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Calculation of the effect of a tank partitioning on a kerosene explosion

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Extended abstract :

The combustion of liquid fuel droplets^{1,2} has received much recent attention because of its importance in power-generating equipment, especially in high output military aircraft propulsion systems. In the course of previous works, we have presented a simple modelling initially developed as part of a novel study on ignition and combustion of classical propulsive powders in order to predict the main characteristics of fuel explosions in a closed or a vented vessel^{3,4}.

The aim of this work is to give a theoretical study on the chain propagation of a kerosene explosion inside a partitioned vessel. A calculation methodology is developed allowing to adapt the numerical simulation to the case of the transmission of the explosion from one compartment to another adjacent compartment by the means of the hot flow through the shared orifice and finally to generalise this methodology to a complex multi-partitioned structure. Simulated predictions have been compared with experimental results obtained in the laboratory in a two-compartment vessel and a special kind of kerosene (F.34) has been studied as part of a contract between the LEES 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 partitioned vessel (tank). The initial conditions for temperature and pressure (T_0, P_0) are supposed to be homogeneous in the vessel. Specific conditions for each compartment may be envisaged for instance such as a gradient of temperature. The various adjacent compartments are connected by inner openings with a variable surface which allow the propagation of the reaction and the progressive establishment of a thermodynamical equilibrium in the vessel. Each compartment is considered as a perfectly wellstirred reactor. The equations introduced in the model need the evaluation of several parameters which characterise molecular collisions, condensation and energy transfers³. The model was initially validated by studies on dust suspensions and two-phase mixtures with the same set of parameters⁴. 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 due to the difference of pressure between two adjacent compartments or the surrounding atmosphere is given by the standard orifice equations⁵. The amount of the liquid fuel and the mass rate of each species transferred between two adjoining areas or discharged through the vent are calculated assuming a global mass rate partition⁴ among the different species in each compartment.

The knowledge of the chemical process and the amount of transferred molecules allows to know by successive time steps, the number of molecules and the mass of each species remaining in each compartment. The numerical integration of equations gives the access for the whole structure 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.

Experiments⁶ have been performed in a cylindrical vessel with a global volume such as $V_0 = 13.2 l$. A horizontal steel plate allows to define two compartments with respective volumes such as $V_{o1} = 4.8 l$ in the upper part and $V_{o2} = 8.4 l$ in the lower part. Both compartments are connected by a small inner opening positioned in the centre of the plate. Several plates may be used corresponding to various inner openings. The thermodynamical conditions are supposed to be homogeneous in the vessel. The ignition of the kerosene vapors may be carried out in both compartments by the means of an exploding wire fixed at the end of a central electrode⁶.



Figure 1 shows the evolution of the maximum pressure for different inner openings with a surface such as $a = 1.76 \text{ cm}^2$ or $a = 16.6 \text{ cm}^2$. The ignition occurs in the first compartment. The experimental measures in each compartment are compared with the model predictions and the corresponding points are plotted in the figure. Experimental results indicate an overpressure in the second compartment The difference of pressure ΔP between both compartments seems to be practically the same, for a given initial pressure, whatever the size of the inner opening. However, for large openings, a homogeneous pressure in both compartments and therefore a decrease of ΔP may be expected. The experimental evolution of ΔP is a function of the initial pressure and extends between 200 and 800 kPa. Most maximum pressures given by the model are in agreement with experimental results with margins of error about 10 to 15 %. It can be noticed that, for large inner openings, the theoretical maximum pressures merge together in both compartments, whereas this effect is not yet experimentally observed. However, the calculated maximum pressure remains quite compatible with the average pressure deduced from both experimental values.

For small inner openings, the model also predicts an overpressure in the second compartment. For intermediate initial pressures (200 - 250 kPa) the theoretical difference of pressure $\Delta P = 150 \text{ kPa}$ is very near the experimental value $\Delta P = 200 \text{ kPa}$. We can notice again, a slight gap about 10 to 15% between the absolute values of theoretical and experimental pressures in each compartment.

