

Combustion of Kerosene-Air Mixtures in a Closed Vessel

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Abstract: 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. The emphasis is on the mechanical effects of the reactive processes. The evolution of the thermodynamical variables (pressure, temperature, concentrations...) is obtained by solving several coupled transport equations for: the mass continuity, the momentum, the temperature and the fuel concentration. This work relies on laminar and weakly compressible flow assumptions. A global one-step chemical reaction is used for the consumption of the homogeneous kerosene-air mixture.

In the present manuscript, the calibration and validation of the model is reported. The modelling results reveal the influence of the tank geometry on the pressure effects of explosion. Outlines refer to other physical parameters to investigate but also to possible model improvements. This work may be useful for the understanding of accidental explosions of aircraft kerosene tank submitted to a projectile.

Keywords: Explosion, CFD, aircraft tank, confined combustion.

1. Introduction

Partially filled kerosene aircraft tanks exhibit fire or explosion risks. Often related to safety issues, the combustion process is presently studied in terms of vulnerability, when the tank is submitted to anti-aircraft ammunition. The risk of explosion originates from the evaporation of the liquid kerosene: the mixing with air in appropriate proportions forms a gaseous media likely to explode if a small amount of energy is deposited.

As the explosion results of the interplay between several physical phenomena, it is addressed in many ways in the scientific literature, with both experimental and numerical tools: some studies focus on the conditions for which explosion is likely to occur, other concern the effects of the combustion process itself. The present work

describes a simple model able to represent both phenomena. It relies on the Comsol V3.4 code. After a detailed description of the model, the present manuscript relates its calibration and validation. Results refer to the influence of the tank geometry on the mechanical effects of explosion.

2. Description of the physical model

2.1 Two dimensional transport equations

The evolution of the thermodynamical variables ensues from the resolution of a system of Partial Differential Equations (PDE) taking into account mass and heat transport phenomena in the vessel.

(1) Mass continuity equation:

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

(2) Navier-Stokes equation:

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

(3) Fuel transport equation:

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

(4) Thermal transport:

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

The PDE system is solved according to laminar and weakly compressible fluid flow assumptions. A deflagrative combustion regime is thus assumed to occur, for the considered fuel and thermodynamical conditions. (shock waves and/or detonations are not expected in the conditions of the present study).

Second order polynomials are used for the velocity, and linear elements for other variables.

An ideal gas behaviour is assumed for the state equation of the reactive mixture: $P = \rho rT$.

A conservative form is retained for Eq. 3, where the fuel concentration $[C_x H_y]$ is also written C .

It is worth noticing that eq. (3) and (4) are strongly coupled since the heat production rate

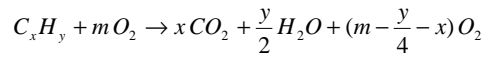
q (W/m^3) is linked to the reaction velocity ω , according to: $q = \omega M_p Q + q_{\text{ign}}$.

Where M_p is the molar mass of kerosene and Q is the heat of combustion of kerosene ($Q = 4.33 \cdot 10^7$ J/kg). The q_{ign} value refers to the ignition process.

As combustion occurs within a closed vessel, the effects of compression are represented in eq. 4 (ideal gas).

2.2 Chemical reaction

The gaseous combustion of kerosene is described with a global one-step chemical reaction. In the present study, only lean or stoichiometric mixtures are considered, so that the oxidation reaction of a C_xH_y kerosene writes:



The values of $x=11$ and $y=21$ are retained in the present study, and $m \geq 16.25$ in the present case.

The velocity ω of the chemical reaction is written in the form:

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

where P is the total pressure (atm) and T the temperature (K). Molar concentrations $[C_xH_y]$ and $[O_2]$ are expressed in mol/cm^3 . The reaction velocity ω is expressed in $\text{mol/cm}^3\text{s}$.

