

19th ICDERS HAKONE Japan

Numerical simulation of gaseous explosions inside a partitioned vessel

J.M. Pascaud, F. Faubert and P. Gillard
LEES – Université d'Orléans
63, avenue de Lattre de Tassigny
18020 BOURGES Cedex, France
Fax : 02.48.23.80.23

Extended abstract :

Over the last past years, a simple modelling initially developed as part of a novel study on ignition and combustion of classical propulsive powders has been presented in order to predict the main characteristics of these explosions in a closed or a vented vessel¹. Then, the model has been adapted to the explosion of dust suspensions and more recently to kerosene droplets.

The aim of this work is to extend the model validation to gaseous mixtures and to give a theoretical study on the chain propagation of a gaseous 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 in one compartment have been compared with results of experimental works available for gaseous mixtures.

We consider that the combustion of the gaseous fuel (methane or propane) results from collisions between all the particles of the gaseous phase. The reactive system is composed of molecules in gaseous phase, active molecules and condensable molecules. The energy flux brought to the gaseous 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 destruction of the gaseous fuel.

The combustion of the gaseous fuel takes place in a closed partitioned vessel (tank). The initial conditions 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 well-stirred reactor which may be fitted with a vent. The equations introduced in the model need the evaluation of several parameters which characterise molecular collisions, condensation and energy transfers¹. 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 . 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 equations². The amount of the gaseous 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 partition¹ 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 reduced pressure in the case of vented explosions.

The proposed development allows the study of varied initial conditions which may differ for the

various compartments, the influence of different parameters such as the vessel volume, the concentration of gaseous additives in a rich or a lean mixture, the venting effects or the vent sizes between the compartments and finally the existence of overpressures.

Figure 1 shows the time evolution of the pressure for varied concentrations in methane or propane extending from lean mixtures to rich mixtures ($p_{sto} = 9.5\%$ for methane and $p_{sto} = 4\%$ for propane) in a large vessel volume such as $V_o = 1900\text{ l}$.

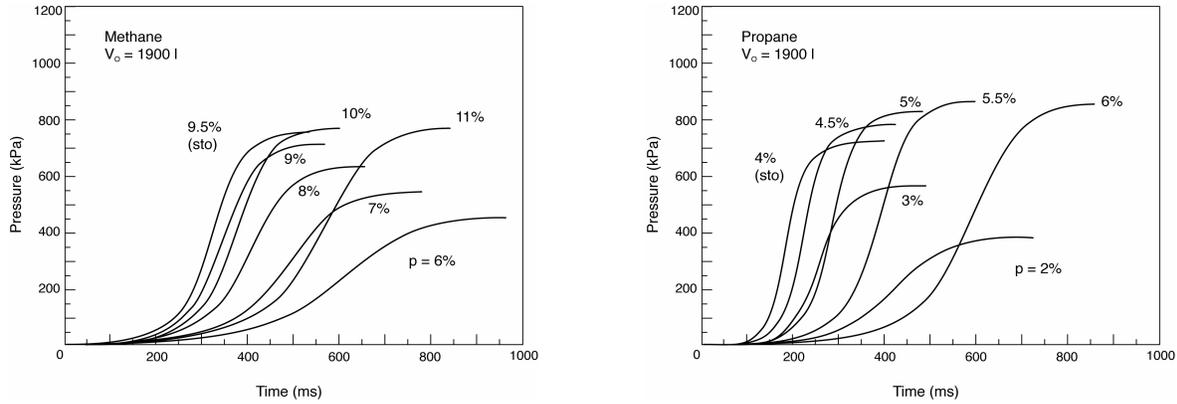


Fig 1 Pressure vs time for different % of gaseous fuel.

For rather rich mixtures, the maximum pressure decreases and the rise time becomes longer. On the contrary, for lean mixtures, the increase in concentration leads to a progressive increase of the maximum pressure and to a very important decrease of the rise time when curves are close to stoichiometric conditions. Stoichiometry appears to be the most favourable environment to get explosive conditions. It can be noticed that according to the model, these conditions still exist on a wide enough concentration range between 9.5 % and 12 % for methane and between 4 % and 6 % for propane. The continuity of conditions close to stoichiometry in a slightly rich mixture is experimentally verified³. The previous evolutions show therefore correctly the transition between lean and rich mixtures and are in good agreement with experimental data³.

