Modelling of Detonation Cellular Structure in Aluminium Suspensions

Arnaud Briand, Bernard Veyssière, Boris A. Khasainov

Laboratoire de Combustion et de Détonique, CNRS UPR 9028
1 av. Clement Ader, 86 961, Futuroscope-Chasseneuil, France

1 Introduction

Heterogeneous detonations involving aluminium suspensions have been studied for many years due to their interest in industrial safety policies, military applications or propulsion applications. As for gaseous detonations, the cellular detonation structure was established to exist in aluminium suspensions in oxidizing atmosphere (see for example [1], [2]), but its characteristic size is larger due to slower chemistry of heterogeneous burning of particles.

The numerical model recently developed by the authors is able to simulate the detonation cell structure, and the calculated cell size agrees with the few experimental results available for suspensions of aluminium particles in air or oxygen [3]. It also displays major differences between heterogeneous and gaseous detonations as far as ignition period is concerned. In the case of aluminium - gas mixtures, particle ignition does not occur first in high pressure zones around the triple point areas, where the aluminium concentration is maximum but the temperature is the lowest, due to the convection of solid particles by the transverse waves. Particle ignition is controlled by the heat exchange rate between gas and particles and occurs outside triple point zones where low concentration of particles allows fast ignition.

Using a two-step model including separated induction and combustion periods for aluminium burning, Briand et al. [4] investigated numerically the detonation cellular structure in aluminium suspensions as function of the characteristic parameters of the particles. For both aluminium - air and aluminium - oxygen mixtures, the detonation cell size was found to be proportional to the particle diameter to the power 1.4, in agreement with other studies [5], [6]. Moreover, like for gaseous detonations, a linear relationship was found between the detonation cell size and the induction length while no obvious correlation was found between the cell size and the combustion zone length [4]. In the present work we improve the predictive ability of our model [4] by incorporating a hybrid model of aluminium combustion similar to that proposed by Zhang et al. [7] and examine correlations between the detonation cell size and the particle diameter.

2 Modelling aluminium combustion behind shock wave

Our previous two-step model for aluminium combustion [4], although simplified, allowed us to easily separate the induction and combustion periods and to study their distinct effects on the detonation cell structure. This model was also used in many studies [5], [8]. However, it requires defining a particle

Correspondence to: arnaud.briand@lcd.ensma.fr

ignition temperature which plays a double role: below this temperature the combustion rate is equal to zero, and beyond it the combustion is triggered. However, definition of an appropriate criterion for aluminium particle ignition in dynamic conditions behind a shock wave is difficult and somewhat arbitrary. Here we incorporate a hybrid model based on that proposed by Zhang et al. [7], [9] which combines in a more realistic way both kinetic and diffusion regimes of aluminium combustion and does not require any ignition temperature. The key point of this hybrid model is in the mass exchange source term J (overall burning rate), which is modelled as follows:

$$J = \left(\frac{1}{J_{kin}} + \frac{1}{J_{diff}} \right)^{-1} \tag{1}$$

where particle burning rates in kinetic regime J_{kin} and diffusion regime J_{diff} are defined respectively with equations (2) and (3):

$$\begin{cases} J_{kin} = \pi d_p^2 n_p Z_{Arr} \exp\left(\dfrac{-E_a}{RT_p} \right) & (2) \\ J_{diff} = 3\sigma \left(1 + 0.276\sqrt{\mathrm{Re}}\right) \Big/ t_p & (3) \end{cases}$$

Here σ is the particle concentration, *Re* is the Reynolds number, t_p is the particle burning time in diffusion-controlled regime, d_p is the particle diameter, n_p is the particle number density, Z_{Arr} is the pre-exponential factor, E_a is the activation energy, R is the universal gas constant and T_p is the particle temperature. The burning time t_p is defined as:

$$t_p = \frac{k d_{p0}^2}{\phi_{ox}^{0.9}} \tag{4}$$

where k is the burning constant and Φ_{ox} is the weight fraction of oxidant.

3 Simulation of the detonation cellular structure with the hybrid model

As for the previous two-step model, three parameters have to be set to describe the chemistry of aluminium combustion. The burning constant k is set to the same value as in our former two-step model: $k = 1.6 \times 10^6$ s/m², as found by Ingignoli [10] for flake-type particles. In addition, the activation energy of the kinetic regime in the mass exchange source term is also set to the same value as before, in the case of reaction between aluminium and oxygen, according to the results of Merzhanov et al. on aluminium wires combustion [11]: E_a = 17 000 cal/mol. Hence, Z_{Arr} is the only best-fitting parameter as compared with the two-step model, due to different definition of kinetic regime. It was varied in a wide range, and the calculated results were compared with experimental ones as in [3] for aluminium - air and aluminium - oxygen mixtures.

Aluminium - air reference mixture corresponds to the experiments of Zhang et al. [2] with flakes (with an estimated equivalent diameter d_p = 13.5 μm). Experimental detonation cell width is $\lambda \approx 40$ cm for a rich mixture (equivalent ratio 1.61) at particle concentration $\sigma = 500$ g/m^3. The pre-exponential factor in the hybrid model is set to $Z_{Arr} = 7.5 \times 10^4$ kg/m²/s.

Aluminium - oxygen reference mixture is that of the experiments of Ingignoli et al. [1] for flakes with an equivalent diameter of d_p = 8.6 μm, for which the detonation cell size has been estimated to be about $\lambda \approx$ 5-10 cm for a mixture at stoichiometry (particle concentration $\sigma = 1500$ g/m^3). The pre-exponential factor in the hybrid model is set to $Z_{Arr} = 3 \times 10^6$ kg/m^2/s.

