Formation of Overpressures in the Combustion of Two-Phase Mixtures inside Partitioned Structures

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1 Introduction and model elements

Two-phase mixture explosions (dust + gas) often have in the past created dramatic situations and consequences. The study of these mixtures has concerned in numerous cases coal dusts in order to improve the general knowledge on safety in industrial plants and more particularly in mines. The association of coal dusts with a gaseous energetic fuel such as methane was frequently analysed. On the contrary very few studies have been interested in the association of agricultural dusts with such gaseous energetic substances. Over the last past years, a simple modelling initially developed as part of a novel study on ignition and combustion of dust suspensions [1] has been presented in order to predict the main characteristics of these explosions in a closed or a vented vessel. It has been also experimentally verified for gaseous mixtures that very important overpressures went on in all the adjoining areas of the ignition compartment for a multi-partitioned vessel [2]. The aim of this work is to verify the pressure pilling effect in the chain propagation of a two-phase mixture explosion composed of agricultural dusts with a gaseous fuel (methane or propane) and the formation of overpressures inside a partitioned structure. The combustion of the two-phase mixture is supposed to be described by collisions between particles of the gaseous phase and those of the solid phase. The reactive system is composed of molecules in gaseous phase and active molecules [1].

The energy flux brought to the solid leads to its degradation by the active molecules and to the dissociation by the other molecules in the gaseous phase. All those phenomena contribute to the solid destruction [1]. The combustion of the solid fuel takes place in a closed partitioned vessel. The initial conditions are supposed to be homogeneous in the vessel. The various adjacent compartments are connected by inner openings with a variable surface which allow the propagation of the reaction and the formation of a progressive thermodynamic equilibrium in the vessel. Each compartment is considered as a perfectly well-stirred reactor which may be fitted with a vent. The vent breaking is obtained when the pressure in the medium reaches the static venting pressure [3].The initial thermodynamic characteristics of the medium are determined (pressure P_o, temperature T_o) or may be calculated (internal energy, total number of gaseous molecules) from oxygen-nitrogen-fuel amounts in the vessel [1]. The evolution of the active or gaseous species is based on the chemical kinetics of the reaction and takes into account collisions on the solid fuel, collisions on the wall or in the gaseous medium [1]. 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 the equations gives the access for the whole structure to the pressure history [1] and more generally to the time evolution of all thermodynamic variables.

2   Comparison with experimental results

Figure 1 presents experimental and theoretical curves relative to a cornstarch + 4% C_3H_8 mixture in the case of the time evolution of the pressure. The model is applied with a size of the cornstarch grain such as $D_g = 10$ μm which corresponds to a medium distribution value representative of experimental results [4]. The experimental curve is due to Senecal [4] for a large spherical vessel volume such as $V_o = 1900$ l. A very good correlation between theory and experiment is noticeable, which brings a first validation of the model for two-phase mixtures. It is also noticeable that the maximum pressure is close to the pressure obtained for a cornstarch concentration $\Delta = 1$ kg/m^3 and without propane [1]. It empirically appears that addition of 1% C_3H_8 produces a medium experimental overpressure of about 100 kPa. This point is comparable with experimental results due to Leuckel [5] for slight amounts of methane. In addition the K_{st} factor may be calculated according to Bartknecht's formula [6]. The calculated value $K_{st} = 43.6$ MPa.m/s approximately corresponds to the experimental value $K_{st} = 42$ MPa.m/s given by Senecal for the cornstarch + 4% C_3H_8 mixture [4].

