Analysis of combustion problems in highly dilute dust and gas mixtures

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1 Introduction

When a cloud of combustible dust is in contact with oxygen in the air at high temperature, a combustion reaction can occur spontaneously, in some cases producing a detonation wave that propagates at high speed. The risk of dust explosion is a threat, known and studied for decades, in all industrial processes where combustible dusts are present. For almost a century spontaneous explosions in coal mines or in corn silos have caused fires and damage at different levels. Nowadays, the dust explosion is studied in different fields, such as ballistics and nuclear energy. In fact, it is known that the powder contained inside the reactor vessel could react violently if in contact with oxygen in the air. It is important to develop accurate predictive tools capable of analyzing these events to ensure safety.

In this paper the combustion of a highly dilute mixture of gases and particles is studied. By considering the volume fraction of particles is nearly zero, and neglecting the pressure on the particles, we obtain a decoupled system of equations easier to solve numerically. A computational finite volume code has been developed to deal with such kind of problems involving multiphase flow and detonation phenomena. Two different experiments existing in the literature have been used to check the reliability of the code, the first one involving combustion of aluminium particles in air, and the second one including the hydrogen-oxygen reaction.

2 Physical model considered

Considering the dilute character of the solid and gas mixtures included in this work, several mathematical models have been studied (see [5]). Let us propose for this study a system of two-phase conservation equations, assuming spherical and incompressible particles [3], and taking into account the combustion source terms. The implemented code, based on the reported equation model, is able to solve 1D, 2D and 3D problems, with non-conformal meshes , but only 1D results are shown in Section 4 because of test's characteristics.

$$\frac{\partial \rho_g}{\partial t} + \vec{\nabla} \cdot (\rho_g \vec{u}_g) = \Gamma_g,$$
$$\frac{\partial \rho_g \vec{u}_g}{\partial t} + \vec{\nabla} \cdot (\rho_g \vec{u}_g \otimes \vec{u}_g + pI) = -\vec{F}_d + \rho_g \vec{g} + \Gamma_g \vec{u}_p,$$
$$\frac{\partial \rho_g E_g}{\partial t} + \vec{\nabla} \cdot (\vec{u}_g (\rho_g E_g + p)) = -\vec{u}_p \vec{F}_d + \rho_g \vec{u}_g \vec{g} + \Gamma_g H_p + Q_d + \alpha Q_c,$$
$$\frac{\partial \rho_g Y_m^g}{\partial t} + \vec{\nabla} \cdot (\rho_g \vec{u}_g Y_m^g) = \Gamma_m, \quad \text{for } m = 1, \ldots, NGSP.$$
$$\frac{\partial \sigma}{\partial t} + \vec{\nabla} \cdot (\sigma \vec{u}_p) = \Gamma_p,$$
$$\frac{\partial \sigma \vec{u}_p}{\partial t} + \vec{\nabla} \cdot (\sigma \vec{u}_p \otimes \vec{u}_p) = \vec{F}_d + \sigma \vec{g} + \Gamma_p \vec{u}_p,$$
$$\frac{\partial \sigma E_p}{\partial t} + \vec{\nabla} \cdot (\vec{u}_p \sigma E_p) = \vec{u}_p \vec{F}_d + \sigma \vec{u}_p \vec{g} + \Gamma_p H_p - Q_d + (1-\alpha) Q_c,$$
$$\frac{\partial \sigma Y_n^p}{\partial t} + \vec{\nabla} \cdot (\sigma \vec{u}_p Y_n^p) = -\Gamma_n, \quad \text{for } n = 1, \ldots, NSSP.$$

where subscripts g and p denote gas and particle phases, ρ is the density, u velocity, p is the pressure, and g is the gravity. $NGSP$ and $NSSP$ are the number of species in gas and solid phase, respectively. The left side terms represent the advection or "Euler" part of the flow equations. The right-hand side terms include interfacial mass, momentum, and energy exchange. Total energy for gases and particles are defined as: $E_g = \frac{p}{\gamma-1} + \frac{1}{2}\rho u^2$, $E_p = \sigma c T_p + \frac{1}{2}\sigma u_p^2$. H_p is total entalphy of particles. F_d represents the drag force over the particles and Q_d the heat transfer in the particle interface. Γ is the phase mass exchange due to combustion ($\Gamma_p = \Gamma_g$) and Q_c represent the released combustion heat. Note that α, the void fraction, cannot be assumed to be equal to 1 inside the combustion energy source term.

