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Combustion of Kerosene-Air Mixtures in a Closed Vessel

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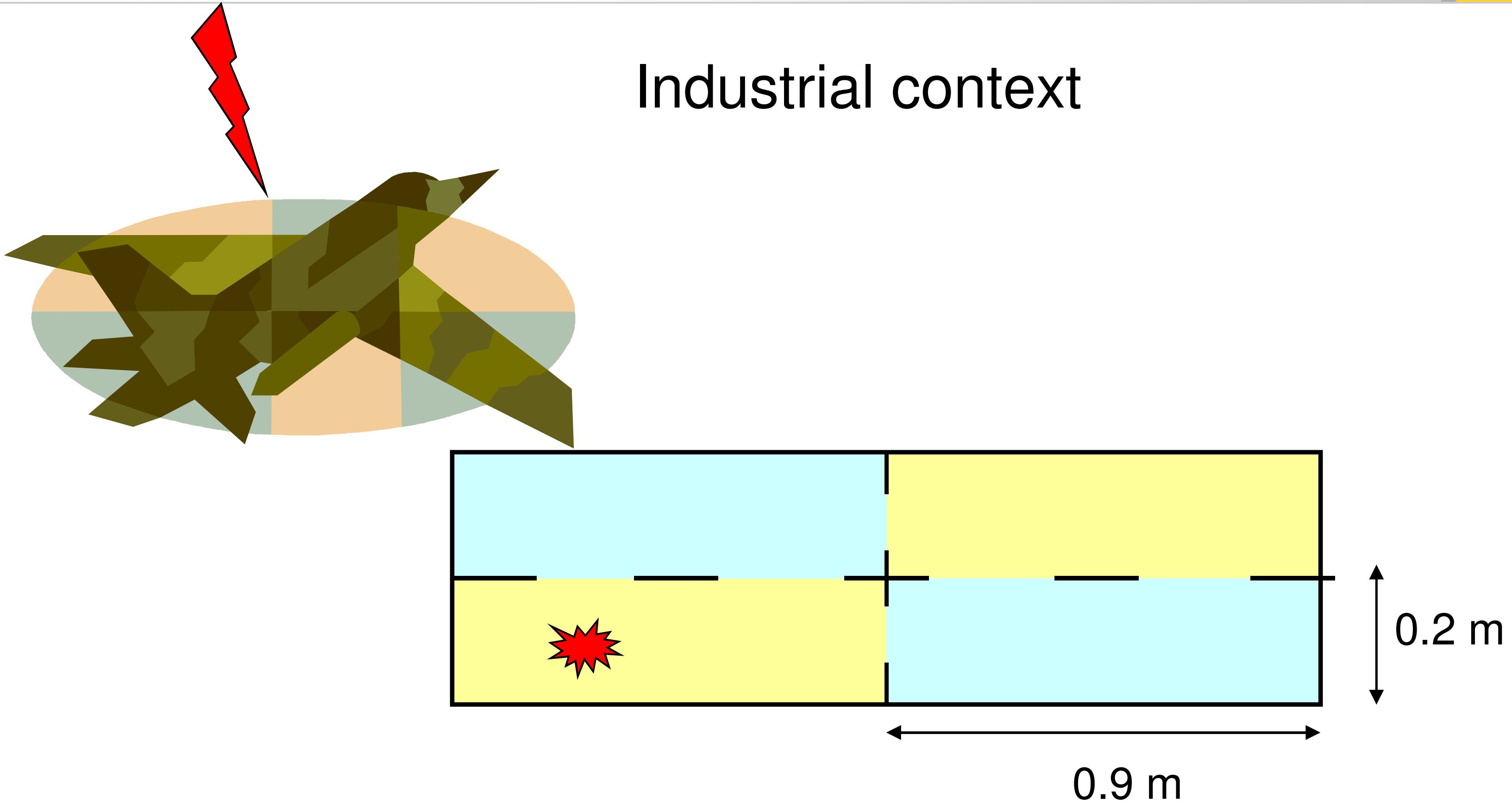
Industrial context



Multi-Compartment Tank filled with kerosene vapours mixed with air

at various initial temperatures and pressures according to the height of flight

Introduction

✓ This is a study performed in the frame of a contractual work (*DGA contract N°2007 25 009 000 51 00 00).*

Aims of the study

✓ Vulnerability of aircraft tanks submitted to a projectile
  - ☑ (i) Ignition
  - ☑ (ii) dynamics of combustion (final pressure, combustion duration)

