Cooling Process Optimization Through A Three-phases Thermo-hydraulic Model

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Introduction

Ammunition cooling process is a critical part of ammunition manufacturing. Adjusting this process to a new type of body shell or melt-cast composition is a time-consuming task. Besides, improvements to an existing production line are difficult to implement. Therefore, THALES uses numerical modelling to better target the experiments to run and define working zones.

A COMSOL application[1] initially developed in 2017 has been improved to include new physics features and more options. Namely, the new version can consider:

- a mixture of liquid and solid phases at the beginning of the process,
- the influence of density difference at the solidification on convection within the liquid phase.

Furthermore, the solving strategy has been improved to reduce substantially computation time.

Theory

The explosive formulation is defined as a liquid in the body and then its solidification occurs inside[2]. This leads to different challenges. At the phase change, a huge energy is released from the solidification front to the outside of the body. Numerically, a modified heat capacity method (see **Figure 1**) is applied since the first version of the app. The phase change is spread over a small range of temperature through a narrow Gaussian distribution so that the global energy generated by the solidification is equivalent fusion enthalpy. While solidifying, the mixture becomes more dense which results in a motion force within the liquid phase. This density difference results in solidification shrinkage. Therefore, Navier-Stokes equations are solved under their weakly compressible form. As the overall volume of the mixture changes, all the equations in it are solved on a moving mesh to conserve the mass balance. Moreover, the solid phase needs to be still even if the Navier-Stokes equation is solved in the area.

One of the methods to reduce cooling time is to pour a mixture that is partially solidified and contains grains (see **Figure 2**, left). To account for this intermediate thermodynamic state, the application computes the specific temperature to apply as an initial temperature of an homogenised mixture (see **Figure 2**, right). This initial temperature is located within the Gaussian distribution used for the fusion enthalpy modelling and depends on the energy that still needs to be released to completely solidify the mixture (see **Figure 1**).

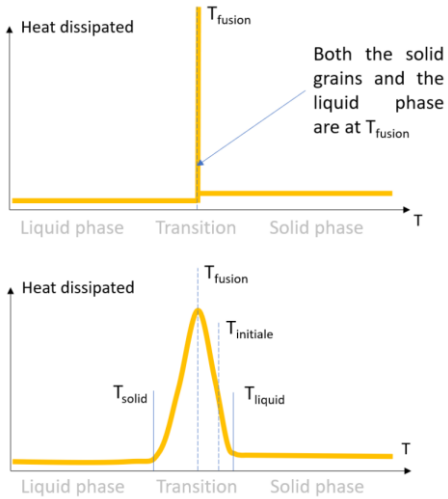

Figure 1 - Diagram of the heat released to vary the temperature of the mixture, including phase change. Top: transition at a single temperature. Bottom: transition across a limited range of temperatures (modified heat capacity method)

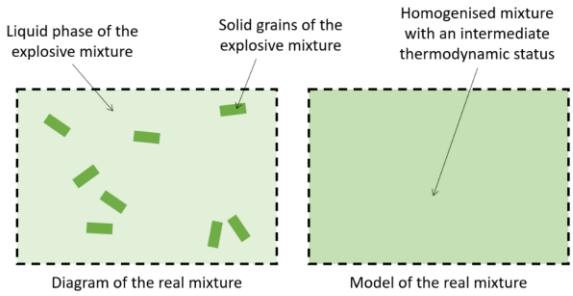

Figure 2 - Partially solidified mixture

Governing Equations

The equations are solved under their axisymmetric form as the geometry of the ammunition and its accessories is invariant by any vertical rotation (see **Figure 3**).

