Numerical study of the structure of detonation in very lean hydrogen-nitrous oxide mixtures

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1 Introduction

In some mixtures or under specific conditions, detonation soot records show sub-structures that appear in the first half of the main cell pattern [1]. Presles et al. [2] reported unsual sub-structures in nitromethane and nitromethane-oxygen mixtures. Contrary to the classical ones, sub-structures in nitromethane based mixtures survive in the second half of the main cell. Further studies [3] demonstrated that for a variety of fuels including H_2, CH_4, and C_2H_6, mixed with NO_2/N_2O_4 such sub-structures also appear. Their existence has been correlated with a non-monotonous energy release in the ZND structure for stoichiometric and rich mixtures [4]. The first step of energy release is fast and attributed to the oxidation by NO_2 whereas the second step is slow and driven by NO. Ng et al. [5] also correlated a two-step energy release with the double cellular structure observed in dimethyl ether-oxygen mixtures. Joubert [3] performed calculations of the ZND structure of various fuels mixed with N_2O over the equivalence ratio range 0.2-2, but detected no non-monotonous energy release. However, Karnesky and Shepherd [6] experimentally showed that very lean H_2-N_2O mixtures exhibit a double cellular structure. In a previous study [7], we demonstrated that, for these lean mixtures, i.e. equivalence ratio $\Phi \leq 0.10$, the ZND structure is characterized by a double-peak thermicity profile. Vasiliev and Trotsyuk [8] also reported double cellular structures in a variety of lean fuel-N_2O mixtures. Numerical simulations by Vasiliev and Trotsyuk [8] and by Guilly et al. [9] demonstrated that the double cellular structure can be reproduced by using a two-step kinetic scheme.
The present paper aims at investigating, by means of 1-D ZND and 2-D Euler simulations, the behaviour of H_2-N_2O detonations in the double energy release region, using realistic reduced chemical models.

2 The ZND detonation structure

The ZND structure of a 1-D stationary detonation can be simulated with the "Shock and Detonation ToolBox" using a detailed kinetic model [10]. The model used in the present study is that of Mével et al. [11]. It is constituted of 203 reactions and 32 species.
Figure 1 shows the evolution of temperature and thermicity [12] in the ZND detonation for H_2-N_2O mixtures at different Φ. It is clearly seen that, for very lean mixtures, $\Phi \leq 0.10$, the thermicity curves exhibit a double-peak shape.
Aiming at a further investigation, the analysis of the energy release per reaction and of the reaction pathways have been performed. The most energetic reaction is $N_2O+H=N_2+OH$ and its energy release curve presents a double peak shape for very lean mixtures. The analysis of H atoms reaction pathways shows that, at the first stage, H atoms are produced by $H_2+OH=H_2O+H$ and then, by $O+OH=H+O_2$. The reaction $H_2+OH=H_2O+H$ cannot sustain very long the H production because of the H_2 lack.

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Thus, the decrease in the heat release is due to a discontinuity in H production. As the importance of O+OH=H+O_2 increases, the energy release is re-intensified, resulting in a second thermicity peak. At greater Φ, there is enough hydrogen molecules, and the two-step energy release is no more observed.

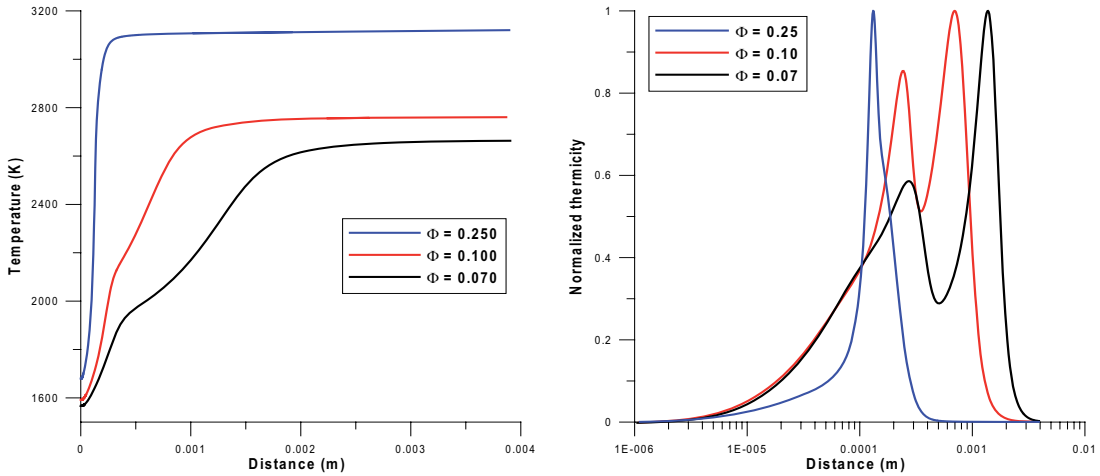

Figure 1: ZND structure in H_2-N_2O mixtures at different equivalence ratios. Left: Temperature profiles. Right: Thermicity profiles. Initial conditions: T_1 = 293 K; P_1 = 70.9 kPa.