✓ These data have to be used as input data for structure vulnerability studies

COMSOL MultiPhysics 3.4 (4.0) used to **determine the sensitivity of the combustion process** to:

✓ Ignition parameters (Position, Size and energy distribution)

✓ The geometry (with internal obstacles)

✓ …

Outlines of the presentation

1. **Description Of The Physical Model**
    a) Basic equations
    b) Kinetic and Fluid properties
    c) Representation of ignition source
2. **Model Calibration and validation**
3. **Numerical Results for a Multi-Compartment Tank**
4. **Conclusions**

Description Of The Physical Model

Assumptions:

- Laminar and weakly compressible fluid flow.
- Ideal gas, pressure vapor of kerosene in equilibrium with liquid (initial condition)
- Liquid phase is not considered during combustion
- One step reaction of combustion

(1) Mass continuity eq.:

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

(2) Navier-Stokes eq.:

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

(3) Fuel transport eq.:
(Diffusion & convection)

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

(4) Thermal transport eq.:
(Conduction & convection)

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

Heat production rate q (W/m^3) linked to the reaction rate ω: **q = ωMpQ + qign.**

Kinetic and Fluid properties, Ignition parameters

Simple kinetic : $C_xH_y + mO_2 \rightarrow xCO_2 + \frac{y}{2}H_2O + (m - \frac{y}{4} - x)O_2$

Najjar (1981) kinetic law : $\omega = AP^{0.3}T[C_xH_y]^{\alpha}[O_2]^{\beta}\exp(-E_a / RT)$

Physico-chemical data

η (Pa.s) = $1.156.\ 10^{-6}\exp(1285.15/T)$ D (m^2/s) = $3.95.10^{-4}.T^{3/2}P^{-1}$

λ (W/mK) = $-4.82.10^{-9}\ T^2 + 5.81.10^{-5}\ T + 7.53.10^{-3}$

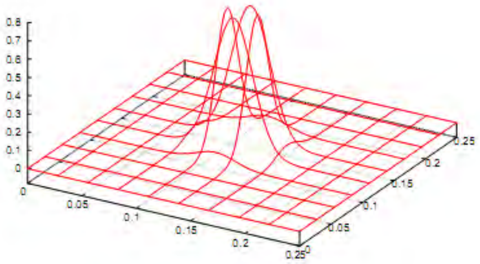
Cp=f(T,C) : dependence to temperature and composition (unburned/burned gases). (Gaseq computations, stoechiometric n-decane/air mixture, adiabatic combustion).

Ignition model

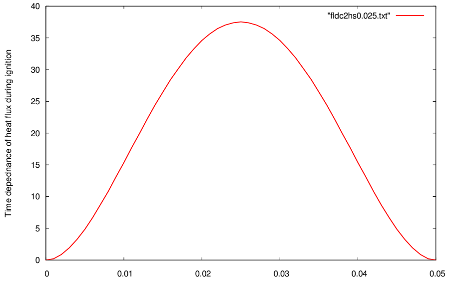
Supply of a heat flux q_{ign} : Gaussian-like space-time distribution.

Total energy provided:

$E_{ign} = 2\pi\sigma^2\ q^{o}_{ign}$



Space distribution



Time distribution

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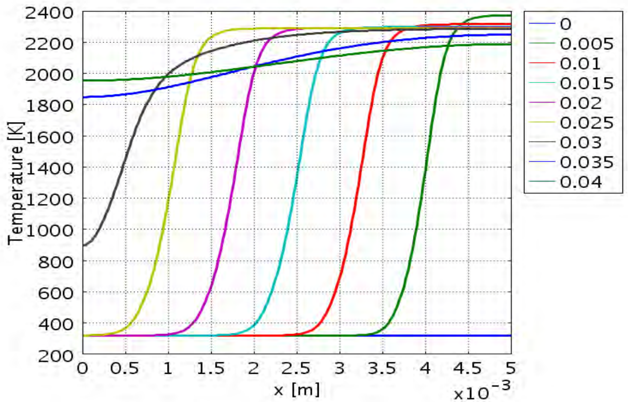
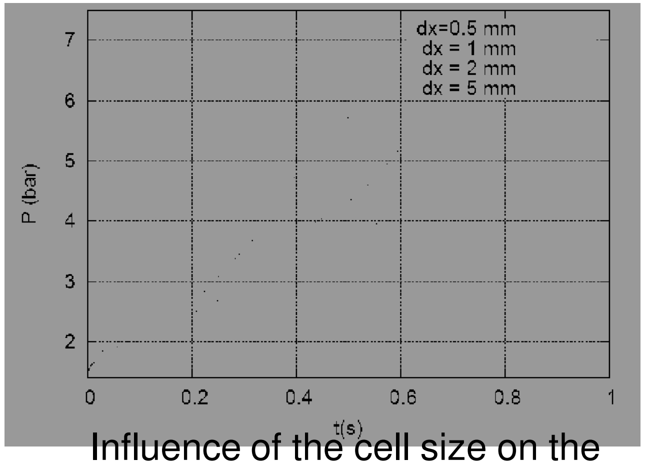
Validation and calibration