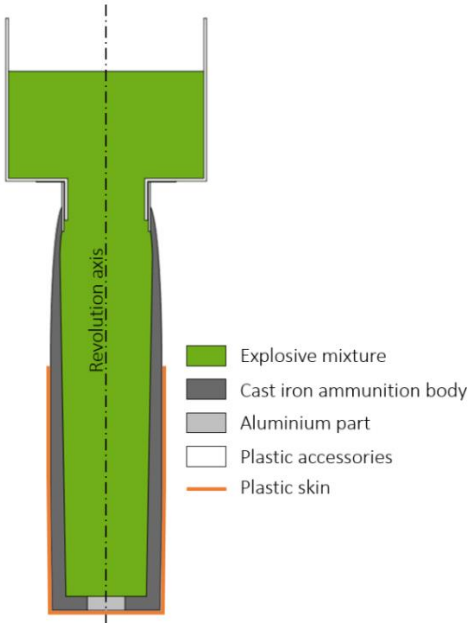

Figure 3 – Cut view of the different bodies of the model

a) Heat transfer

The classical time dependent heat equation is solved on all the domains of the geometry:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \boldsymbol{u} \cdot \nabla T - \nabla.(k \nabla T) = 0$$

where ρ is the density, C_p is the heat capacity, T is the temperature, t is the time, k is the heat conductivity and $\boldsymbol{u}$ is the fluid velocity field in the mixture computed by the Navier-Stokes equations.

At the boundaries of the domain an outward normal heat flux is applied:

$$q = h \cdot (T_{ext} - T)$$

with h a heat transfer coefficient which depends on the height, the surrounding fluid, the flow regime and the surface orientation[1].

The heat capacity is modified to include the fusion enthalpy across a narrow range of temperature (see **Figure 1**).

The initial temperature is computed by a dichotomy method within the temperature range where the modified heat capacity method. This initial temperature accounts for the intermediate thermodynamic state of the mixture.

b) Navier-Stokes equations

The weakly compressible Navier-Stokes equations are solved within the solid and liquid phases of the mixture:

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \nabla \cdot [-p\boldsymbol{I} + \boldsymbol{K}] + \boldsymbol{F}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

$$\boldsymbol{K} = \mu(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T) - \frac{2}{3}\mu(\nabla \cdot \boldsymbol{u})\boldsymbol{I}$$

with $\boldsymbol{I}$ the identity matrix, $\boldsymbol{F}$ the volume forces and μ the viscosity. Because of the low Reynolds number (< 20 across the whole simulation), the flow is considered laminar and no turbulence modelling is included.

At the interface between the mixture and its container (see **Figure 3**) a Navier slip is applied to allow the mixture to slide along the container walls during the process:

$$\boldsymbol{u} \cdot \boldsymbol{n} = \boldsymbol{0}$$

$$\boldsymbol{K_n} - (\boldsymbol{K_n} \cdot \boldsymbol{n})\boldsymbol{n} = \frac{\mu}{\beta}[\boldsymbol{u} - (\boldsymbol{u} \cdot \boldsymbol{n})\boldsymbol{n}]$$

with $\boldsymbol{K_n} = \boldsymbol{K} \cdot \boldsymbol{n}$, $\beta = h_{min}/2$, h_{min} the minimum element size.

To model the free surface at the top, a $p = 0$ pressure is applied.

In the solid phase, a high viscosity μ_{solid} is applied to model the zero-velocity field. This approach finds its limit when the ratio of liquid to solid viscosity is too small or when the solving time is longer than the characteristic time of motion within the viscous solid phase.

In the liquid phase, the natural convection is accounted for through the Boussinesq approximation:

$$F = -g\rho\beta \cdot (\mathrm{T} - \mathrm{T_{fusion}})$$

with g the gravitational acceleration and β the thermo-dilatation coefficient. This approximation is selected here because of the low density variation within the liquid phase.

c) Moving mesh

The moving mesh is applied all over the mixture domain. A Yeoh smoothing is applied to the mesh.
All the above-mentioned equations are solved on the deformed domain which undergoes a dr, dz displacement computed by the moving mesh method.

At the free surface, the normal mesh velocity is set equal to the fluid normal velocity.

d) Coupling

A two-ways coupling is applied to the different equations solved here. They indeed depend significantly on one another (see **Figure 4**) and different variables are transferred during the solving process.

