Simulation of the combustion of kerosene vapors by a multi-physics model

J.M. Pascaud, P. Gillard, N. Gascoin

Institut Prisme – Université d'Orléans
63, avenue de Lattre de Tassigny 18020, Bourges, France

1   Elements of modelling and results

Over the last past years, there has been a considerable effort to precise the characteristics of the combustion of kerosene [1] which 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 is to present a simple multi-physics simulation able to describe the combustion of kerosene vapors in a closed vessel with subsequent applications to vent openings. Simulated predictions have been compared with experimental results [2], [3] available for 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). In a first time, a global one-step chemical reaction has been envisaged for the decomposition of kerosene C_xH_y with the following expression given at the stoichiometry :

$$C_xH_y \; + \; (x + \frac{y}{4})O_2 \rightarrow \; xCO_2 \; + \frac{y}{2}H_2O$$
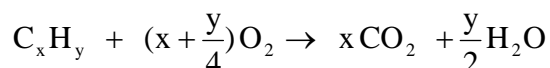
The velocity ω of the chemical reaction may be written in the form [4] :

$$\omega \; = A \, P^{0.3} \, T \, [C_xH_y]^\alpha \, [O_2]^\beta \, \exp(- \, E_a/RT)$$

where P and T are the pressure and the temperature in the ambient medium.

The initial characteristics of the gaseous mixture are known [2], [3] (pressure P_o, temperature T_o) or may be calculated [3] in a rich or a lean mixture or in the stoichiometric conditions (p_{sto} = 1.3% for kerosene). The evolution of the thermodynamical variables (pressure, temperature, concentrations…) is obtained by the resolution of a system of partial differential equations (PDE) taking into account heat and transport phenomena and the flow in the vessel which could give the access to the fundamental flame velocity.

* Mass continuity equation :

$$\vec{\nabla} \bullet (\rho \vec{V}) \; + \; \frac{\partial \rho}{\partial t} \; = \; 0$$

where ρ is the fluid density.

* Navier-Stokes equations :

They describe the motion of combustible molecules with a laminar flow velocity $\vec{V}$ (u,v,w) in a gaseous mixture and with the following expression in the assumption of a weakly compressible fluid :

Correspondence to: Jean-Marc.Pascaud@bourges.univ-orleans.fr

$$\rho \frac{\partial \vec{V}}{\partial t} + \rho \vec{V} \bullet \vec{\nabla} \vec{V} = \vec{\nabla} \bullet [-PI + \eta(\vec{\nabla}\vec{V} + (\vec{\nabla}\vec{V})^T) - \frac{2}{3}\eta(\vec{\nabla}\bullet\vec{V})I] + \vec{F}$$

where :

F represents body forces acting on the fluid such as gravity for example.

I is the 3x3 identity matrix.

* Heat conduction-convection equation :

$$\rho C_p \frac{\partial T}{\partial t} + \vec{\nabla} \bullet (-\lambda\vec{\nabla}T) = q - \rho C_p \vec{V} \bullet \vec{\nabla}T$$

The initial heat supply q (W/m^3) is given by :

$$q = \rho\omega QV_m$$

where :

Q is the heat of combustion of kerosene.

V_m is the molar volume depending on the initial conditions.

* Transport-diffusion equation :

$$\frac{\partial C}{\partial t} + \vec{\nabla} \bullet (-D\vec{\nabla}C) = -\omega - \vec{V} \bullet \vec{\nabla}C$$

where C = [C_xH_y] is the concentration of kerosene.

The physico-chemical data used in the previous expressions such as the thermal conductivity λ, the dynamic viscosity η, the specific heat capacity C_p or the diffusion coefficient D are generally depending on the temperature and have been determined either from works performed in the laboratory or from data available in the literature. The closure of the system of PDEs is obtained by linking thermodynamical variables with the perfect gas law.

