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Closed and vented explosions with kerosene droplets

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Extended abstract :

Over the last past years, there has been a considerable effort to precise the characteristics of the combustion of liquid fuel droplets¹. The combustion of kerosene has received much recent attention because of its importance in power-generating equipment, especially in high output military aircraft propulsion systems.

The aim of this work consists in presenting a simple modelling, initially developed for ignition and combustion of dust suspensions² and studying the model transposition to liquid kerosene droplets in order to predict the main characteristics of these explosions in a closed or a vented vessel. Simulated predictions have been compared with experimental results available in the literature and a special kind of kerosene (F.34) which has been studied as part of a contract between the laboratory and the Ministry of Defence (DGA).

We consider that the combustion of the liquid droplets results from collisions between particles of the gaseous phase and those of the liquid phase. The reactive system is composed of molecules in gaseous phase, active molecules and condensable molecules.

The energy flux brought to the liquid fuel leads to its degradation by active or condensable molecules and to the dissociation by the other molecules in the gaseous phase. All those phenomena contribute to the liquid fuel destruction. The combustion of the kerosene droplets takes place in a closed vessel, fitted with a vent and considered as a perfectly well-stirred reactor.

The liquid fuel evaporates. Some molecules change from the liquid phase to the gaseous phase. The equilibrium between both liquid and gaseous phases is obtained when the partial pressure of the fuel vapor reaches the saturated vapor pressure. We obtain for the fuel ratio :

$$\varphi = \frac{m_{sto}}{m} = m_{sto} \cdot \frac{P_{po}}{P_o - P_{po}}$$

where P_o is the initial pressure in the vessel.

The evaluation of the partial pressure P_{po} has been carried out for kerosene F.34 or deduced from literature for other kinds of kerosene.

The equations introduced in the model need the evaluation of several parameters which characterize molecular collisions, condensation and energy transfers³. The model was initially validated by studies on dust suspensions² and two-phase mixtures³ with the same set of parameters. The same values have been conserved for the combustion of the kerosene droplets.

In the case of vented explosions, the vent breaking is taken into account by the calculation code when the overpressure in the medium reaches the static venting pressure P_v . If the vent opens when the mixture ignites, we have then $P_v = P_o$. The total mass rate of gaseous substances from the

confining volume to the surrounding atmosphere is given by the standard orifice equations⁴. The amount of the liquid fuel and the mass rate of each species discharged through the vent are calculated assuming a global mass rate partition among the different species.

The knowledge of the chemical process and the amount of evacuated molecules allows to know by successive time steps, the number of molecules and the mass of each species remaining in the vessel. The numerical integration of equations gives the access to thermodynamical factors and to the calculation of the time evolution of the pressure, the rate of pressure rise and the regression velocity of the kerosene droplets.



Figure 1 shows the evolution of the ratio P_{max}/P_o as a function of the temperature for a closed vessel such as $V_o=33$ *l* and various kinds of kerosene. Different curves are presented for initial pressures rising from 100 to 300 kPa. The same kind of evolution is observed for the different initial pressures with a sort of translation effect and a maximum corresponding to relatively rich mixtures ($\varphi \approx 1.3$). The peaks seem to be more or less close according to the nature of the kerosene. The ratio P_o/P_o

The peaks seem to be more or less close according to the nature of the kerosene. The ratio P_{max}/P_o has been experimentally studied⁵ for kerosene F.34. It has been etablished that this ratio was nearly constant and close to 6 for the different initial pressures. The model also gives a constant ratio which slightly differs according to the kerosene used. The ratio is close to 6.7 for kerosene F.34, to 8.2 for kerosene JP.4 and to 5.8 for kerosene JP.5. Furthermore, the temperature evolution of the ratio P_{max}/P_o has been carefully experimentally studied⁵ for $P_o = 300$ kPa and for kerosene F. 34. A similar evolution to the theoretical curve is obtained, but with slightly higher temperature values. The maximum of the ratio P_{max}/P_o calculated by the model for $P_o = 300$ kPa corresponds to a temperature close to T = 350 K. The experimental results lead to 360 K. Also the experimental decrease is slower and extends over a larger temperature range $\Delta T \approx 15$ K. The influence of the studied kerosene on the temperature evolution can be mentionned. For kerosene F.34, the curves obtained present a maximum which varies between 310 and 350 K. For kerosene JP.5, the maximum varies between 350 and 410 K which corresponds to a noticeably higher and slightly larger temperature range. For kerosene JP.4, the maximum varies between 250 and 280 K