The other constants in the formula (frequency factor, exponents and activation energy) are chosen from data available in the literature (Najjar, 1981). However, the frequency factor has been adapted, as explained further in section 3. With the previous units we have:

$$A = 2 \cdot 10^3 ; \alpha = 0.5 ; \beta = 1 ; E_a/R = 13600$$

2.3 Mixture composition

The mixture formation is now considered: the liquid fuel is introduced into the tank containing air at the initial temperature T_o . Then it evaporates. The equilibrium between both the liquid and gaseous phases is obtained when the partial pressure of the fuel vapor reaches the saturated vapor pressure. In the present study, the mixture of kerosene vapors and air is assumed to be perfectly stirred. The fuel equivalence ratio ϕ is determined by the thermodynamic conditions in the vessel and therefore by the characteristics

of the gaseous phase. The experimental determination of the partial pressure P_{po} of the considered kerosene was carried out in the laboratory by Sochet et al. (1998, 2002). For the studied range of temperatures, the partial pressure writes:

$$P_{po}(\text{Pa}) = \exp[18.5 - 3506.6/T_o]$$

It must be noticed that the partial pressure of kerosene, and consequently the equivalence ratio ϕ , depend on the initial temperature. The equivalence ratio is also sensitive to the initial pressure.

2.4 Physical data

The physical and chemical data used in the previous equations (1), (2), (3) and (4) such as the thermal conductivity λ , the dynamic viscosity η , the specific heat capacity C_p , or the diffusion coefficient C generally depend on the temperature. They are computed as follows:

$$\eta (\text{Pa.s}) = 1.156 \cdot 10^{-6} \exp(1285.15/T)$$

$$D (\text{m}^2/\text{s}) = 3.95 \cdot 10^{-4} \cdot T^{3/2} P^{-1}$$

$$\lambda (\text{W/mK}) = -4.82 \cdot 10^{-9} T^2 + 5.81 \cdot 10^{-5} T + 7.53 \cdot 10^{-3}$$

The value of the global heat capacity C_p depends on each species present in the vessel. A constant chemical composition is assumed for the fresh and the burned gases, so that:

$$C_p = (1 - \xi)C_{p_{\text{pug}}} + \xi C_{p_{\text{pbg}}}$$

where the progress variable $\xi \in [0,1]$ is defined as a function of the molar fraction of the fuel x_c and its initial value x_{co} : $\xi = 1 - x_c / x_{co}$

The specific heat capacity of unburnt gases $C_{p_{\text{pug}}}$ and burned gases $C_{p_{\text{pbg}}}$ (J/mol.K) are sixth order polynomial expressions of temperature, see [1] for more details.

2.5 Ignition process

In the present study, ignition is caused by a fragment of anti-aircraft ammunition. It is modeled by the supply of a heat flux q_{ign} described by a Gaussian space-time distribution. The spatial part of q_{ign} is a function such as:

$$f(x, y) = q_{\text{ign}}^o \exp \left[-\frac{(x - x_p)^2}{\sigma^2} - \frac{(y - y_p)^2}{\sigma^2} \right]$$

where q_{ign}^o is the heat generation rate (W/m^3) initially brought to the mixture, x_p and y_p are the

coordinates of the hot point, and σ is the width of the Gaussian function. The area of ignition is then $a = \pi \sigma^2$.

In the same way, the part depending on time has a similar shape centered on a time t_o , with a total duration of $2 \cdot dt$. The area of the time function is normalized to unity.

The total energy E_{ign} provided to the ignition is therefore: $E_{ign} = \pi \sigma^2 q_{ign}^o$

3. Model Calibration and validation

The thickness of the flame for a fully premixed fuel-air media represents an order of magnitude of 0.1mm in the investigated conditions. Consequently an appropriate mesh should present a cell size dx (more or less) lower than this value. Figure 1 represent the temperature profiles obtained at several instants for a (pseudo) 1D computation. The domain is 5 mm long, it is opened at the right extremity (outlet condition). Adiabatic walls with slipping conditions are used as boundary conditions elsewhere. Ignition is produced by a high temperature zone near the opened extremity.

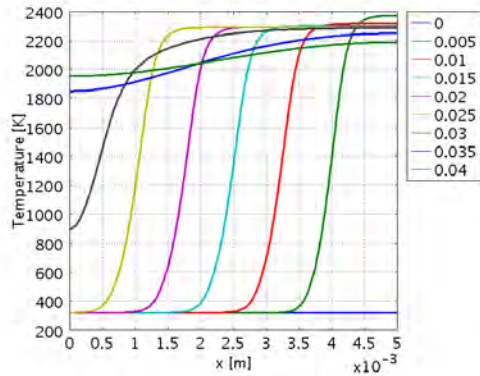


Figure 1. Temperature profiles for a 1D computation ($dx=0.068\text{mm}$), at several instants ($dt=0.005\text{s}$).