3 Reduction of the detailed kinetic scheme

An automatic reduction procedure [13] has been applied to the detailed kinetic scheme for a H_2-N_2O mixture with Φ=0.07. The inital conditions are: T_{ini}=1567 K and P_{ini}=3.45 MPa, corresponding to a shock travelling at the CJ velocity.

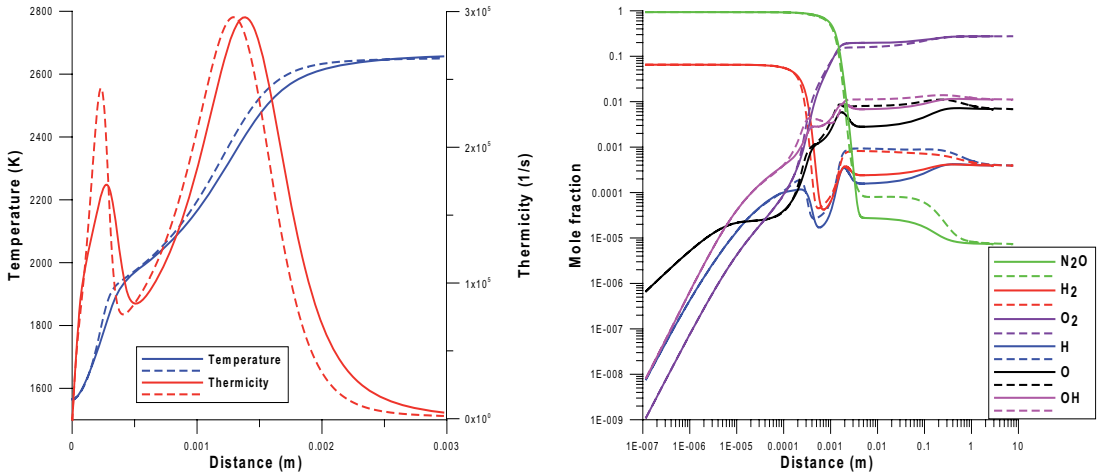

Figure 2: Comparison between the detailed and the reduced chemical schemes for ZND simulations. Left: Temperature and thermicity profiles. Right: Species mole fraction profiles. Solid lines: detailed scheme. Dotted lines: reduced scheme. Initial conditions: Φ=0.07; T_1=293 K; P_1=70.9 kPa.

The automatic reduction leads to a reduced scheme including 23 reactions and 18 species. In order to further reduce the model, the less important reactions among the remaining ones are deleted and a scheme with 13 reactions and 14 species is obtained.
Figure 2 compares the temperature, the thermicity, and the major species profiles obtained with the detailed and the reduced schemes for conditions corresponding to a 1-D stationary detonation travelling at CJ velocity in a H_2-N_2O mixture with Φ=0.07 at T_1=293 K and P_1=70.9 kPa. It can be seen that the agreement is quite good for these conditions. Previous numerical simulations of detonation in H_2-N_2O mixtures [13] have shown that the velocity of the leading shock typically varies between 1.6 and 0.8 the CJ velocity along a detonation cell. The reduced model gives also satisfactory results for conditions corresponding to this shock velocity range.

4 The 2-D detonation structure

Euler solver based on a Weighted Essentially Non-Oscillatory (WENO) scheme of the fifth order has been used to carry out 2-D simulations of detonations in a H_2-N_2O mixture with Φ=0.07. The kinetic model is the reduced scheme presented in the previous section. In addition, another simulation has been performed with a modified reduced scheme that exhibits a monotonous energy release profile in the ZND solution. With this reduced model, the maximum of energy release rate is located at the position of the second thermicity peak and its magnitude is 2.5 times higher.
The simulation results presented below are obtained for a 30 mm wide domain. The computational mesh is structured with the finest resolution of 25 μm. Periodicity conditions are imposed on the flow-wise boundaries. Other simulations performed for 30 and 60 mm wide domains with symmetry boundary conditions yielded very similar soot records but with less regular pattern of major cells.