Hence : P = ρ rT

The experiments [2] have been performed in a closed cylindrical vessel with a diameter D = 20.5 cm and a height h = 40 cm corresponding to a volume V_o = 13.2 l. The ignition was produced by a capacitor discharge which could be moved vertically along the central axis. Due to the axial symmetry of the studied geometry, the tank may be likened to a rectangular surface with dimensions 20.5 cm x 40 cm for the resolution of the previous equations with the help of the Comsol multi-physics solver. The ignition may be taken into account in the calculation by an increase of the wall temperature able to correspond to the studied experimental conditions (supply of a nominal ignition energy around a few tens of joules). The ignition may be envisaged either on a side area, or at the base of the tank.
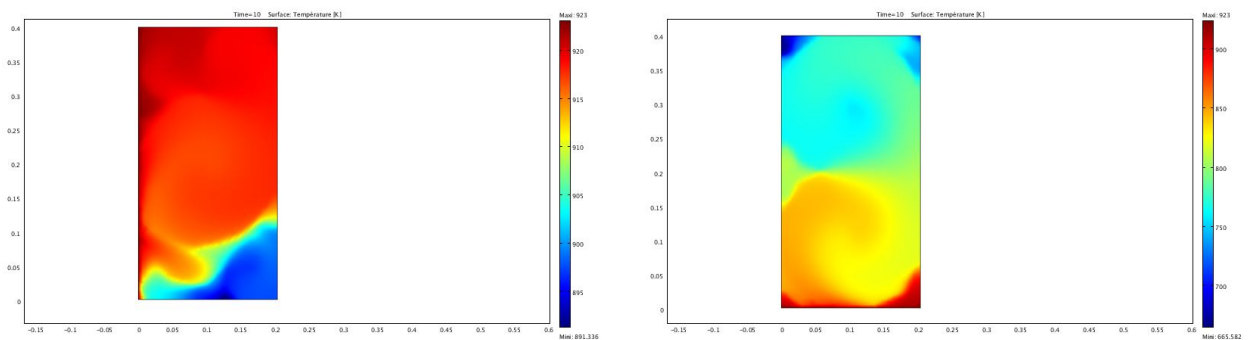

Fig 1   Surface temperature for different locations of the ignition energy

Figure 1 shows the temperature evolution in a section of the tank for a side ignition (left part) and a base ignition (right part). The studied mixture is stoichiometric with thermodynamical conditions such as P_o = 130 kPa and T_o = 323 K. Both parts of the figure show a distribution of temperatures in the different areas of the tank, around 300 K for the blue-tinted areas and up to 900 K for the red zones. The layout of the colours also shows the progression of the flow and the influence of body and gravity forces. The side ignition is characterized by a distribution of higher mean temperatures and a more important development of the flow phenomena with hot locations near the ignition zone.

Figure 2 shows the time evolution of the pressure for a side ignition and a selected point P close to the centre of the tank defined by x = 10.25 cm and y = 25 cm.
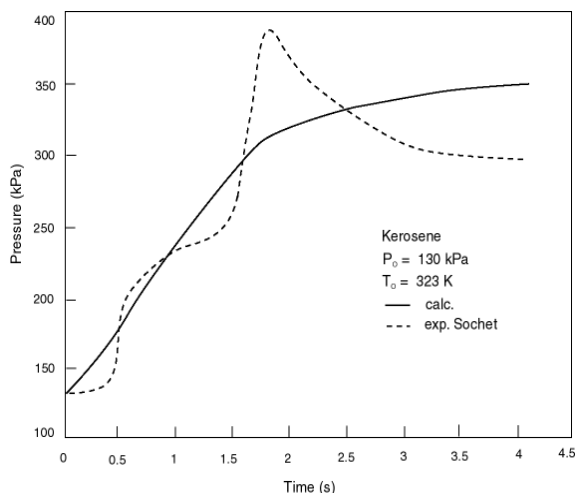

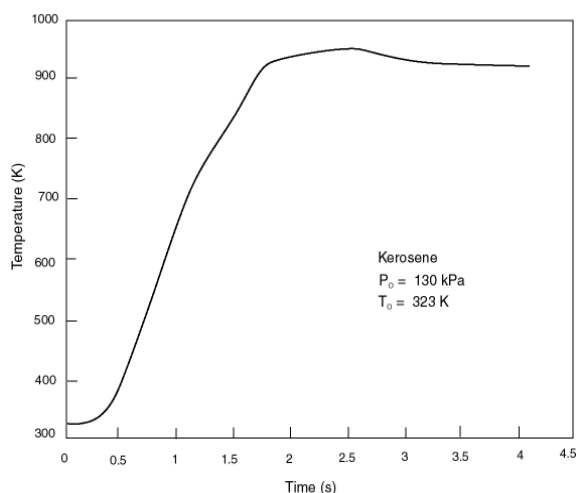Fig 2   Pressure vs time   Fig 3   Temperature vs time

The calculated maximum pressure is then P_{max} = 350 kPa with rise times around 2.5 to 3.5 s.