Figure 2 shows the time evolution of the pressure for different vessel volumes between 200 and 10 000 l in order to get a wide enough study range in the conditions of a cornstarch + 4% C_3H_8 rich mixture such as $\Delta = 0.5$ kg/m^3. It is noticeable that the same value of the maximum pressure $P_{max} = 780$ kPa is practically obtained for the different volumes. The maximum pressure is therefore independent of the vessel volume. This result is in accordance with Bartknecht's experiments [6].
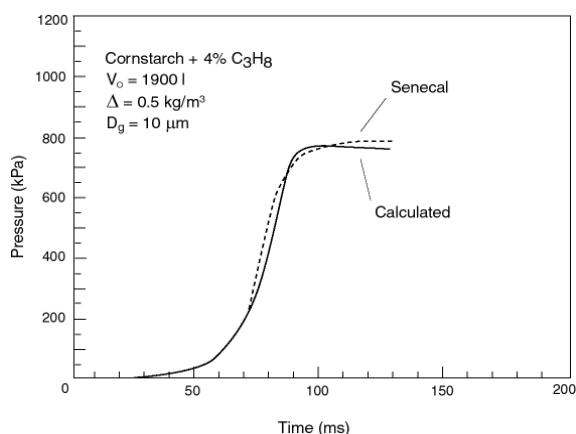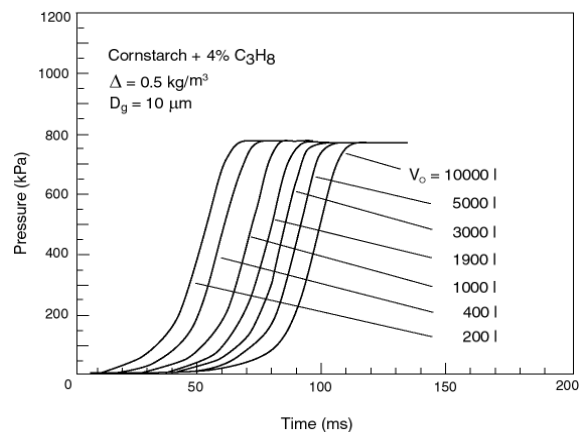

Fig 1   Pressure of explosion vs time.

Fig 2   Pressure vs time for different vessel volumes.

Furthermore, it can be observed that the smaller the vessel volume is, the quicker P_{max} can be reached in about 60 to 120 ms.

Then, the time evolution of the pressure is presented for propane and for two different cornstarch concentrations in figure 3.

For the smallest solid concentration corresponding to a lean mixture ($\Delta = 0.15$ kg/m^3), the increase of the percentage of propane first leads to a progressive increase of the maximum pressure and to a decrease of the rise time. The system gets nearer to stoichiometric conditions (p = 2.6 %). It appears that addition of 1 % of propane in a lean mixture leads to a medium overpressure around 100 kPa. This result is consistent with the results deduced from Leuckel's experiments [5]. Furthermore, the increase of the solid concentration for a given gaseous supply in a lean mixture also leads to a more important maximum of pressure and to a shorter rise time. These elements present a strong analogy with phenomena observed for mixtures only composed of dust suspensions or gaseous fuels [5],[6]. Then, addition of solid fuel or gas progressively creates a rich mixture whose evolution is reversed in comparison with lean mixtures and remains in accordance with the previous results. It appears that

supplementary addition of energetic gaseous substances in a lean mixture is favourable to the combustion of these mixtures. The evolution towards stoichiometric conditions creates a considerable overpressure (10 to 15 % of overpressure for 1 % of added gas).
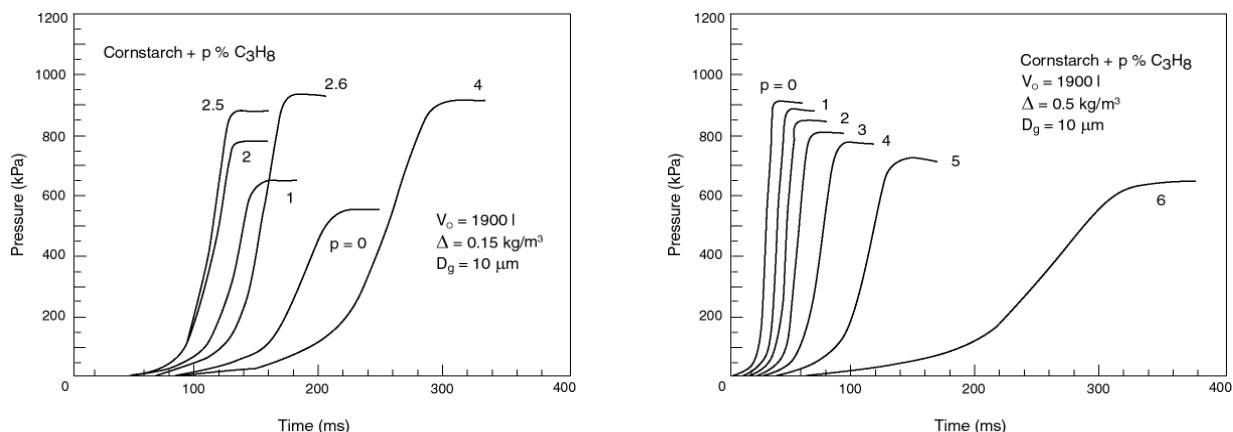