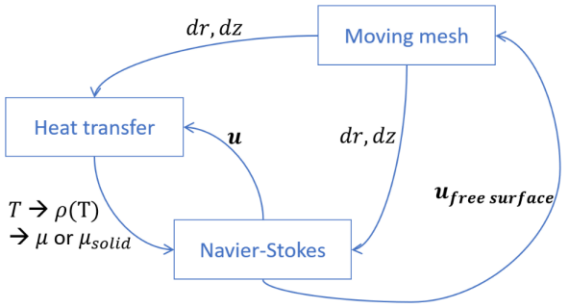

Figure 4 - Coupling between the different equations

Constitutive relations

The constitutive relations proposed here are not restrictive and other possibilities are available. However, the present relations are relevant for the present case:

a) Thermal properties

The different materials have various properties and the explosive composition behaves differently when it is solid and liquid. Besides, at phase change the fusion enthalpy applies. The different material properties are listed in **Table 1**.

Item	k $[W/(m.K)]$	C_p $[J/(kg.K]$	ρ $[kg/m^3]$	T_{fusion} $[K]$	**Fusion latent heat** $[kJ/kg]$
Exp. Mixt.	Confidential data				
Cast iron	30	477	7200		
Alu.	229	898	2710		
Plastic	52	1900	925		

Table 1 - Thermal properties

b) Fluid properties

Whereas the cast iron, aluminium and plastic are only under their solid forms, the melt-cast formulation can be liquid and solid. Therefore, its properties are required in the Navier-Stokes equation. The properties required are displayed in **Table 2** even if the numerical value is not available to the reader.

Item	μ $[Pa.s]$	β $[1/K]$
Explosive Mixture	Confidential data	

Table 2 - Fluid properties

Solving method

COMSOL Multiphysics® 5.5 software is used to build and solve the numerical system defined previously.

The method used here is composed of two steps. Because initial conditions apply different temperatures to contiguous domains, a few timesteps are made with the single heat equation. During this step, the velocity in the fluid domain is set to zero.

Then, a second step consists in solving both heat and Navier-Stokes equations on the deformed meshes in the time domain with the result of the first step as initial condition.

A Newton-Raphson algorithm is used, with a 0.2 damping. The linear system is solved by a direct linear Pardiso solver. Besides a maximum timestep of 5 s is applied.

Interface

The first version of the interface (GUI) was developed by SIMTEC in 2017 with THALES requirements and THALES support through the COMSOL Application tools. This application has been used by THALES since then and a continuous development of the GUI has been made by SIMTEC with new features and modelling options every year. Two views of the interface are available in **Figure 6** and **Figure 7**.

Results and discussion

Thanks to the model presented previously, the cooling phase of new melt-cast composition can be quickly optimised. A case study is presented here. After filling the ammunition shell with “fusible / melted” explosive formulation, the cooling process is started. Several variations of the process are quickly tested through the interface.

One of the sequences predicted is presented in **Figure 5**. This sequence shows that the cast explosive shrinks while cooling and that the liquid phase flows from the plastic accessories to the body shell to compensate. It implies that warm explosive mixture circulates and transfers heat to cooler areas. Thanks to the numerical simulations, it is possible to quantify this heat flow and its impact on the quality

of solidification. More specifically, it allows for avoiding the formation of liquid cavities which would result in shrinkage porosity.