Figure 2 presents the evolution of the reduced maximum explosion pressure P_{red} as a function of the vent area for a vessel volume such as from $V_o = 1000\text{ l}$ in the case of methane-air or propane-air mixtures and for a static venting pressure $P_v = 10\text{ kPa}$ around the stoichiometry. The theoretical curves are obtained plotting the different values of P_{red} calculated for each vent opening.

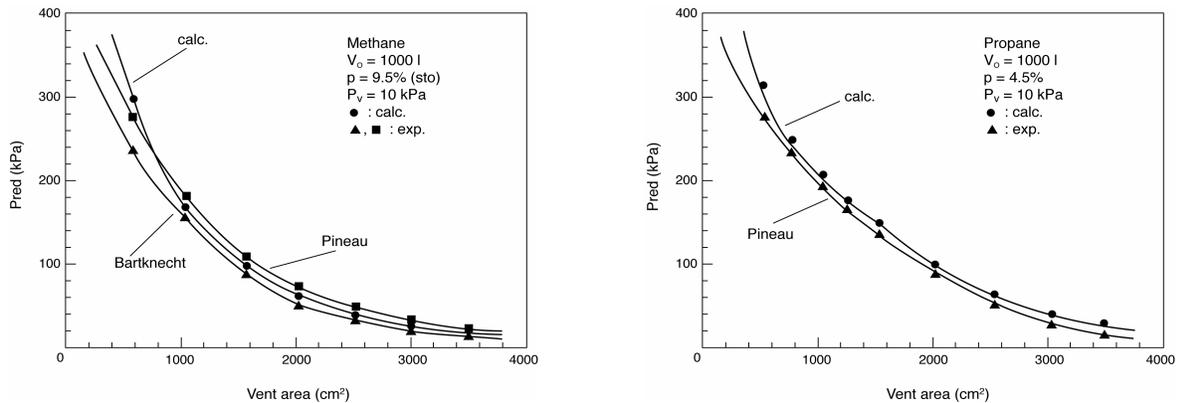


Fig 2 Evolution of the reduced maximum explosion pressure with the vent area.

The experimental curves are due to Pineau⁴ or Bartknecht⁵ in the same conditions. The general trend of the curves has the aspect of a decreasing hyperbola. For large vent areas, the reduced pressure strongly declines towards a residual overpressure.

An excellent correlation is noticeable between theoretical and experimental results which brings another validation of the model.

The existence of overpressures in the adjoining areas of the ignition compartment has been experimentally observed in industrial installation vessels interconnected by pipelines. After ignition in the first vessel, the laminar flame is accelerated when it enters the pipeline and becomes turbulent. According to Bartknecht, for identical combined vessels⁵, the length of the connecting line does not significantly influence the course of the explosion, but in the second vessel the maximum explosion pressure may be increased by approximately 10 % for gaseous mixtures. This value may be modified and strongly increased when the explosion propagates from the larger vessel into the smaller one⁵. Also, the diameter of the connecting pipeline is an important parameter.

On the contrary, the propagation of a flame in a tube composed of different compartments by the means of obstacles (large vent areas) increases the turbulence in the mixture but does not lead to the formation of significant overpressures^{6,7}.

Between these results, the case of partitioned vessels is intermediate and seems interesting to investigate by the simulation. So, we consider a set-up composed of a cylindrical vessel with a global volume such as $V_o = 2000 \text{ l}$. A vertical steel plate allows to define two compartments with respective volumes such as $V_{o1} = V_{o2} = 1000 \text{ l}$. 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 thermodynamical conditions are supposed to be homogeneous in the vessel. The combustion of the gaseous mixture may be carried out in both compartments by the means of a central ignition corresponding to 68 J.

Figure 3 gives the time evolution of the absolute pressure in each compartment for a small inner opening $a = 100 \text{ cm}^2$ in the case of methane at 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 thermodynamical equilibrium is obtained in the mixture and the pressure evolution is shared by both compartments.