First Case : open tube (1D)

- ✓ S_u= 0.15 m/s
  → **consistent burning velocity** for a stoichiometric mixture in similar conditions (0.2-0.4 m/s)
- ✓ **But thin mesh !**
  (dx=0.068 mm ≈ flame width / 10)
  → **a 1m² tank computation is out of reach** (2e8 cells !)
- ✓ **Problem**: for coarser meshes, the solution becomes dependant on the cell size !
- ✓ **Retained solution (calibration):**
  - ☑ Coarse mesh (dx=20 mm)
  - ☑ Reduced reaction rate (x10^{-3})



Temperature profiles at several instants (dt=0.005s) within an open tube. (1D computation, dx=0.068mm)



Influence of the cell size on the pressure evolution for a closed vessel (0.1x0.05m, 2D computation).

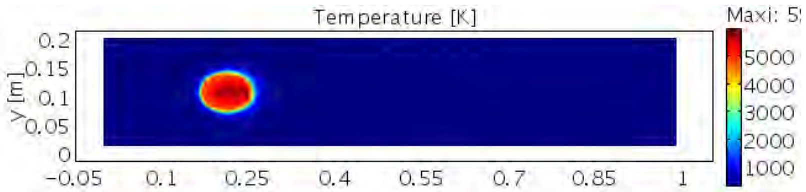
Validation and calibration

Validation of the results: 1x0.2 m closed vessel (2D)

✓ **Qualitative behavior**

☑ Concentration and velocity profiles across the flame

☑ Flame propagation



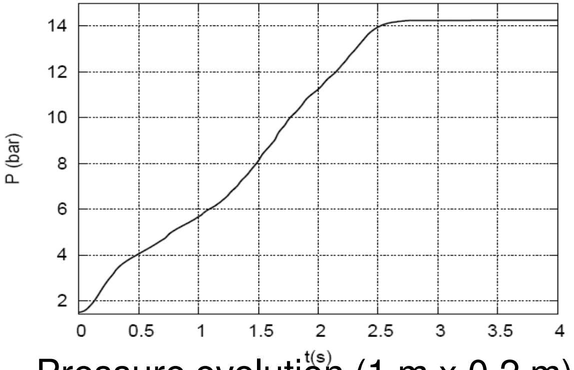
Temperature field at 0.06s.

✓ **Quantitative results**

☑ **Burning velocity**: **consistent** with experiment Su=0.2-0.4m/s (1m of mixture burned in 3s)

☑ Temperature fields: locally overestimated (2700-4000K) (adiabatic, V=cst temperature: 2900K)

☑ **Final pressure**: **good results** PComsol=14.1 bar; PGaseq=14.4 bar (0D adiabatic, V=cst)



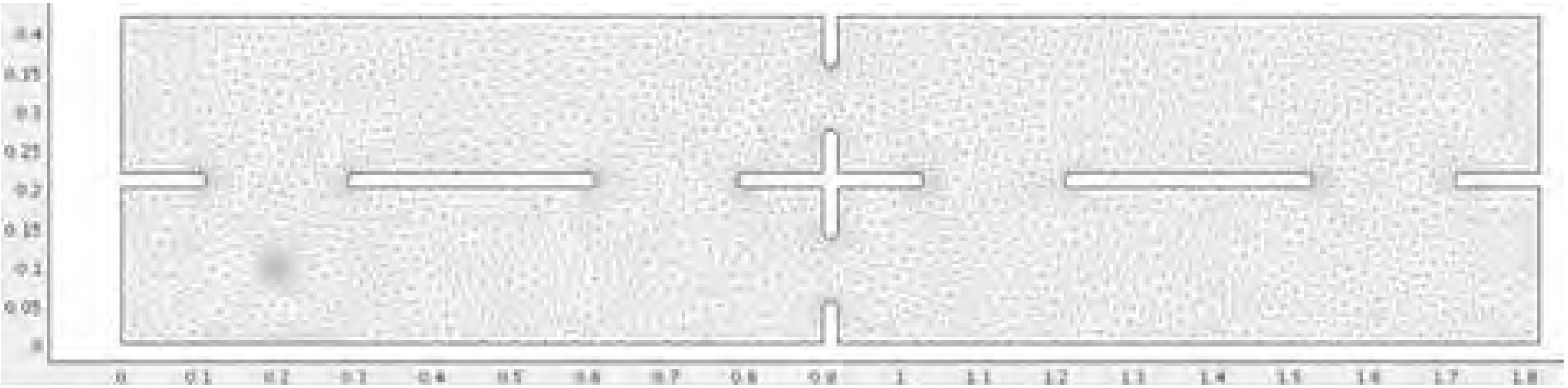
Pressure evolution (1 m x 0.2 m)