A classical stabilization of the maximum pressure reached is observed for very long times.

The result of the calculation is relatively close to experimental data [2] (P_{max} = 390 kPa ; t_{rise} = 2s). Experimentally, the rise time seems to be quicker, which can be explained by difficulties to estimate the ignition energy really dissipated in the gaseous mixture (generally 10 to 20% of the capacitor discharge). Figure 3 shows the time evolution of the temperature in the same conditions as previously. A relatively quick increase in temperature may be noticed with a maximum near $_{max}$ = 920 K and rise times around 2 to 2.5 s. Then, the temperature slightly decreases towards a limit value close to 900 K.
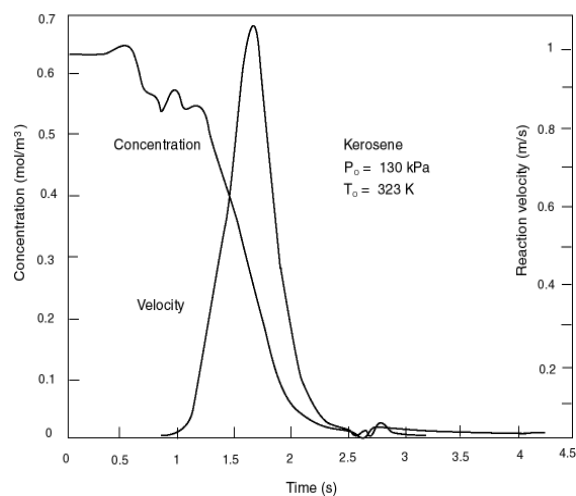

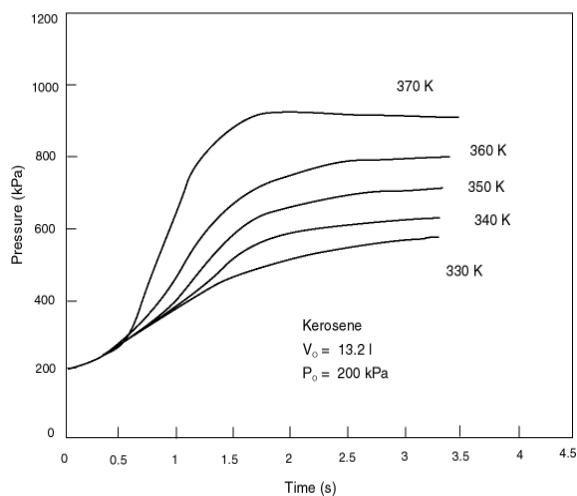Fig 4   Concentration and reaction velocity vs time   Fig 5   Pressure vs time at different temperatures

Figure 4 shows the time evolution of the kerosene concentration and the reaction velocity at point P. The combustion classically decreases after an initial latent period. The concentration becomes very closed to zero for times comprised between 2 and 2.5 s corresponding to a maximum in pressure and in temperature. Beyond this range, the reaction expands no longer. The evolution of the reaction velocity comes in the form of a peak centred around 1.7 s corresponding to the maximum velocity. It can be noticed that for times quicker than 1s, the reaction does not expand and the concentration remains practically constant. Furthermore, the time corresponding to the maximum reaction velocity is a point of symmetry in the evolution of the kerosene concentration.

Figure 5 shows an example of the time evolution of the pressure in the same conditions as previously and for a temperature range extending from lean mixtures to rich mixtures (330-370 K).

