GENERAL DYNAMICS
Ordnance and Tactical Systems–Canada

POLYTECHNIQUE MONTRÉAL
LE GÉNIE EN PREMIÈRE CLASSE

Simulation of the cooling and phase change of a melt-cast explosive

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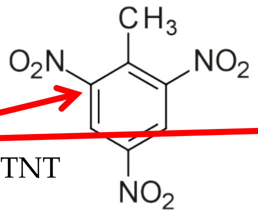
Outline

1. Background
2. Objectives
3. State of the art
4. Key steps
    5.1 Solidification
    5.2 The cooling of the solid – Thermal stress and stress relaxation
    5.3 Adhesion to the mold walls
5. Results and lessons learned
6. Conclusion

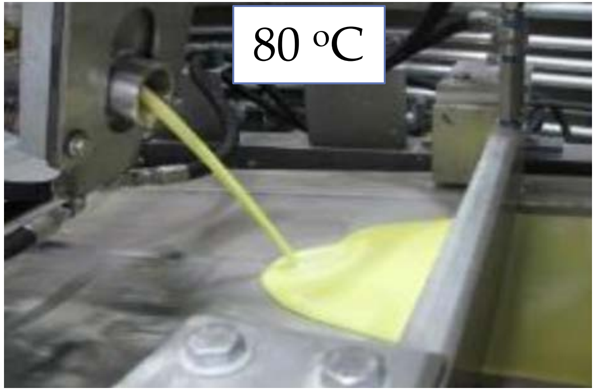
Melt cast explosives:

Composition B



TNT

Such casting has long been conducted on a trial-and-error basis before new product improvements in the field called for more precision.



- Generic Process:

Source C. Coulouarn, and al., NEXTER Munitions, c.coulouarn@nexter-group.fr

- Cooling Process:

Source: Eurenco

The cooling and solidification process come along with factors affecting the material performance:

- Higher density
- Air/void entrapments
- Thermally induced mechanical stress and debonding at the wall

Challenges

Melt casting of explosives is a proven process but the production remain a major challenge in today's economical environment:

- Inadequate cooling cycle.
- Albeit some imprecision, temperature measurements (via thermocouples) are the only reliable data captured during casting.
- No information on stress development during casting.
- Formulations are changing, new products are being used, therefore the manufacturing cycle must be adapted.

