio (Φ) obtained by sampling the reaction rate of (a) R_1: $H+O_2=OH+O$; and (b) R_2: $H+O_2(+M)=HO_2(+M)$. ZND detonation in H_2-air mixtures initially at 298 K and 101.325 kPa were considered. The color in the black-grey strips is proportional to the probability density. Black dashed lines denote the limit of values obtained by sampling the reaction rate of R_1 or R_2. Red lines represent the extreme values obtained by setting the rates of the top ten sensitive reactions to their extreme values; Experimental data are from [17].

2.4 Numerical cell width

We further studied the impact of chemical kinetics on the detonation cell width by performing 2D numerical simulations using the in-house code RESIDENT (REcycling mesh SImulations of DEtoNaTions), whose detailed description can be found elsewhere [18]. Based on the sensitivity analysis and the uncertainty quantification, two extreme reaction models predicting the smallest and largest induction lengths were prepared by setting the rate constant of all the sensitive reactions to their extreme value, within their respective uncertainty range. We refer to them as MechLow, and MechHigh, respectively. The cell widths predicted by these two mechanisms for H_2-air mixtures are shown in Figure 3. Clearly, the two mechanisms predict very different cell width, which can vary by several orders of magnitude, especially for very lean and very rich mixtures. Considering a stoichiometric mixture initially at 298 K and 101.325 kPa, the steady detonation induction zone length predicted by MechLow and MechHigh are 93

μm and 1.4 mm, respectively. The two extreme mechanisms were employed to perform 2D numerical simulations with an effective resolution of up to 20 pts/Δ_i. Figure 4 presents the 2D numerical soot foils and temperature fields obtained using the two extreme reaction models. First, it is interesting to note that a much more regular cellular structure was obtained when using the MechLow. In Figure 4 (a), a highly regular soot foil is observed with an essentially unique cell width of approximately 3.2 mm, which is approximately consistent with the value of 4.8 mm predicted using Eq. 1, but is 5 times smaller than the experimental value [17]. The temperature field also demonstrates the high regularity of the structure with a very smooth reaction zone front and well-defined keystone features. Unreacted pockets of gas are observed behind the front and exhibit smooth contours. In Figure 4 (b), a rather irregular soot foil is observed with a wide range of cell widths. Such an irregular behavior makes it difficult to distinguish between actual detonation cell and potential sub-structures and complicates the determination of the cell width. It seems the dominant cell width is in the range 30-70 mm, which is consistent with λ = 47.3 mm obtained with Eq. 1, but is 2 to 4.5 times larger than the experimental value. Although the temperature field is still characterized by well defined keystone features, the reaction zone front appears much more corrugated than in the simulation performed with MechLow. Unreacted pockets of gas away from the front are also present in this simulation but do not seem much more numerous than in Figure 4 (a).



(a) MechLow (b) MechHigh

Figure 4: Two-dimensional numerical soot foils and temperature fields obtained using two extreme reaction models predicting very small and very large induction zone lengths. Φ = 1; T = 298 K; P = 101.325 kPa.

3 Conclusion

In the present study, an accurate detailed reaction model for simulating detonation in hydrogen-air mixtures was selected through a quantitative comparison with experimental shock tube data. A reduced version of this model was employed to perform a UQ analysis on the detonation cell size predicted by the correlation of Ng et al. It was shown that, by sampling the reaction rate constant ($\ln k$), which obeys a joint normal distribution of ($\ln A$, n, E_a/R), the obtained probability distribution of cell width follows a GEV distribution. Besides, reaction R_1: H+O_2=OH+O and R_2: H+O_2(+M)=HO_2(+M) are the two most sensitive reactions to predict the cell width for stoichiometric H_2-air mixture initially at 298 K and 101.325 kPa. The contribution of R_1 and R_2 to the probability distribution of cell width was evaluated over a wide range of conditions. In addition, two extreme reaction models were developed based on

the maximum uncertainty of the rate constant of each of the most sensitive reactions, and were used to perform 2D numerical simulations of detonation in a stiochiometric H_2-air mixture. It was observed that the resulting cell width could change by as much as 20 times and that the regularity of the cellular structure could significantly vary depending on the characteristics of the chemical mechanism used.

Acknowledgements

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