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# Modelling of melt cast cooling and solidification processes for explosives

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The search for high-energy but low-sensitivity explosives has been the focus of many studies. It has been found that the use of cyclo-trimethylene-trinitramine (RDX) or cyclo-tetramethylene-tetranitramine (HMX) can maximize the energy of the explosive while minimizing its sensitivity. However, the preparation and processing of such explosives is a major challenge for military applications.

Melt casting and mechanical pressing are two of the most used approaches for explosives production. Of the two, melt casting is more economical for large-scale filling in munitions applications. A large amount of charge can be cast, even with very special shape. Explosives melt casting has traditionally been based on a trial-and-error approach. Further process and product improvements call for the development of a comprehensive numerical model that allow a systematic study of the melt casting process parameters and offer a better understanding of the physical mechanisms involved. The numerical modelling and simulation presented here are used to determine optimized casting parameters. High quality explosives can not be produced without well-controlled casting parameters.



## Problems to be solved

- Product non-uniformity
- Porosity and cavities
- Void formation
- Shrinkage
- Cracks and micro-defects





#### **Model**

Heat transfer by conduction equation:



Incompressible Navier-Stokes:

$$\begin{split} \rho \frac{\partial \vec{u}}{\partial t} - \nabla \mu \left( \nabla \vec{u} + (\nabla \vec{u})^T \right) + \rho \left( \vec{u} \nabla \right) \vec{u} + \nabla p &= \vec{F} \\ \frac{\partial \rho}{\partial t} + \nabla \left( \rho \vec{u} \right) &= 0 \end{split}$$
• Phase change during solidification:  $C_p = C_{p \text{ solide}} + \frac{\Delta H_f}{T_f} (flc 2hs(T - T_f, 1)) + \Delta H_f \cdot \exp\left(-\frac{(T - T_f)^2}{\sqrt{\pi}}\right)$ 

#### Inputs for the Model

- Explosive properties:
  - Density: ρ
  - Melting point: T<sub>f</sub>
  - Latent heat of solidification:  $\Delta H_{I}$





Thermal conductivity: k
Thermal expansion coefficient: α
Viscosity: η

Conditions:

• Initial temperature of metal and explosive: T<sub>0</sub>

• Ambiant air temperature: T<sub>ext</sub>

• Cooling conditions: conduction, free convection, forced convection

### **Results of COMSOL 3.4 simulation:**

- Validation of the model : comparison between measured temperature and simulated temperature
- Solidification front evolution versus time is observed to determine the best cooling conditions





#### Visualisation of stress/strain and shrinkage



This new model is a cost and time-effective tool to optimize the process parameters