3 Combustion models utilized

3.1 Hydrogen oxidation

The hydrogen air detonation has extensively been studied and the kinetics is well understood. In the reaction process, we can distinguish between the induction stage and exothermic recombination stage. In our model, we consider the one step, global reaction mechanism:

$$2H_2 + O_2 \xrightarrow{\dot{\omega}} 2H_2O \tag{1}$$

where the reaction rate is given by a general Arrhenius law of the form:

$$\dot{\omega} = H(T - T_s) A \rho^3 Y_{H_2}^2 Y_{O_2} T^{-b} \exp(-T_a/T) \quad (\text{in mol} \cdot \text{m}^{-3} \cdot \text{s}^{-1}) \tag{2}$$

where $H(y)$ is the Heaviside function, T_s the threshold temperature ($T_s = 1200$K), $A = 1.1725 \cdot 10^{14}$ (in units consistent with International System), $T_a = 8310$K and $b = 0.91$. Then the reaction rate of each component is given by $\dot{\omega}_{H_2} = -2W_{H_2}\dot{\omega}$; $\dot{\omega}_{O_2} = -W_{O_2}\dot{\omega}$; $\dot{\omega}_{H_2O} = 2W_{H_2O}\dot{\omega}$.

3.2 Metal combustion. Aluminium particles

Ogle et al. [4] proposed to use a model developed by Markstein (1966), where the aluminium droplet oxidation process takes place through a number of six homogeneous and heterogeneous reactions. However, the overall reaction can be expressed as:

$$2Al + \frac{3}{2}O_2 \rightarrow Al_2O_3 \tag{3}$$

The rate of reaction can be transformed into a quasi-homogeneous reaction rate (Slattery, 1981) and, in mass units, can be written as:

$$\dot{r}_{Al} = \alpha_{Al} S_v k \rho_m^{3/2} Y'_{Al} Y'^{0.5}_{O_2} \quad \left(\frac{\text{kg}_{Al}}{\text{m}^3 s}\right). \tag{4}$$

where the surface to volume ratio of the aluminium droplet cloud is $S_v = 6/d_p$; $\alpha_{Al} = Y'_{Al}\frac{\rho_m}{\rho_{Al}}$; $\rho_m = \rho_g + \sigma$; Y'_i represent the mass fraction of the species i related to total mass and k is the lumped parameter rate coefficient, which is written in Arrhenius form: $k = Aexp\left(-E/R_gT\right)$, with a value for the Arrhenius constant equal to $A = 3.8 \times 10^5$ (m^3/kg) $^{1/2}\cdot$ s^{-1} and a value for the activation energy $E = 100$ kJ/kmol. R_g is the gas constant (about 0.237 kJ/kgK for air) and T is temperature in Kelvin.

Using the conservation of total mass for a reacting mixture ($\sum_{i=1}^{N} \dot{r}_i = 0$), the rates of the reaction can be related to equation 4:

$$\dot{r}_{O_2} = s \cdot \dot{r}_{Al}; \quad \dot{r}_{N_2} = 0; \quad \dot{r}_{Al_2O_3} = \dot{r}_{Al} - \dot{r}_{O_2} = -(s+1)\dot{r}_{Al} \tag{5}$$

The amount of gas consumed in the reaction, Γ can be computed as the sum of all rates of reaction of gas phase. In the present case, only oxygen will react (as nitrogen behaves as inert).

The heat of combustion (absorbed or released) can be computed as the enthalpy change of reaction:

$$Q_c = \dot{r}_{Al_2O_3}\frac{\Delta H^0_{Al_2O_3}}{W_{Al_2O_3}} - \dot{r}_{Al}\frac{\Delta H^0_{Al}}{W_{Al}} - \dot{r}_{O_2}\frac{\Delta H^0_{O_2}}{W_{O_2}} \approx \dot{r}_{Al_2O_3}\frac{\Delta H^0_{Al_2O_3}}{W_{Al_2O_3}} \tag{6}$$

4 Numerical results

4.1 Combustion of Al particles. Chen Test

As a test, to check the results obtained with our finite volume numerical code, some suitable experimental results have been searched within the literature. An interesting test with experimental data has been found in Chen [1]. It consists of a large, horizontal combustion tube containing a mixture of aluminium powder. It is considered that the gas phase inside the tube is atmospheric air (oxygen and nitrogen). The rate of oxygen in air is 21% molar. A uniform suspension of dust is assumed along the tube. The particle diameter is 6 μm and the particle concentration of the mixture is $\sigma = 500$ g/m^3. Initial conditions are given by a pressure of 1 bar and the ambient temperature $T = 300$ K for the entire tube. The ignition temperature of aluminium $T_{ig} = 1350K$. Both phases (gases and particles) are considered initially at rest. The mass fraction of aluminium is maximum, $Y_1^p = 1$, initially and it decreases as combustion goes on. The tube diameter is 0.14 m (circular cross section) and its length 20m.