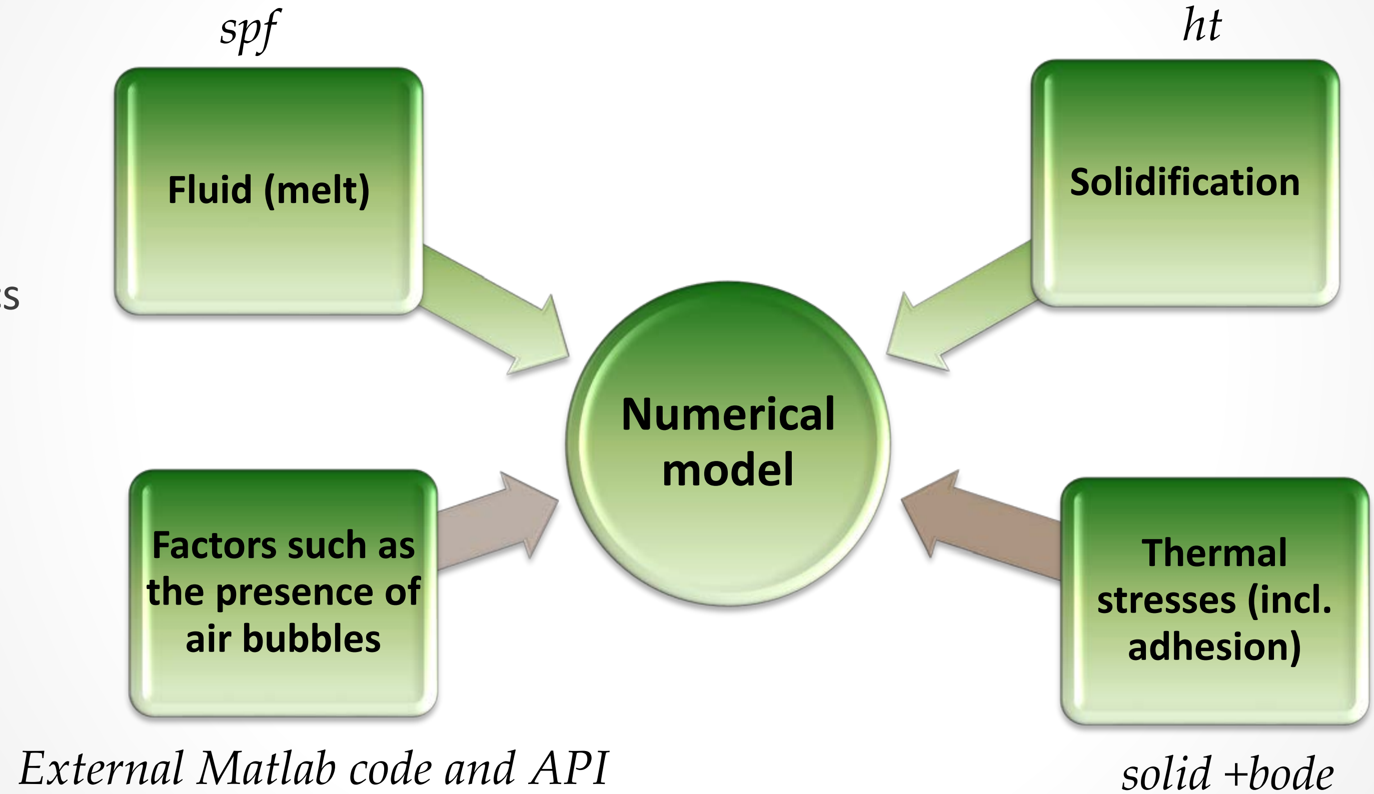
Develop a <u>numerical model to optimize cooling process parameters for melt cast explosives charges</u>.

- Use a multiphysics approach (Comsol Multiphysics®) to simulate phase change and cooling.
- Study the effect of thermal stresses on the casting of explosive melts.
- Investigate the lasting effect of factors such as the presence of air bubbles entrapped during the casting process.

Required model inputs:

Material properties (explosive, mold, funnel etc.)	**Cooling conditions**
Density	Water bath temperature
Thermal conductivity	Ambient air temperature
Specific heat	Loading temperature
Viscosity	Projectile and funnel temperature
Latent heat	Immersion depth of projectile
Solid to slurry temperature (melting point)	Probe heating, if any
Thermal expansion coefficient	Heaters temperature, if any
Poisson’s ratio	
Young’s modulus	

Multiphysics approach:



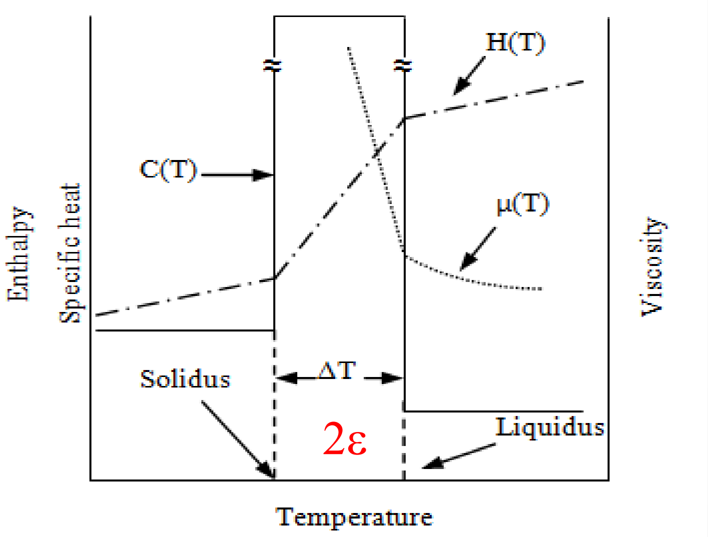
- Use of numerical modeling tools for casting applications ≈ 30 years old (Bellet & Thomas, 2007)
- Modeling of explosive casting process is much younger:

  Sun et al, (2005), Coulouarn et al (2007, 2013)
- Characteristics spotted by authors:
  - High Prandtl number (long casting time compared to steel casting, for example).
  - Viscous dissipation remains negligible due to very small velocities (Sun, Annapragada, Garimella & Singh, 2007)
  - Few studies for the analysis of stress development and defect formation resulting from phase change

$$\mathrm{Pr} = \frac{\text{momentum diffusivity}}{\text{thermal diffusivity}} = \frac{\mu c_p}{k}$$

- Solidification process: Very difficult to distinguish which portion of the liquid has been solidified at a given time.
  - Hence, a progressive approach must be devised in terms of a "fraction" of solid increasing in time (or fraction of liquid decreasing with time).
  - The popular enthalpy method:

Voller, V., & Prakash, C. (1987).	**(Marin, 2006)**	**(Sun *et al.*, 2007)**
Enthalpy method	Modified enthalpy method based on temperature	Enthalpy method



(Reddy & Gartling, 2000)

Solidification

- Progressive solidification process.

1. Heat equation with a *modified Cp* to include latent heat.

$$c_p^*(T) = c_p(T) + L\delta_{2\varepsilon}(T - T_m)$$

$$\rho c_p^* \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = \nabla \cdot (k \nabla T) + Q$$

2. Use of a solid fraction : F_s
   - Tm : "Average" melting temperature
   - ε : half-transition width (zero if pure material)

Temperature dependence : $\frac{df_l(T)}{dT}$

$$F_s(T) = \begin{cases} 1 & T < T_m - \varepsilon \\ \dfrac{T_m + \varepsilon - T}{2\varepsilon} & T_m - \varepsilon \le T < T_m + \varepsilon \\ 0 & T \ge T_m + \varepsilon \end{cases}$$

3. Jump conditions at the interface

$$k_s \left.\frac{\partial T}{\partial \mathbf{n}}\right|_X - k_l \left.\frac{\partial T}{\partial \mathbf{n}}\right|_X = \rho L \frac{\partial X}{\partial t} = \rho L \mathbf{u}^*$$

Heat and flow coupling

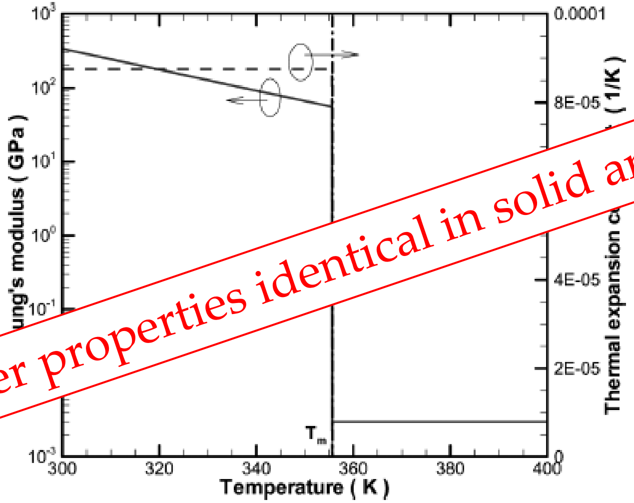
Flow:

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \mu\nabla^2\mathbf{v} + \rho\mathbf{g} + \frac{(1-f_l)^2}{f_l^{\,3}+q}C\mathbf{v}$$

If the temperature is below the solidus, the solidification term (in red) severely damps the acceleration resulting from the momentum equation and thereby imitates solid behaviour. In our simulations, we use $C \approx 10^5$ and $q = 0.001$