✓ **Model validated for 2D computations of pressure evolution (laminar conditions).**

Outlines of the presentation

Results for A Multi-Compartment Tank

Geometry, mesh, initial and boundary conditions



Geometries: 26L / compartment, orifices (~50% area blockage)

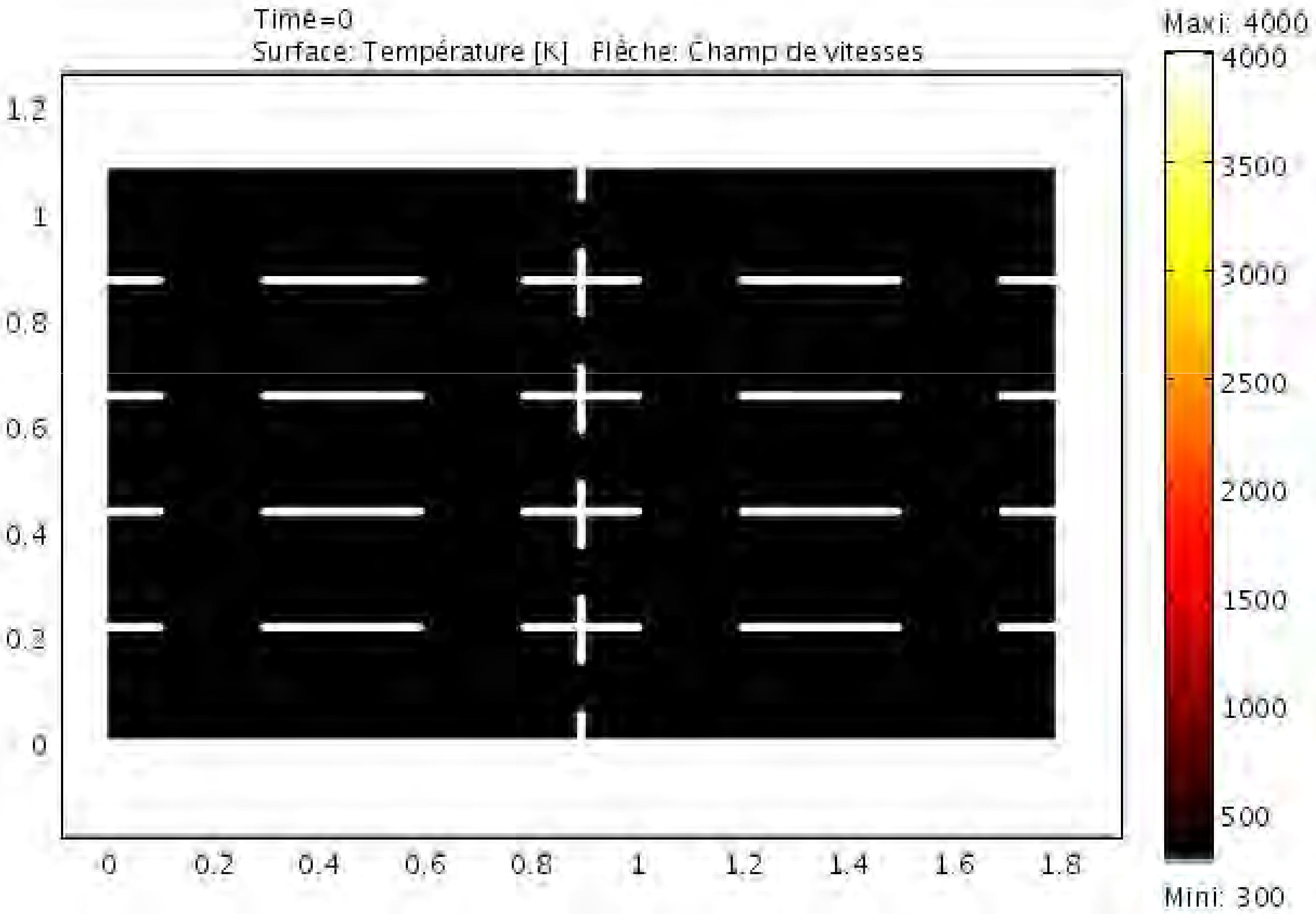
Boundary conditions: Adiabatic, non-slipping conditions at the walls.