Finally, an initial ignition state has been computed in the first two cells of the unidimensional domain. This implies to force the reaction of all the aluminium or oxygen present in these two cells, adding the resultant heat for both solid and gas phases. The initial ignitionstarts a self-sustaining reaction. The increase in pressure and the resulting high temperature leads to a phenomenon of DDT (Deflagration-to-Detonation Transition). As time progresses, the detonation front moving at high speed towards the other end of the tube, while all aluminium particles burn progressively. The distribution of variables along the tube is shown in Figure 1, where blue color has been used for variables corresponding to particles (u_p, σ, T_p and Y_p), red color for those corresponding to the gas phase (u_g, ρ_g, T_g and Y_g) and green for the variables of the ignition state. The history of the pressure variable in different x coordinates in the tube is shown in Figure 2.

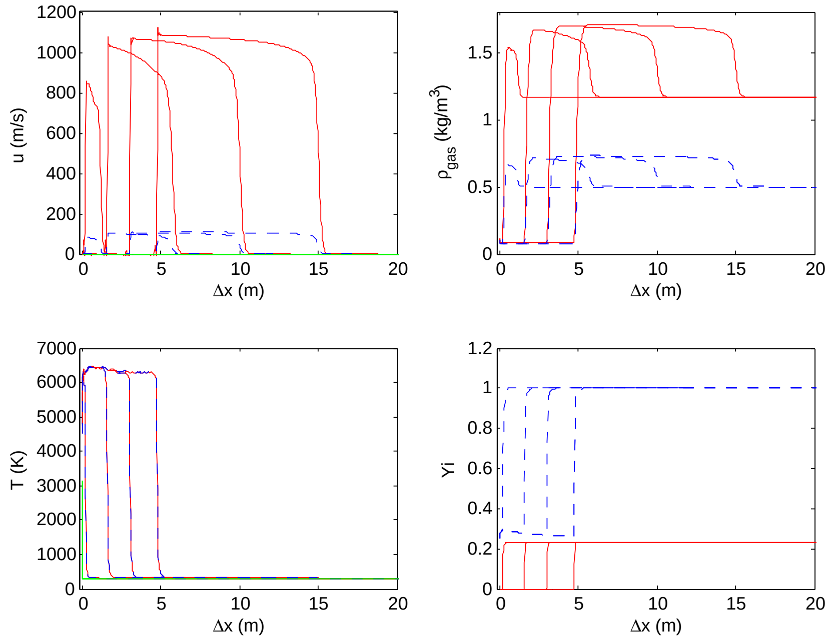

Figure 1: Chen test: Distribution of several variables along the tube at t= 0.003, 0.017, 0.030 and 0.044s.

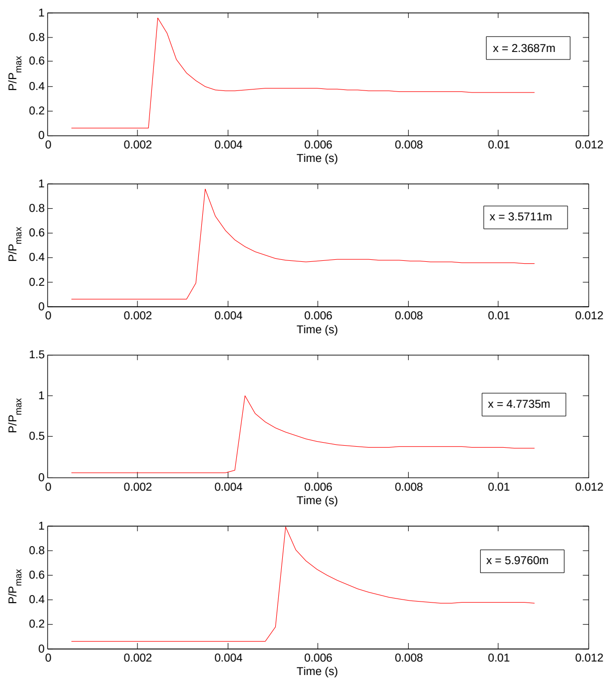

Figure 2: Chen test: History of pressure over time for different positions: x = 2.3687, 3.5711, 4.7735 and 5.9760m.

4.2 Combustion in both phases. Veyssiere Test

The next stage in our study is to analyze the problem of combustion of both phases. That means not only particles will burn, but also some species from the gas phase. A new reacting species (H_2) has been added within the components of the gas mixture. Now, two general combustion chemical reactions are considered to take place simultaneously in the problem (Eqns. 1 and 3). These reactions will be mathematical and numerically modelled as two different processes, although oxygen will be a common species in both of them. The combustion model used here for solid phase is similar to that used in previous sections of this work. The model for the hydrogen combustion has been extracted from Beccantini (2001) and it is based on the Arrhenius approach.