- Thermal stresses:
  - Highly non-linear problem in the field of continuum mechanics.
  - Melt is often modeled as a single material with :

$$E = E(T)$$



All other properties identical in solid and liquid phases

$$\alpha = \alpha(T)$$

Temperature dependent Young's modulus and thermal expansion coefficient (Sun et al., 2007)

Air bubbles – multiphase flow

- Use of a phase field method to track the liquid-air interface through a scalar function ϕ.

$$V_{f1} = \frac{1-\phi}{2} \qquad V_{f2} = \frac{1+\phi}{2} \qquad \phi \in [-1,1]$$

$$\rho = \rho_1 + (\rho_2 - \rho_1) V_{f2}$$

- An advection equation for ϕ adds to the Navier-Stokes equations:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \left(M \nabla \psi \right)$$

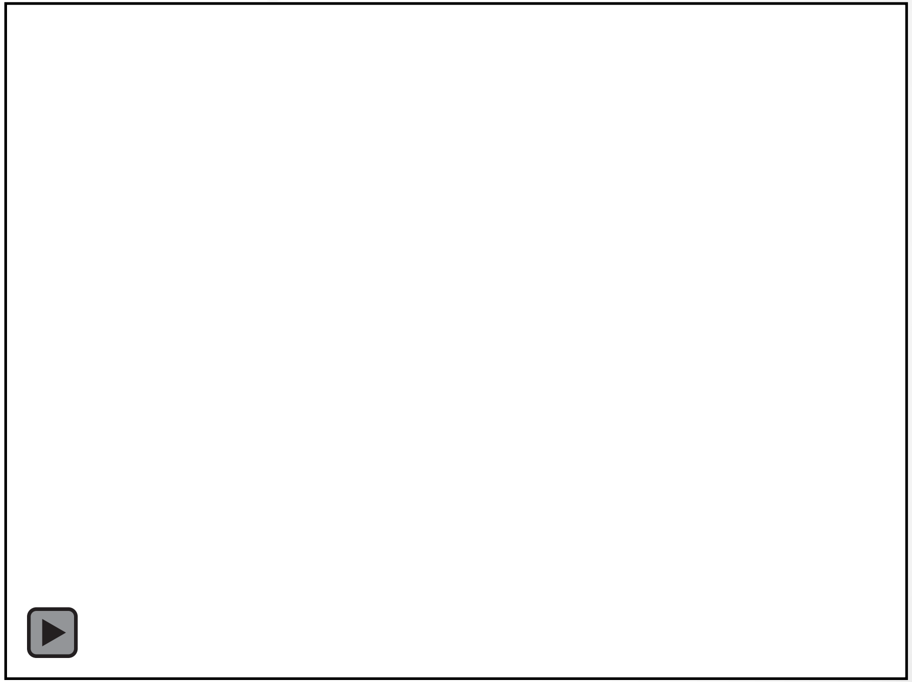
M : mobility factor

ψ : chemical potential

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \boxed{\mathbf{F}_g + \mathbf{F}_{ST} + \mathbf{F}_s}$$

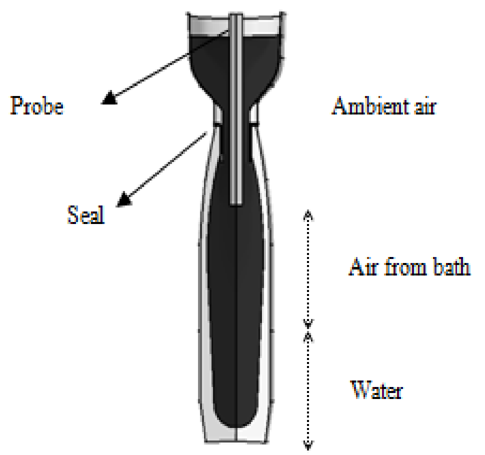
5.2 Air bubbles – multiphase flow

Matlab script to generate and position bubbles randomly throughout domain: *generate a geometry file that can be imported in Comsol*