corresponding to a narrower area and to much lower temperatures. The evaluation of the partial pressure⁶ of the kerosene vapors explains these different evolutions. Kerosene F.34 appears as an intermediate kerosene, between kerosenes JP.4 and JP.5 both for the ratio P_{max}/P_o and the temperature evolution area.

Figure 2 shows the time evolution of the absolute pressure for different initial temperatures and pressures $P_o = 200$ and 300 kPa in a closed vessel such as $V_o = 33 l$.



Fig 2 Pressure vs time for different temperatures and a given initial pressure.

For $P_o = 200$ kPa, the temperature corresponding to stoichiometric conditions is close to 325 K and for $P_o = 300$ kPa, the value obtained is near 340 K. The increase of the temperature in a lean mixture leads to a progressive increase of the maximum of pressure and to a very important decrease of the rise time. The system gets nearer stoichiometric conditions. The increase of the temperature in slightly rich mixtures leads to a nearly constant maximum of pressure and to much longer rise times. Finally for richer mixtures, the maximum of pressure quickly slows down towards the initial conditions. Similar phenomena are observed for gaseous mixtures or dust suspensions³. The model also allows the description of thermodynamical conditions resulting from a vent

opening. Experiments have been performed in a cubic tank such as $V_0 = 33 l$ with a global vent area $A_v = 2 \text{ cm}^2$.



Figure 3 compares the time evolution of the theoretical reduced pressure with an experimental result for initially given conditions and for a static venting pressure $P_v = P_o$.

The theoretical simulation is obtained for a spherical vessel geometry and gives a rather good correlation. Despite the vent opening, the pressure in the reactive mixture quickly grows and reaches a maximum around 120 ms. Then, the pressure decreases and tends towards the

atmospheric conditions after a long enough time around 800 ms. The theoretical maximum of pressure is closed to 520 kPa and remains higher than the experimental value ($P_{max} = 450$ kPa). The insertion in the calculation of a cubic geometry is presented in figure 4. The maximum of the reduced pressure is close to 420 kPa which corresponds to a fall of about 100 kPa in comparison with the spherical geometry and the rise time is slightly shorter around 100 ms. An excellent correlation of the theoretical simulation can be observed with both limit curves deduced from experimental studies. A more systematic study of the venting effects can be carried out to improve safety in industrial plants.



5 Pressure vs time for a vent area A, static venting pressures.

Figure 5 shows the time evolution of the reduced pressure for a given vent area $A_v = 20 \text{ cm}^2$ and for different values of the venting pressure. Stoichiometric conditions ($T_o = 337 \text{ K}$) and a slightly rich mixture are presented. For fuel ratios near the stoichiometry, the rise time is very short and the various curves are characterized by a high peak of pressure whose time position remains approximately constant around 18 ms.

The same behaviour can be noticed for higher values of the venting pressure in slightly rich mixtures, but the rise time is much longer and the overpressure remains limited to well-defined initial conditions. Finally, a slight inflexion in the pressure evolution also occurs at the vent breaking for the lowest values of the venting pressure.

The previous results show a good ability of the model to the description of closed or vented kerosene explosions for very wide use conditions, such as the fuel ratio of the mixture, the influence of thermodynamical factors, the thermal exchanges or the venting effects. The first results let appear correct tendencies in the predictions and it seems interesting to precise this evaluation.

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