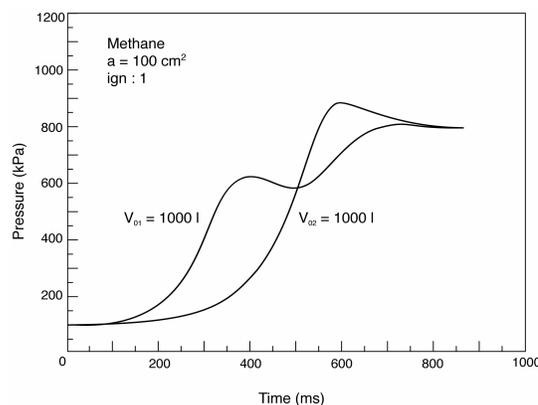


Fig 3 Pressure vs time in both compartments and different locations of the ignition energy.

It can be observed that the maximum of pressure obtained is higher in the adjacent compartment than in the initial one, where ignition occurs. The effective overpressure $\Delta P = 80 \text{ kPa}$ is much more reduced than in the case of kerosene⁸ but quite consistent with experimental results⁵ due to Bartknecht for comparable volumes (about 10% of overpressure). 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 $V_o = 2000 \text{ l}$. 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 figure 4 for vessel volumes such as $V_{o1} = 5000 \text{ l}$ and $V_{o2} = 1000 \text{ l}$.

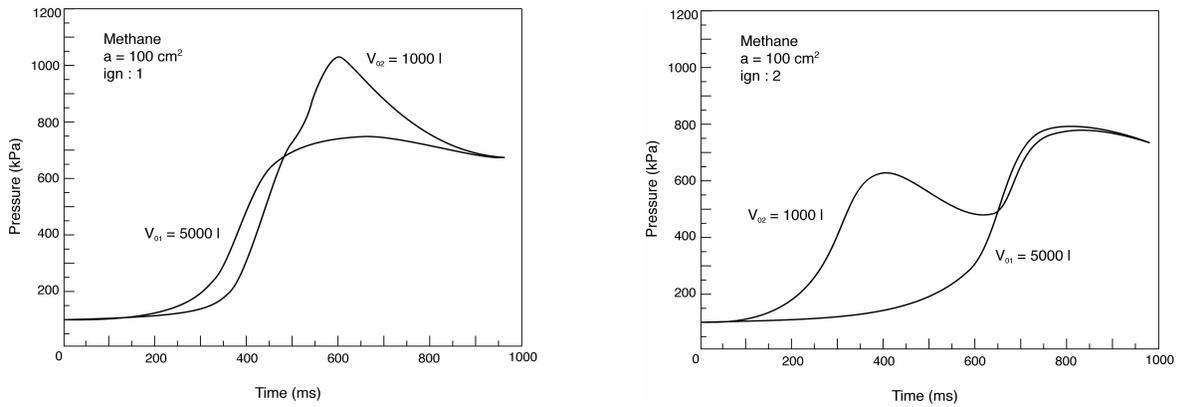


Fig 4 Pressure vs time in both compartments and different locations of the ignition energy.

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.

The overpressure is very strongly marked when it occurs in the small compartment. In this case, the effective overpressure $\Delta P = 300$ kPa is increased by approximately 50 % in comparison with the ignition compartment with rise times close to 550 ms. Similar data with sometimes more important overpressures have been observed by Bartknecht⁵ for comparable volumes interconnected by a pipeline. Experimental data depend strongly enough in this case on the diameter of the connecting line 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 a 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 however strongly delayed and the effective overpressure remains very limited ($\Delta P = 30$ kPa). Similar results are obtained by Bartknecht⁵ 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 richer ($\Delta t = 350$ ms at the stoichiometry).

Figure 5 shows the time evolution of the absolute pressure in each compartment of a simple multi-partitioned structure composed of nine cubic identical compartments (3×3) such as $V_{ok} = 1000$ l and $1 \leq k \leq 9$, for initial conditions corresponding to the stoichiometry. All the adjoining compartments are connected by a small inner opening $a = 100$ cm².