Figure 1 shows the flame speed stabilizes at a value of 0.15 m/s. In this well known configuration, the unburned gases remain quiescent. Consequently, the observed flame velocity equals the burning velocity. The value of 0.15 m/s is in fairly good agreement with the laminar burning velocity 0.2-0.4cm/s observed for kerosene in usual temperature and pressure conditions at stoichiometry.

It is important to note that for this computation, the A constant of the reaction rate is $A=2e6$, in agreement with Najjar et al [2].

However, it is clear that with the same approach, a three or even two-dimensional computation of combustion is not appropriate for wide domains: for a one square meter tank, such a thin mesh (2D) would include about 2.10^8 cells.

When considering coarser meshes, solution becomes dependant to the cells size. Indeed, the numerical diffusion tends to increase the heat diffusion and consequently accelerates the flame propagation with increasing cell sizes. This point is illustrated in figure 2, where the combustion duration decreases with an increasing cell size.

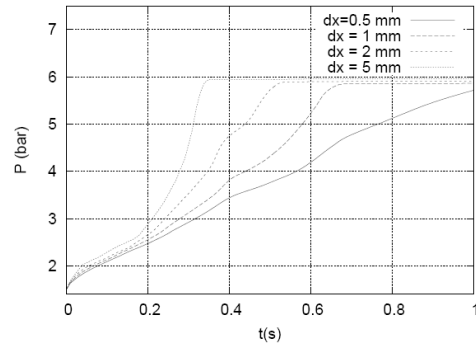


Figure 2. Influence of the mesh cell size on the pressure evolution for a closed 0.1x0.05m vessel.

Several approaches are possible to treat such problems. The simplest one is used in the present study: it consists in using a coarse mesh, with an artificial reduction of the reaction rate so that the correct flame velocity is reproduced. The model calibration led to the following parameters: the cell size is kept approximately constant at $dx=0.02\text{m}$ and the pre-exponential factor of the reaction rate is set to $A=2 \cdot 10^3$.

More advanced methods are briefly evoked in the “outlines” section.

In the present two-dimensional case, the modelled flame thickness is about one cell size, which corresponds to high numerical diffusion conditions. Nevertheless, our investigations showed the computations provide pertaining results on a phenomenological point of view. For instance, in the case of a single compartment (1 x 0.2m), the flame exhibit a typical spherical shape at 6 ms, see fig. 3. At later instants, the flame propagates within the whole tank in 3s. Quantitatively speaking, the mixture contained in a one meter length tank is burned in 3s. This

value is consistent with that of a 1D adiabatic constant pressure combustion, as the laminar burning velocity is about 0.2-0.4 m/s in these conditions.

It was also checked that satisfying results are obtained for concentration profiles across the flame. The burned gases temperature is overestimated (2800-4000K) in the early stages of combustion, as the theoretical value for an adiabatic combustion at constant volume is about 2900K (non dissociated products). This is (partly) caused by the energy deposited during ignition.

The final combustion pressure is about 14.1 bar, see fig. 4. This value agrees with the adiabatic combustion pressure (14.4 bar), computed with the Gaseq code [3] for the same conditions (constant volume).

All these results show the model is well calibrated and can be considered as validated.

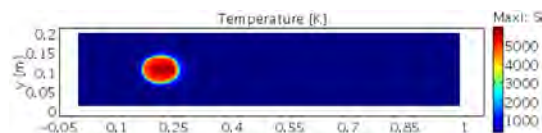


Figure 3. Temperature field at 0.06s.

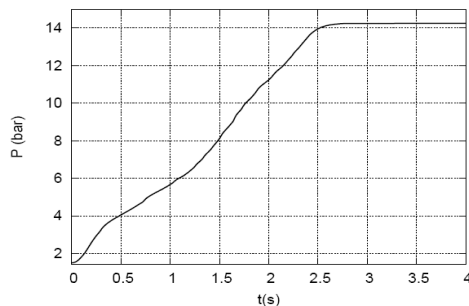


Figure 4. Pressure evolution for a stoichiometric mixture. (1 m x 0.2 m tank, single compartment)

4. Numerical Results

4.1 Framework of the study

The Comsol CFD code is used to evaluate the effects of several parameters on the mechanical effects of explosion within a kerosene tank. In this respect, the present model provided interesting results in a previous study [1]. Among other results, the computations evidenced a strong influence of ignition location for a tank made of several internal compartments. By contrast, the amount of

ignition energy does not influence the pressure evolution in the range of investigated ignition volumes, provided that deposited energy is sufficient to initiate a sustained combustion. Furthermore, the value of this minimum ignition energy is in good agreement with results obtained with a 1D code developed at our laboratory, featuring a detailed chemistry description [4].