Fig 3   Pressure vs time for different % C_3H_8 and 2 different cornstarch concentrations

For higher initial solid concentrations in rich mixtures ($\Delta > 0.253$ kg/m^3 for cornstarch), it appears that the maximum pressure regularly decreases as a function of the percentage of added gas and that the rise time becomes progressively longer like for gaseous mixtures [5].

The influence of the size of the cornstarch grain is also interesting to study. The modelling conditions have generally been fixed such as $D_g = 10$ μm but the diameter of the cornstarch grain may experimentally vary over this value. The time evolution of the pressure is presented for different grain sizes in figure 4. The presented curves have been obtained for $\Delta = 0.15$ kg/m^3 + 2.6 % C_3H_8 in conditions near the stoichiometry. For a given gaseous supply, we notice that the same value $P_{max} = 940$ kPa is practically obtained for the various grain sizes but decreases for very large diameters. Furthermore, the quicker rise times also correspond to smaller sizes for the cornstarch grains and P_{max} can be reached between 150 and 600 ms for propane. Finally, the risk of explosion is all the more important as the solid particle size is smaller [6].
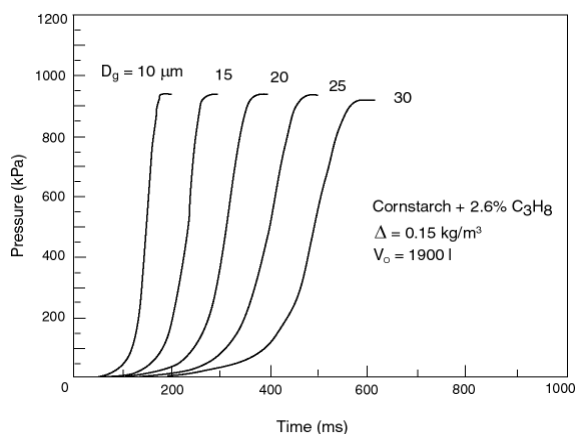

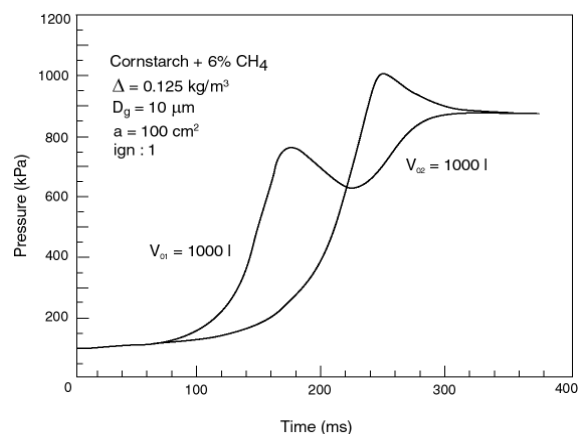Fig 4   Pressure vs time for different grain sizes.   Fig 5   Pressure vs time in both compartments.

All the results presented in a single compartment seem to be in good agreement with experimental works about two-phase mixtures and bring a first validation of the model.

Then, different elementary cases with two compartments are analysed in order to test the model predictions. The existence of overpressures in the adjoining areas of the ignition compartment has been experimentally observed in industrial installations with interconnected vessels. After ignition in the first vessel, the flame is accelerated when it enters the second one and becomes very turbulent. According to Bartknecht [6], for identical combined vessels, the maximum explosion pressure in the second vessel may be increased by approximately 10 %. This value may be modified and strongly increased when the explosion propagates from the largest vessel into the smallest one [6].