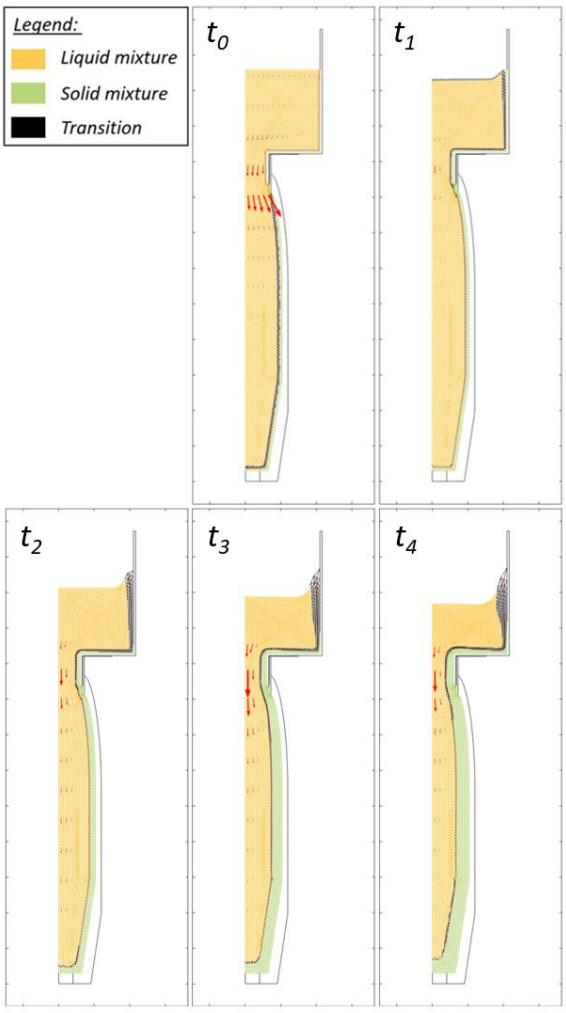

Figure 5 - Cooling with solidification shrinkage

Conclusions

An improved numerical model is presented in this document. This model predicts the solidification front evolution of melt-cast composition in its ammunition during the cooling process. This model considers the liquid-solid phase change, a wide variety of cooling methods and solidification shrinkage. It is possible to model different cooling fluids, with a control on the fluid circulation velocity, on the area which undergoes the fluid circulation, and on variation during the cooling process of these configurations. A heating of the top part of the ammunition and the funnel can also be adjusted. The different geometry parameters and process possibilities can be defined easily in the COMSOL Application developed by SIMTEC for THALES. A secured https internet connection enables remote confidential computations. Thanks to this application, different process possibilities can be tested on the new configurations. After this simulation step, only the relevant cases are experimented. This is a powerful way to optimise the process while rationalising the development costs.

References

1. Wheeler, J.-D., Coulouarn, C., Benade, E. & Namy, P. Optimization of an explosive mixture cooling process including a phase change. in *COMSOL Conference* (2017).
2. Coulouarn, C., Aumasson, R., Lamy-Bracq, P. & Sta, F. Focus on the melt-cast technology – Main properties of XF®11585. in *Presentation at the 44th ICT* (2013).

Appendix: Interface

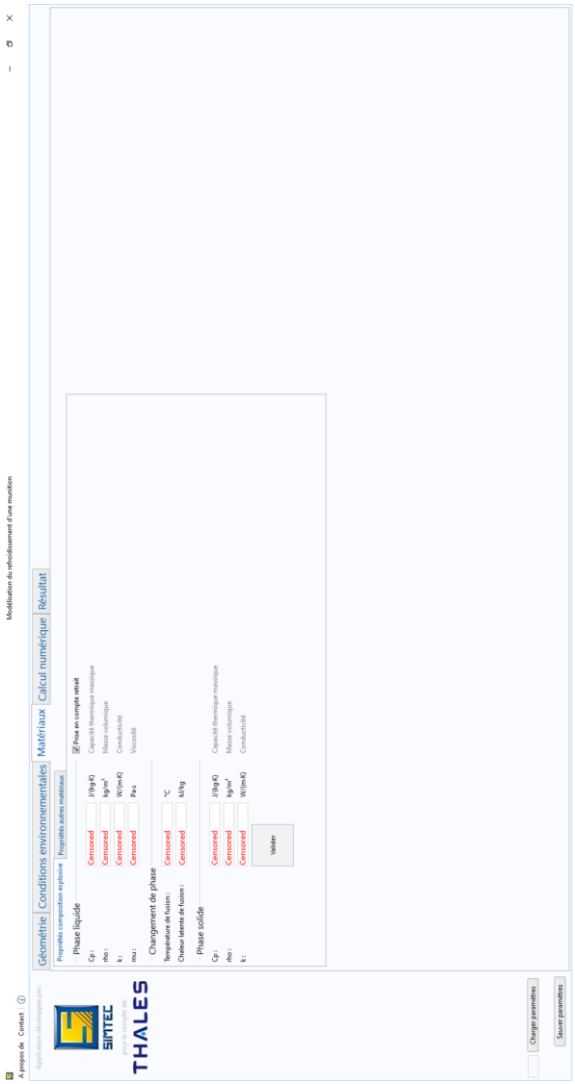

Figure 6 - Interface overview, material properties (landscape layout)

Figure 7 - Interface overview, environmental condition parameters (landscape layout)