Typical cellular structures, obtained by numerical simulations performed using this set of parameters, are displayed in Fig. 1. For aluminium – air mixture, the average detonation cell size is $\lambda \approx$ 40 cm, while in the case of aluminium – oxygen mixture it is $\lambda \approx 10$ cm. These results are in reasonable agreement with experimental observations. Compared with our previous model [3], these calculated detonation cell sizes are a little bit larger. Further characteristics may be derived from the examination of Fig.1: the cellular structure appears to be less regular for aluminium – air mixture while for aluminium – oxygen mixture, the trajectories of transverse waves seem to be thicker and

amplitude of pressure variations less important. This might be attributed to an effect of the longer induction length (kinetic regime) ensuing from the hybrid model for aluminium – oxygen mixture, since the detonation cell size is $\lambda \approx 10$ cm, while the value of λ was only ≈ 7.5 cm with the two-step model (see next section).

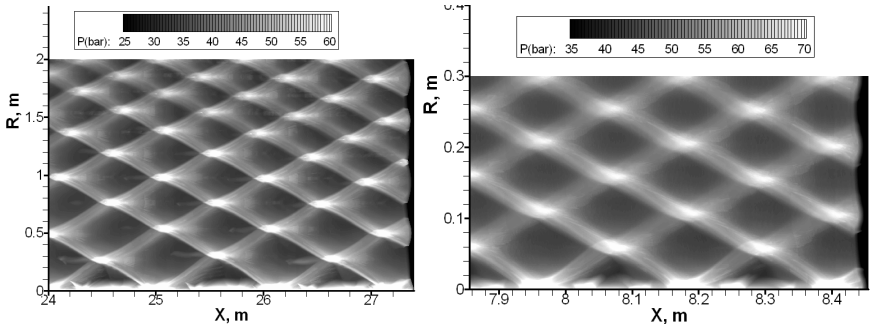

Figure 1. Detonation cells obtained using the hybrid model. Left: aluminium – air mixture, equivalent particle diameter 13.5 µm, richness 1.61. Right: aluminium – O_2 stoichiometric mixture, particle diameter 8.6 µm.

From Fig. 2, one can observe that this model is consistent with previous results on ignition and combustion regimes in the case of aluminium – air detonation [3], [4], [7]. Indeed, before ignition, the overall burning rate J is superposed on kinetic regime curve J_{kin} (up to 4.1 cm behind the front). After a transition zone of about 2.8 cm, the overall burning rate J then coincides with diffusion regime curve J_{diff}. Moreover, particles start to burn when their temperature T_p is of about 1100 K, which is consistent with usual experimental and numerical values.

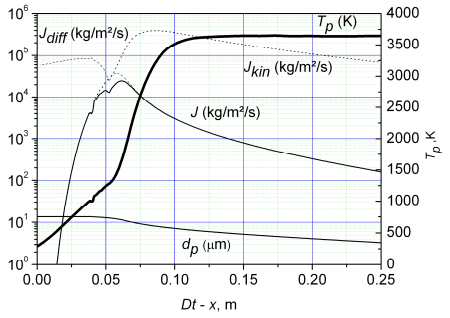

Figure 2. Combustion regimes and ignition parameters for aluminium – air mixture.

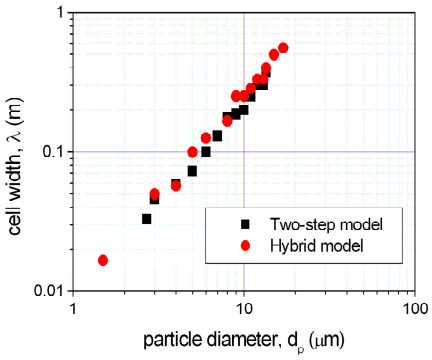

Figure 3. Detonation cell size as function of particle diameter for both models (aluminium - air mixture)

4 Influence of the particle diameter on the detonation structure

From numerical simulations with the two-step model, it has been found that the detonation cell size was proportional to the particle diameter to the power 1.4 for both aluminium – air or oxygen mixtures, the induction length being linearly dependent on the particle diameter, and the combustion zone length proportional to the particle diameter to the power 1.8 [4]. With the present hybrid model, the same behaviour is observed for aluminium – air mixtures for particle diameter varying from 1.5 µm to 17 µm. The case of aluminium – oxygen mixtures is currently under investigation and preliminary results give the same expected tendency. Examination of temperature evolution behind the leading shock wave shows that the aluminium particle radius begins to significantly decrease when particle temperature is close to that imposed by the two-step model. Detonation cell sizes and combustion zone lengths are very close to those obtained with the two-step model, the induction length being a little bit higher with the hybrid model. Dependences of the detonation cell size on

particle diameter are compared in Fig.3 between the two-step and hybrid models for the aluminium – air mixture. One can observe good agreement between the models.

Linear dependence is found between the detonation cell size and the induction length (kinetic regime), with proportionality factor *K* of the order of 11, compared to a value of 8 for the two-step model [4]. This dependence is analogous to that exhibited for gaseous detonations where *K* ranges from about 10 to 100. No obvious correlation was observed concerning dependence of the cell width on the combustion zone length (diffusive regime).

5 Conclusion

The hybrid model used in this study appears to be more realistic in terms of aluminium combustion modelling as compared with our previous two-step model. Moreover, aluminium particle ignition is automatically controlled by transition between kinetic-limited regime and diffusion-limited burning regime, which overtakes the difficulty of selecting an appropriate ignition temperature of particles behind a shock wave. Furthermore, the characteristic correlations displayed with the two-step model between the cellular structure and particle diameter are confirmed by the hybrid model, and our preceding conclusions remain valid.

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