In fact, very few quantitative data are available about explosions of two-phase mixtures in partitioned vessels and between these different results, the formation of overpressures leading to a pressure pilling phenomenon seems interesting to investigate by the simulation. So, we consider a set-up composed of a cylindrical vessel with a global volume such as $V_o = 2000\ l$. A vertical steel plate allows to define two compartments with respective volumes such as $V_{o1} = V_{o2} = 1000\ l$. Both compartments are connected by a small inner opening positioned in the centre of the plate. Several plates may be envisaged corresponding to various inner openings. The thermodynamic conditions are supposed to be homogeneous in the vessel. The combustion of the two-phase mixture may be carried out in both compartments by the means of a central ignition corresponding to 50 J.

Figure 5 gives the time evolution of the absolute pressure in each compartment for a small inner opening $a = 100\ cm^2$ in the case of a cornstarch + 6 % CH_4 mixture near the stoichiometry.

The ignition occurs in the first compartment and induces there a quicker pressure rise. This effect involves a molecule transfer towards the adjacent compartment, which modifies the concentrations in the reactive mixture and therefore, the maximum pressures reached. At the end of the reaction, a thermodynamic equilibrium is obtained in the mixture and the pressure evolution is shared by both compartments. It can be observed that the maximum pressure obtained is higher in the adjacent compartment than in the initial one, where ignition occurs. The effective overpressure $\Delta P = 130$ kPa is stronger than Bartknecht's experimental results [6] for comparable volumes with dust suspensions (about 10% of overpressure) but remains consistent with results obtained by Hu [2] for gaseous mixtures in partitioned vessels. Furthermore, the maximum pressure reached at the end of the reaction nearly corresponds to the value obtained in a closed vessel with a single compartment such as $V_o = 2000\ l$. The observed phenomena do not depend on the mixture which may be rich, lean or stoichiometric. It is therefore interesting to study the evolution of the maximum pressure in similar conditions, but for dissymmetric volumes. These evolutions are plotted in figures 6 and 7 for vessel volumes such as $V_{o1} = 5000\ l$ and $V_{o2} = 1000\ l$. The ignition may occur in the first or in the second compartment. In both cases and as previously, an overpressure appears in the compartment adjacent to the ignition compartment but both behaviours however remain very different.
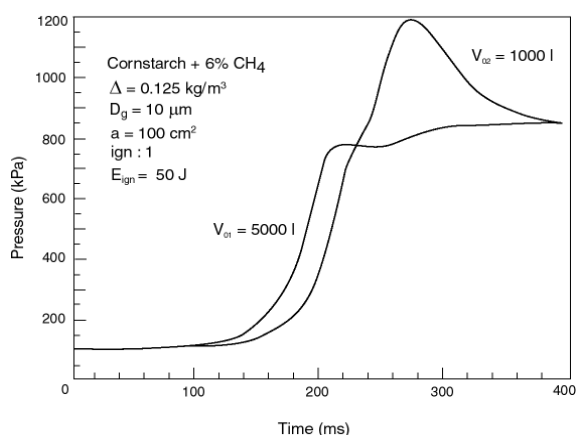

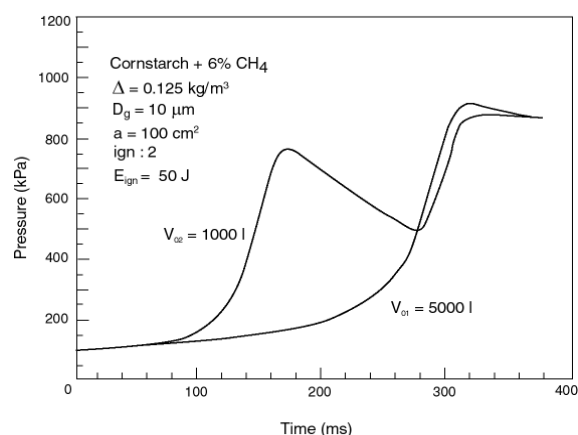Fig 6   Pressure vs time in both compartments and different locations of the ignition energy.

Fig 7   Pressure vs time in both compartments and different locations of the ignition energy.

The overpressure is very strongly marked when it occurs in the small compartment. In this case, the effective overpressure $\Delta P = 350$ kPa is increased by approximately 40 % in comparison with the ignition compartment with rise times close to 240 ms. Similar data with sometimes more important overpressures have been observed by Bartknecht [6] for comparable interconnected volumes. Experimental data depend strongly enough in this case on the inner opening and on the turbulence created by the propagation of the flame front. The volume effect created in these conditions is maximum and can lead to the destruction of the vessel structure.