Figure 2 gives the theoretical time evolution of the pressure in each compartment around the stoichiometry and for a small inner opening such as $a = 2 \text{ cm}^2$.

We consider a global volume $V_0 = 33 l$ comprising two compartments such as $V_{01} = 25 l$ and $V_{02} = 8 l$. The ignition may occur in the first or in the second compartment. In all cases and as previously, an overpressure appears in the compartment adjacent to the ignition compartment⁶.

The overpressure seems to be of the order of 15 to 20 % of the average of the maximum pressures. The overpressure is more particularly marked when it occurs in a small compartment. The coupling



Fig 2 Pressure vs time in both compartments and different locations of the ignition energy.

between the fuel ratio and the volume may therefore in some conditions lead to destructive effects on the vessel structure. When ignition occurs in the largest compartment ($V_{o1} = 25 l$), the overpressure is delayed in the second compartment ($V_{o2} = 8 l$). More detailed considerations show that the delay is all the shorter since the mixture is richer. Finally, when ignition occurs in a small compartment, the initial reaction, limited by the number of available molecules is quickly slowed down by the molecular transfer and the overpressure increases faster in the adjacent compartment.



Fig 3 Pressure vs time in a vessel partially composed of inert compartments.

Figure 3 shows the time evolution of the pressure in a vessel comprising one or several inert compartments and for initial conditions near the stoichiometry. The first part of the figure is relative to a two-compartment system such as $V_{o1} = 25 l$ and $V_{o2} = 8 l$. The second part is relative to a three-component system such as $V_{ok} = 13 l$ and $1 \le k \le 3$. Only the initial compartment is filled with kerosene. The next compartments are filled with air and are inert with regard to the reaction. The ignition occurs in the first compartment. It can be noticed, that no overpressure is obtained in the inert compartments. On the contrary, the pressure quickly mitigates and involves the extinction of the reaction in the first compartment. This phenomenon is particularly short with the three-compartment system. In this case, the maximum of pressure reached in the ignition compartment is strongly reduced and close to 400 kPa, instead of 600 kPa with two compartments. It seems that the addition of several successive inert systems significantly mitigates the maximum of pressure in the ignition compartment. This technique may be used in the field of the risk assessment for adapted compartment volumes and mixtures.

Figure 4 shows the time evolution of the pressure in each compartment of a vessel composed of nine identical compartments (3x3) such as $V_{ok} = 13 l$ and $1 \le k \le 9$, for initial conditions near the stoichiometry. All the adjoining compartments are connected by a small inner opening $a = 2 \text{ cm}^2$.



Fig 4 Pressure vs time in simple partitioned structures and different locations of the ignition energy.

The first part of the figure corresponds to an ignition in the compartment 1 which defines one of the corners of the structure. The reaction progressively expands in the adjoining areas with a delay time and leads to the formation of a progressive overpressure. On account of a possible symmetry in the thermal exchanges and the transfers of matter in the course of the reaction, the overpressure in each compartment corresponds to approximately constant rise times between 230 and 260 ms. The pressure is the same in the symmetrical compartments in comparison with the ignition compartment. The maximum of pressure reached varies between 450 kPa in the first compartment, and 800 kPa in the furthest compartment, which is consistent with the previous results.

The second part of the figure, corresponds to a central ignition in the compartment 5. The pressure evolution due to the symmetry is the same in different compartments. A slight overpressure about 80 kPa exists between the corners of the structure and the central compartment for rise times in the region of 200 ms. All the cases observed indicate two kinds of situations :

- in the course of a central ignition, the overpressure remains slight and the pressure evolution in each compartment is close to the pressure obtained in the global volume without partitioning.
- in the course of a side ignition, a very important overpressure progressively forms with a maximum in the furthest part of the structure.

The location of the ignition energy considerably influences the thermodynamical evolution of the mixture and the possible destruction of the structure. The description proposed for partitioned systems seems to be globally in good agreement with experimental data and it seems interesting to precise this evaluation by studying complex multi-partitioned structures.

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