Initial conditions: T_0=320.5K and P_0=1.5 bar (stoichiometry)

Ignition: radius of the ignition zone is = 5 mm (area a=0.78cm²)
An energy of E_{ign}=157J is deposited during 5 ms.

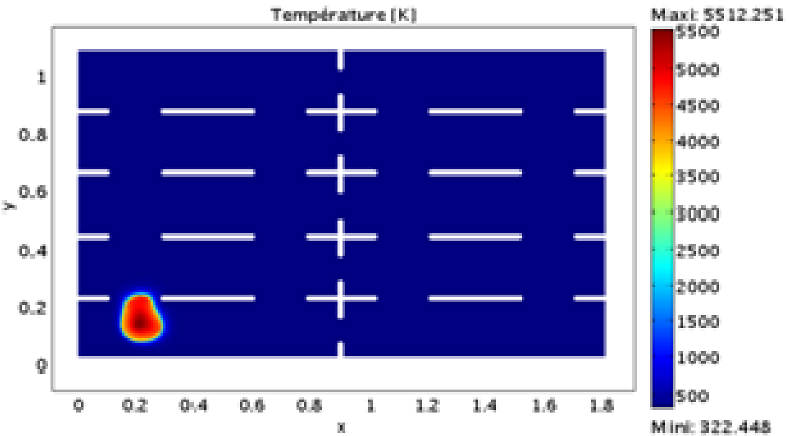
Solving: (V3.4) UMFPACK or (V4) PARDISO + non linear damping.

Results for A Multi-Compartment Tank : Influence of tank geometry

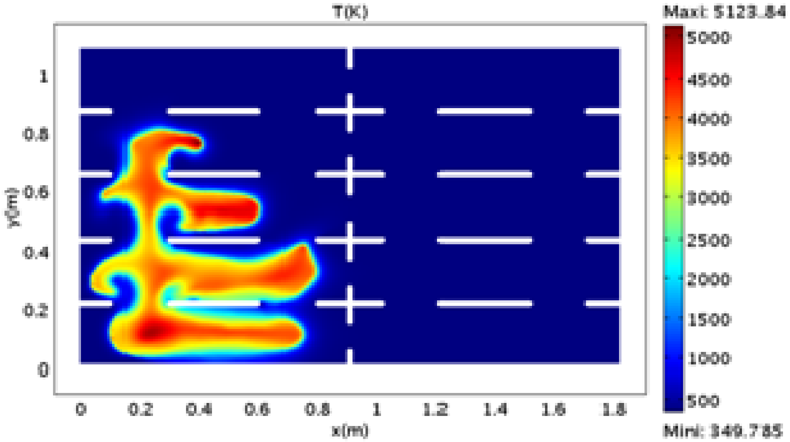


Evolution of temperature fields for a 2x5 compartments tank

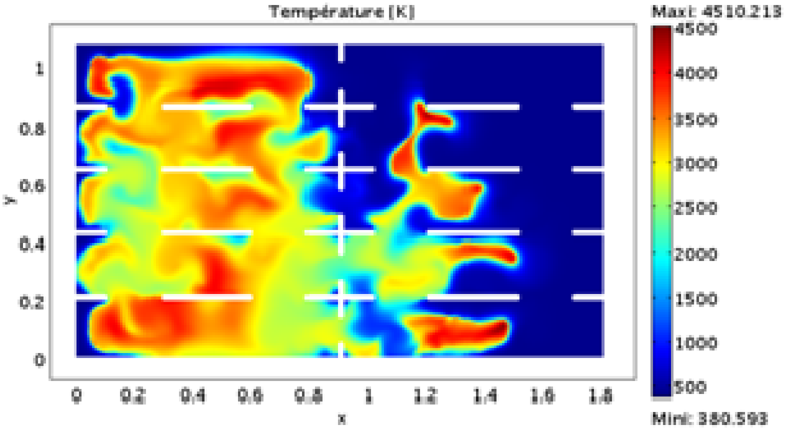
Results for A Multi-Compartment Tank : Influence of tank geometry