On the contrary, when ignition occurs in the small compartment ($V_{o2} = 1000$ l), the initial reaction, limited by the number of available molecules is quickly slowed down by the molecular transfers and the overpressure increases faster in the adjacent compartment than in the initial one. The rise time in the large compartment is delayed and the effective overpressure remains very limited ($\Delta P = 60$ kPa). Similar results are obtained by Bartknecht [6] with an effective overpressure of the order of 7 to 8 %. Finally, more complete studies show that the delay is all the shorter since the mixture is close to stoichiometric conditions. These different examples clearly show the formation of overpressures in the combustion of two-phase mixtures but also the influence of a volume effect in each compartment, consistent with experimental results [2],[6].

3   Application to simple multi-partitioned structures and conclusion

Figure 8 starts the same kind of study again, with a more developed structure composed of nine identical compartments (3x3) such as $V_{ok} = 1000$ l and $1 \leq k \leq 9$. All the adjoining compartments are connected by a small inner opening a = 100 cm^2.

The first part of the figure corresponds to a weak ignition in 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 final pressure in each compartment corresponds to relatively close rise times between 440 and 500 ms. The pressure is the same in the symmetrical compartments in comparison with the ignition compartment. The maximum pressure reached varies between 850 kPa in the first compartment, and 1160 kPa in the furthest compartment (about 35 %), which confirms the amplification of the pressure pilling effect in the course of the propagation.

The second part of the figure corresponds to a central ignition in compartment 5. The pressure evolution due to the symmetry is the same in different compartments. A reduced overpressure about 90 kPa exists between the corners of the structure and the central compartment for final rise times comprised between 360 and 400 ms.
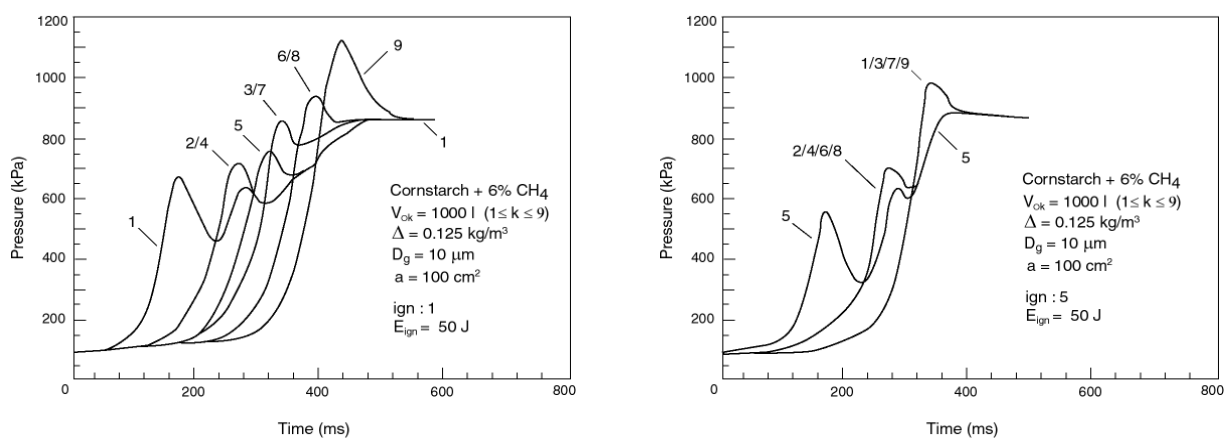

Fig 8   Pressure vs time in a simple partitioned structure and different locations of the ignition energy.

Finally in conclusion, all the cases observed indicate two kinds of situations :
-   in the course of a central ignition, the overpressure remains limited and the maximum pressure in each compartment does not sensibly differ from 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 compartment considerably influences the thermodynamic evolution of the mixture and the possible destruction of the structure. Comparable results are obtained with other dust suspensions or gaseous fuels and other equivalence ratios. The description proposed for partitioned systems seems to be globally in good agreement with experimental data and it seems possible to extend the simulation to the description of more complex multi-partitioned structures.

References :

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