In the present section, the focus is on the influence of the tank geometry. The results reported below are also a part of this previous study [1].

4.2 Description of the computational cases

Geometry: The geometries considered in the present study are relatively simplified for this academic study. Nevertheless, the largest ones are fairly representative of aircraft fuel tanks. They consist of one or several identical compartments. Their size is 920x200 mm. The walls separating two compartments feature two horizontal or a vertical orifices, so that the global area blockage is about 50% for each wall. The openings display rounded shapes. The wall thickness is 20 mm.

Initial conditions: The gaseous mixture contains air perfectly mixed with kerosene vapors. The initial temperature and pressure are $T_0=320.5\text{K}$ and $P_0=1.5\text{bar}$, so that the fuel equivalence ratio is stoichiometric.

Ignition occurs within the bottom-left compartment ($x_p=0.2\text{ m}$, $y_p=0.1\text{ m}$). The radius of the ignition zone is $\sigma=5\text{ mm}$. Consequently the mesh is strongly refined at this location. The duration and amplitude parameters respectively equal $dt=5\text{ ms}$ and $q_{\text{ign}}^{\circ}=2\text{MW/m}^2$. The ignition energy is then 157J.

Boundary conditions: Adiabatic and non-slipping conditions are applied at the wall. It is worth noticing the geometry is represented by a single domain.

Solver and numerical parameters: The direct UMFPACK Solver of Comsol V3.4 is used. A memory allocation factor of 1.2 (instead of 0.7) slightly reduced the computational costs. Galerkin Least Square artificial diffusion is used for the momentum equation. Isotropic diffusion ($\delta=0.5$) is used for the equations of temperature and concentration. For the 2x2 compartments case, the computational time is about 4.5 days for a quadricore 2.6GHz Xeon processor.

The model can also be used with Comsol V4.0, with the PARDISO solver and the highly non linear damping option.

4.3 Computational Results

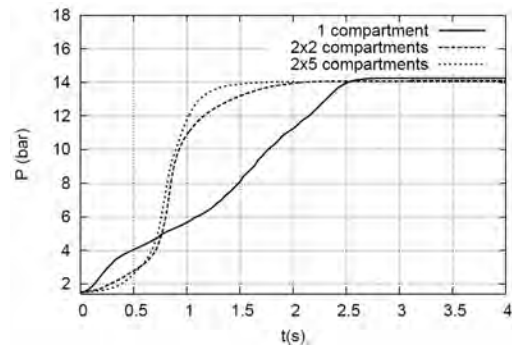


Figure 5. Pressure evolutions for different geometries (made of identical compartments).

Figure 5 reports pressure evolutions for several geometries. The final pressures are identical and in good agreement with the adiabatic pressure of combustion for a constant volume vessel. A recent work [5] reports that this pressure could be exceeded for vessels made of several compartments, even for a deflagrative combustion. The phenomenon is called “Pressure Piling”. In the present case, the compartments feature the same volume, and the blockage area is nearly 50%. For these two reasons, pressure piling is unlikely to occur, which confirms the relevance of the computed final pressure.

One can also remark on fig. 5 that the highest rates of pressure rise are obtained for multiple compartment tanks. This effect results of the acceleration of the combustion process in presence of obstacles. It is explained in the following: for the 2x2 compartments case, the maximum rate of pressure rise is observed between 0.65 and 0.9 s, which corresponds to the propagation of the flame from the left compartments to the right ones, see fig. 6. In fact, the length of the flame contour is moderate in the early stages of combustion. The global rate of combustion and the subsequent rate of pressure rise are then relatively low. As the flame propagates, it moves the unburned gases as a result of the burned gases expansion (this phenomenon is known as the ‘piston effect’). This induces an unsteady jet flow of unburned gases through the vertical orifices separating the

compartments. When the flame reaches the left compartments, it is then distorted by the residual flow. The length of the flame contour is thus increased, so that the global combustion rate is higher. It must be underlined that despite relatively simplified modelling hypotheses, the model reproduces the expected phenomenology (i.e. the flame acceleration) in presence of obstacles [6].