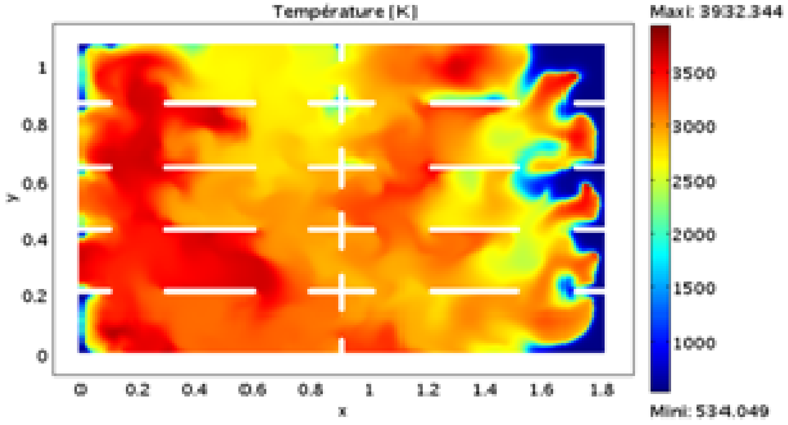
t = 0.1 s



t = 0.4 s



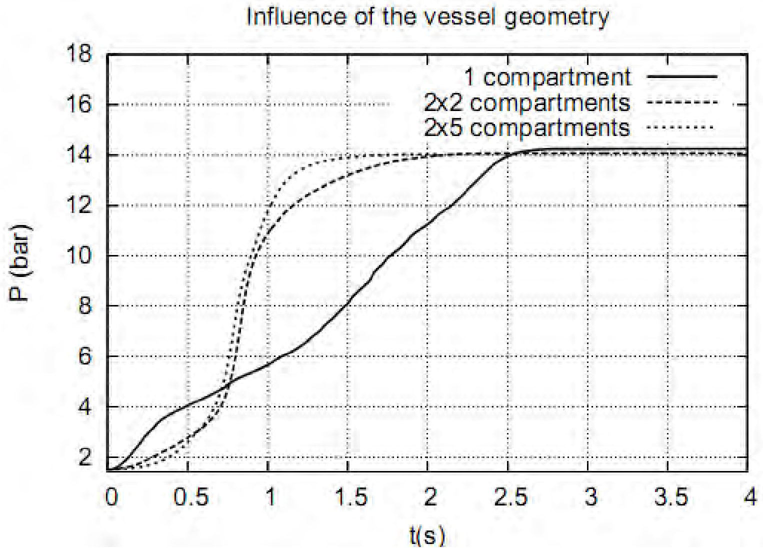
t = 0.1 s



t = 1 s

Temperature fields at several instants for a 2x5 compartments tank

Results for A Multi-Compartment Tank : Influence of tank geometry



✓ **Final pressures agree with the 0D adiabatic constant volume case.**

Relevant even with several compartments since :

☑ The blockage area is moderate

☑ All the compartments feature the same volume (no pressure-pilling, see [Benedetto et al])

✓ **Highest rates of pressure rise obtained for multi-compartment tanks**

☑ Acceleration of the combustion process in presence of internal orifices well reproduced [Ciccarellia et al]

☑ The largest tank features the fastest pressure rise.
→ unexpected as in the 1D case combustion duration decreases with volume

CFD simulation of the explosion of kerosene vapor in a closed vessel

Conclusion

- ✓ A single model describes both ignition and laminar flame propagation.
- ✓ The model is calibrated and validated for such large geometries
  - ☑ Flame velocity in the suitable range for a laminar combustion
  - ☑ Final pressures accurately reproduced
- ✓ Influences of tank geometry is also analyzed:
  - ☑ Internal obstacles accelerate the combustion process.
  - ☑ Influence of volume is not straightforward
- ✓ This model is highly flexible and allows various simulations in a context of safety applied to aircrafts with kerosene tanks.

In progress

- ☑ Tank draining of through vents
- ☑ Heat exchange with walls
- ☑ Turbulence and/or large scale combustion methods

Thank you for your attention

✓ References

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- ☑ Benedetto A.D., Salzano E., CFD simulation of pressure piling, Journal of Loss Prevention in the Process Industries, 23, 498 – 506 (2010).
- ☑ Ciccarellia G, Dorofeev S., Flame acceleration and transition to detonation in ducts, Prog Energ Combust Sci, 34, 499–550 (2008).