Among several possible tests is the work of Veyssiere (1984), who reported some data on various experiments in the detonation tube. The author used their data to study the influence of various parameters on the double-front detonation process that occurs in two-phase mixtures of a detonable gas with aluminium particles in suspension. We will focus on his results concerning a mixture of atmospheric air and hydrogen with aluminium particles. There are three gas species: $H_2 + XO_2 + ZN_2$ following the relationship: $Z/X = 3.76$ and $r = 0.78$ (being $r = 1/\lambda$ the fuel-oxidizer rate). The concentration of aluminium particles (mean diameter 10μm) was set to $\sigma = 65g/m^3$. The fluid domain considered is a horizontal simple tube, whose geometrical dimensions have been extended to $L = 60$m and $D_{internal} = 69$mm, so that we can observe the development of detonation. This domain has been modelled in 1D and split into longitudinal cells with $\Delta x = 0.4m$.

As in the previous test, in the first two cells of the domain sudden combustion is forced over the minority species. This produces a detonation shock which propagates rapidly, inflaming in its way the H_2 and Al present in the tube. The detonation front propagation can be seen in Figure 3.

Pressure history in different positions along the tube has also been depicted (Figure 4). One can easily see how the main pressure peak is followed by another peak of lower intensity. This can be interpreted as the double-front detonation Veyssiere reported on his work. However, this second front is not as sharp as expected, possibly because of the simplicity of the Arrhenius-type model used. Remains as future work to improve the combustion model used.

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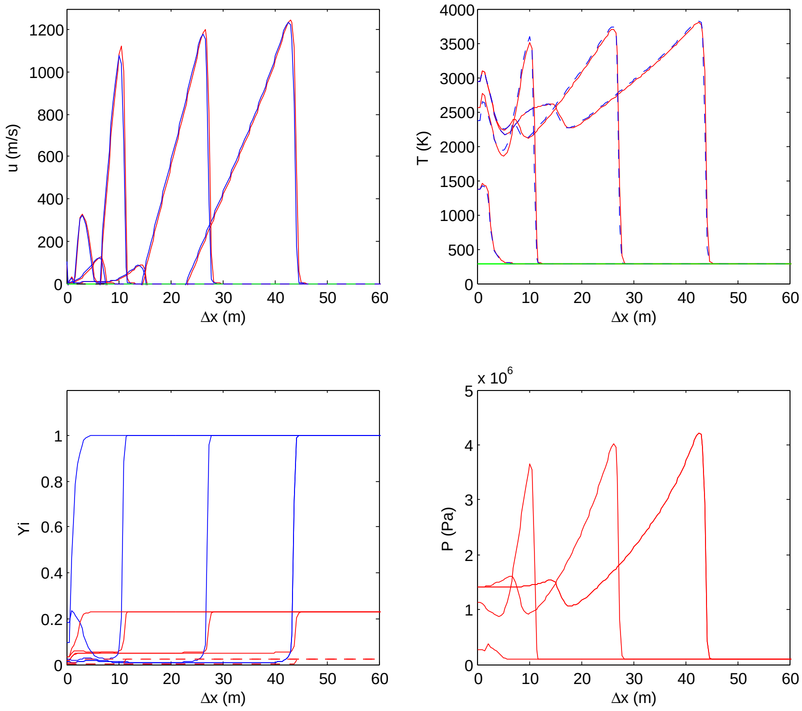

Figure 3: Veyysiere test: Distribution of several variables along the tube at t= 0.005, 0.010, 0.015 and 0.020s.

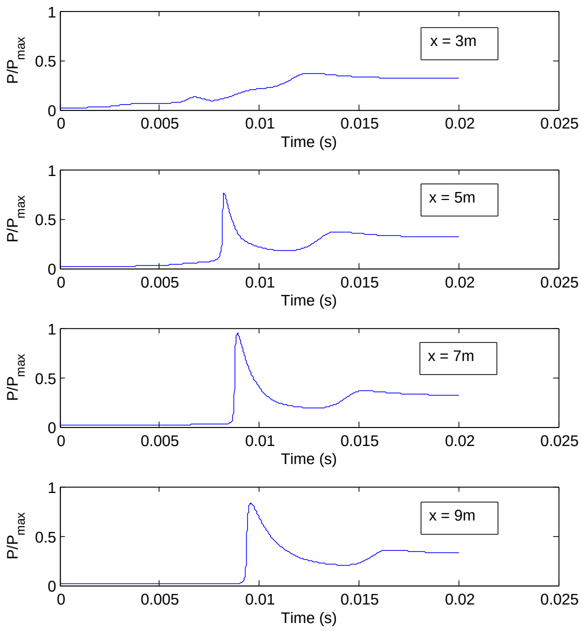

Figure 4: Veyssiere test: History of pressure over time in several x coordinates.