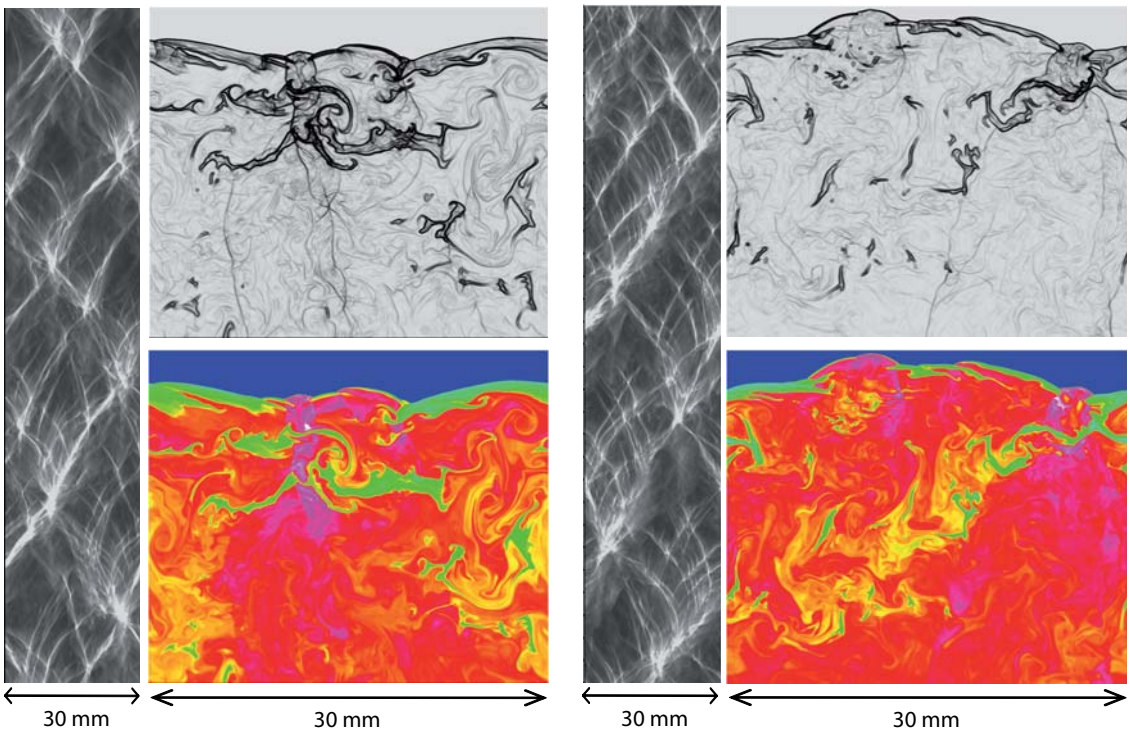

Figure 3: Numerical soot foils, Schlieren pictures and temperature fields of detonations in a H_2-N_2O mixture. Left: Double energy release. Right: Single energy release. Initial conditions: Φ=0.07; T_1=293 K; P_1=70.9 kPa.

Figure 3 shows numerical soot foils, Schlieren pictures and temperature fields obtained for H_2-N_2O mixtures with the two different schemes. Initial conditions are: T_1=293 K ; P_1=70.9 kPa. From the soot foil patterns, it can be seen that, for both reduced schemes, sub-structures appear within the main cells, which are 30 mm wide in most cases. The Schlieren pictures clearly show double Mach reflections of smaller size at the detonation front. Both Schlieren pictures and temperature fields demonstrate that large pockets of unburnt gas survive far dowstream from the detonation front.
On the contrary to what was observed by Guilly et al. [9] in their numerical simulations of detonation in H_2-NO_2/N_2O_4 mixtures, the non-monotonous energy release cannot be related to the existence of sub-structures in our simulations. Moreover, the soot records obtained by Guilly et al. [9] appear very different from our results. This distinct behaviour might be explained by some differences existing between the kinetics of H_2-N_2O and H_2-NO_2/N_2O_4 mixtures. First, in H_2-NO_2/N_2O_4 mixtures, the amplitude of the thermicity peaks are several orders of magnitude different whereas in H_2-N_2O mixtures, the peaks are of the same order of magnitude. Second, in H_2-NO_2/N_2O_4 mixtures, the distance between both peaks is much larger. Third, in H_2-N_2O mixtures, the smaller peak is followed by the higher one whereas it is the opposite in H_2-NO_2/N_2O_4 mixtures. Finally it can be noted that, in H_2-N_2O mixtures, the double thermicity peak is not present in the first part of a cell as the leading shock is largely overdriven. Thus it might be concluded that some critical conditions have to be fulfilled for the thermicity profile to generate "nitromethane-like" sub-structures.

5 Conclusion

In the present paper, the structure of detonation in very lean H_2-N_2O mixtures has been investigated in the double energy release region through numerical simulations using a realistic kinetic scheme. The ZND structure has been explained through a discontinuous energy release. A reduced kinetic model has been obtained and used for 2-D numerical simulations. Numerical results have clearly shown the complexity of the detonation front structure which exhibits similar features for both cases of single and double thermicity peaks.

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