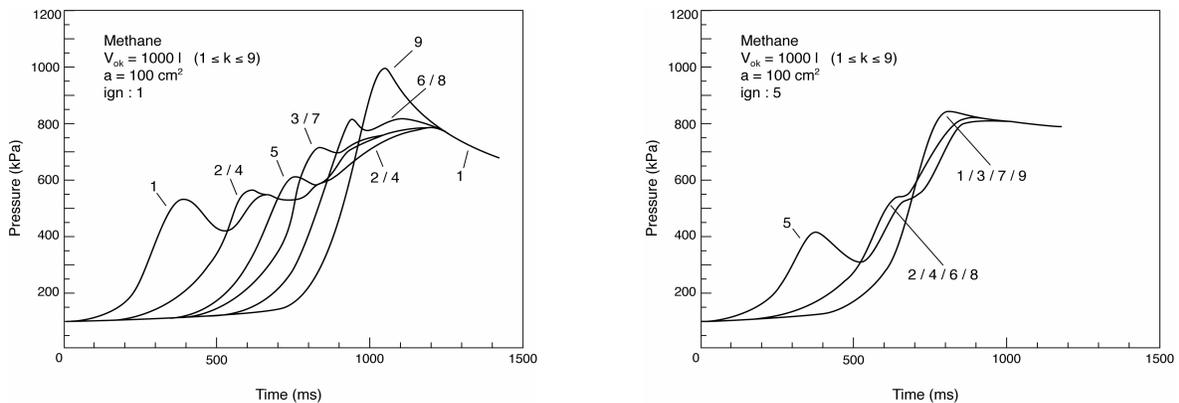


Fig 5 Pressure vs time in simple partitioned structures and different locations of the ignition energy.

The first part of the figure corresponds to an ignition in 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 maximum pressure in each compartment corresponds to relatively close rise times between 1000 and 1200 ms. The pressure is the same in the symmetrical compartments in comparison with the ignition compartment.

The maximum of pressure reached varies between 780 kPa in the first compartment, and 1000 kPa in the furthest compartment (about 25 %), which is consistent with the previous results.

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 slight overpressure about 50 kPa exists between the corners of the structure and the central compartment for final rise times comprised between 800 and 900 ms.

All the cases observed indicate two kinds of situations :

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

The location of the ignition compartment considerably influences the thermodynamical evolution of the mixture and the possible destruction of the structure. Comparable results are obtained with propane. The description proposed for partitioned systems seems to be globally in good agreement with experimental data and it seems possible to adapt the simulation to the description of complex multi-partitioned structures.

References :

- 1. Pascaud J.M., Brossard J., Lombard J.M.** , "Numerical simulation by the molecular collision theory of two-phase mixture explosion characteristics in closed or vented vessels", European Physical Journal A.P., Vol 7, p. 227, 1999.
- 2. Bradley D., Mitcheson A.**, "The venting of gaseous explosions in spherical vessels", Combustion and Flame, Vol 32, p. 221, 1978.
- 3. Leuckel W., Nastoll W., Zarzolis N.**, "Experimental investigation of the influence of turbulence on the transient premixed flame propagation inside closed vessels", 23rd Int. Symp. on Combustion, Orleans, 1990.
- 4. Pineau J.P., Chaineaux J., Ronchail G.**, "Influence on gas and dust explosion development of lengthening and presence of obstacles in closed or vented vessels", 5th Int. Symp. Loss Prevention and Safety Promotion in the Process Industries, Cannes, 1986.
- 5. Bartknecht W.**, Explosionen, Ablauf und Schutzmassnahmen, Springer-Verlag, Berlin, 1978.
- 6. Pu Y.K., Mazurkiewicz J., Jarosinski J., Kauffman C.W.**, "Comparative study of the influence of obstacles on the propagation of dust and gas flames", 22nd Int. Symp. on Combustion, p. 1789, 1988.
- 7. Pu Y.K., Tai C.S., Jarosinski J., Kauffman C.W., Sichel M.**, "The investigation of the feature of dispersion induced turbulence and its effects on dust explosions in closed vessels", 22nd Int. Symp. on Combustion, p. 1777, 1988.
- 8. Sochet I., Gillard P., Moreno A., Delrieu L.**, " Influence of a partitioning of tank on the transmission of the kerosene vapor explosion", 3rd Int. Symp. on Hazards , Prevention and Mitigation of Industrial Explosions, Tsukuba , 2000.