For lean mixtures, the increase in temperature leads to a progressive increase of the maximum pressure and to a similar 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 temperature range which remains experimentally [1], [5] verified in slightly rich mixtures.
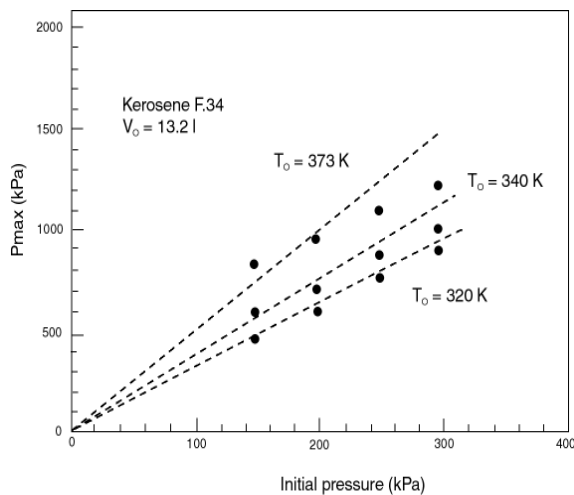

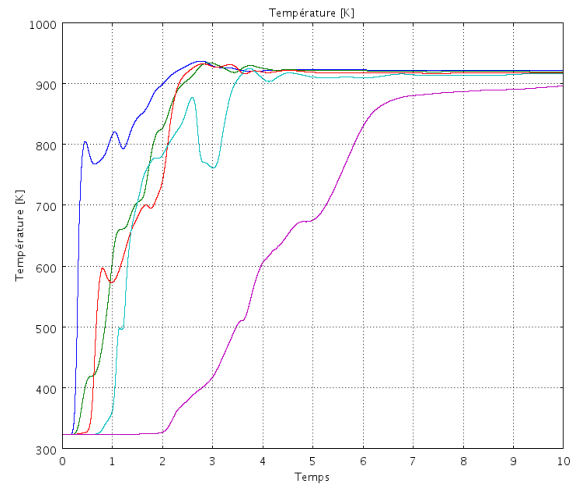Fig 6   Calculated Pmax vs the initial pressure

Fig 7   Temperature vs time at different places

Figure 6 shows the theoretical evolution of the maximum pressure calculated from pressure-time curves as a function of the initial pressure for different temperatures at point P. Then, the data obtained are plotted in the figure. Three calculated curves are presented for initial temperatures such as $T_o = 320$, 340 and 373 K. A straight dotted line, linearly increasing from the origin may be drawn in each case. The ratio P_{max}/P_o is therefore a constant for a given temperature, which is consistent with experimental results [2], [5] . We obtain the following values :

P_{max}/P_o	Theory	Experiment [2]
$T_o = 373$ K	5	5.5 ± 0.5
$T_o = 340$ K	3.5	4.5 ± 0.4
$T_o = 320$ K	2.6	2.7 ± 0.3

The experimental values of the ratio P_{max}/P_o are deduced from experiments performed in the LEES [2] and are relatively consistent with the calculation. Another example of the model applications is the representation of the time evolutions of a thermodynamical variable at different places of the tank which is illustrated in figure 7. On the vertical line x = 12.25 cm the points such as y = 0, y = 13.33, y = 26.66 and y = 40 cm, regularly spaced have been chosen to represent the time evolution of the temperature. Wherever the location of the point is, the maximum temperature is the same around 920 K. On the contrary, the rise time is much slower at the base of the tank and much quicker in the high part. These evolutions correspond to the influence of the flow phenomena and to body gravity forces whose effects have been already observed with the evolution of the surface temperature.

The results obtained are both a qualitative and quantitative illustration of some experimental data previously known [2], [5] and whose evaluation should be completed by applications to a partitioned tank and to vented vessels.

References

[1] Sirignano W.A., Continillo G. (1988). Numerical study of multicomponent fuel spray flame propagation in a spherical closed volume, 22nd Int. Symp. on Combustion, Seattle.

[2] Sochet I., Reboux A., Pascaud J.M., Brossard J. (1998). Inflammabilité et/ou explosivité du kérosène, Rapport DGA n° 020087/CEG-DSI-DV.

[3] Pascaud J.M., Gillard P. (2006). Study of the propagation of kerosene explosions inside a partitioned vessel , Journal of Loss Prevention in the Process Industries Vol 19(2-3), pp 271-279.

[4] Najjar Y.S.H., Goodger E.M., (1981). Soot formation in gas turbine using heavy fuels, Fuel, Vol 60, p. 980.

[5] Bartknecht W. (1978). Explosionen, Ablauf und Schutzmassnahmen, Springer-Verlag, Berlin.