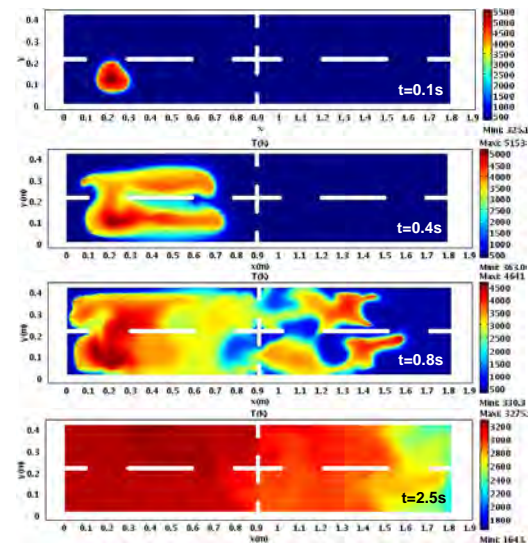


Figure 6. Explosion within a 2x2 compartments tank: Temperature fields at several instants.

The 2x2 and 2x5 compartments cases are then compared each other: the pressure traces are similar up to 0.9s, but the combustion duration is slightly shorter for the 2x5 case (1.5s instead of 2s). This effect was not expected, since for simplified 1D geometries, the combustion duration generally increases with the volume. It is explained as follows: for the considered 2D geometry, the distance from the ignition point to the furthest wall is identical for both 2x5 and 2x2 cases (for a horizontal or vertical path). The combustion duration should be similar, if considering that the flame celerity remains approximately constant. It is even shorter for the 2x5 case, as the strong rate of pressure rise is maintained for a longer duration.

4.4 Outlines

One has to note that other strategies have been published in the scientific literature for the modelling of large scale combustion. Some of them are reported below. Probably the most straightforward method is to use an unsteady

mesh refinement strategy. Maybe the multi-grid solver of Comsol V3.4 could be used for this purpose. Nevertheless, one has to keep in mind that the refinement algorithm can be time consuming and that the transport equations still feature exponential source terms. An other possibility consist in modelling an artificially thicker flame by modifying both the reaction rate and the diffusion coefficient in function of the local cell size, so as a prescribed burning velocity is reproduced. The later is provided by another submodel. If the so-called 'beta flame model' requires some corrections for the flame curvature and near the walls [7], the flame propagation occurs correctly with a limited amount of numerical diffusion. Therefore one can expect moderate computational cost, even for large domains. The computational effort is all the more reduced that the corresponding reaction rate does not exhibit an exponential form. Otherwise, one can consider the flame as a discontinuity and track it with specified approaches such as Level Set or SIF Methods [8]. At the moment, the improvement of the model under the Comsol environment is in progress and some of these approaches are currently tested.

On a more physical point of view, the sensitivity of the pressure evolution to several parameters will be the subject of future works: heat transfer at the walls, external venting, and fuel equivalence ratio heterogeneities. As turbulence is also expected to play an important role in the explosion process, it will be represented in further studies with a RANS approach. It is worth noticing that as the thickness of the (average) turbulent flame is generally more important than in the laminar case, the requirements for the meshes are lower. The use of a specific solving strategy would probably not be necessary in our case, excepted at the early stages of combustion.

5. Conclusions

In a framework related to aircraft vulnerability, a Comsol model is proposed to represent the ignition and combustion of kerosene vapors within aircraft tanks. Calibration and validation works are first reported for the retained approach. Modelling results describe the influence of the tank geometry on the mechanical effects of explosion. As expected, the maximum

pressure is independent of the geometry for the retained set of hypothesis and geometries. Moreover, it appears that the tank volume is not a sufficient parameter to describe the combustion duration: the geometry also plays an important role *via* the ignition location and the presence of internal obstacles. Indeed, the latter accelerate the combustion process. These results show the model proposed for the Comsol code provides pertaining results for the retained set of hypothesis. Outlines are proposed to improve the approach on both a numerical and a physical points of view.

6. References

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