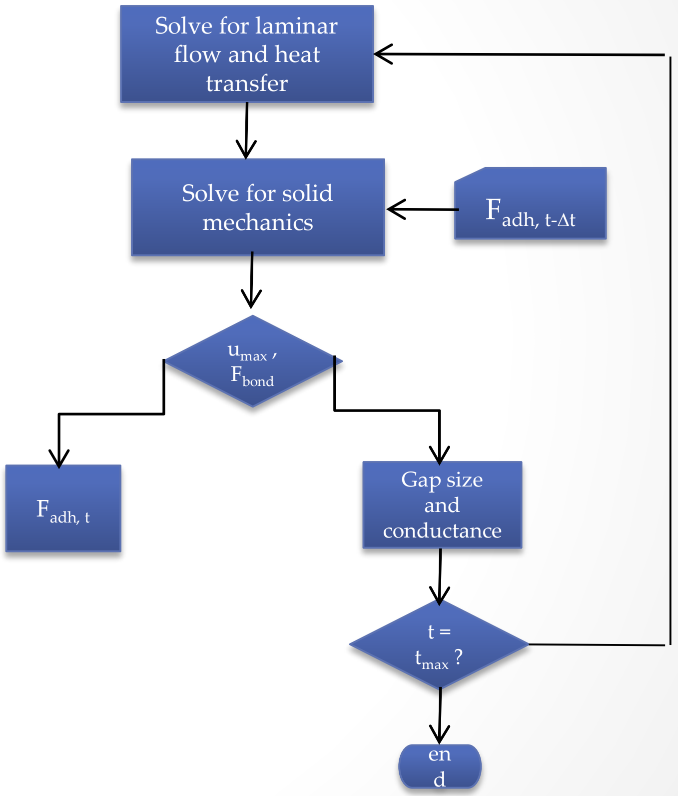
The cooling of the solid – Thermal stress and relaxation

- During cooling, both the mould and the explosive will **contract** and the latter **may or may not detach** from the surface of the mould.
- Knowledge of the **adhesive forces and the surface tension** between the explosive and the mould is critical in predicting the resulting behaviour.
- Strong adhesion may result in cracking and the presence of air bubbles may worsen the phenomenon.
- **It is useful to optimize the cooling process for optimal stress relaxation.**



Coupling methodology:

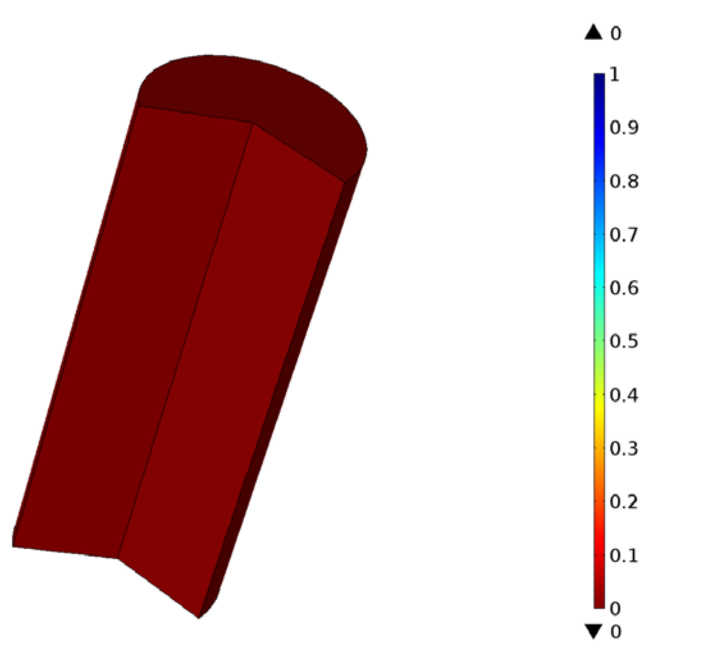
at a given time *t*



Solidification: cylinder

Evolution of the solid front (only explosive domain shown, mold walls omitted)

- solid = 1 and liquid = 0
- cooling conditions: water bath (40 °C); top exposed to ambient air (25 °C)
- solidification front rising and from the sides: main mode is upward solidification.



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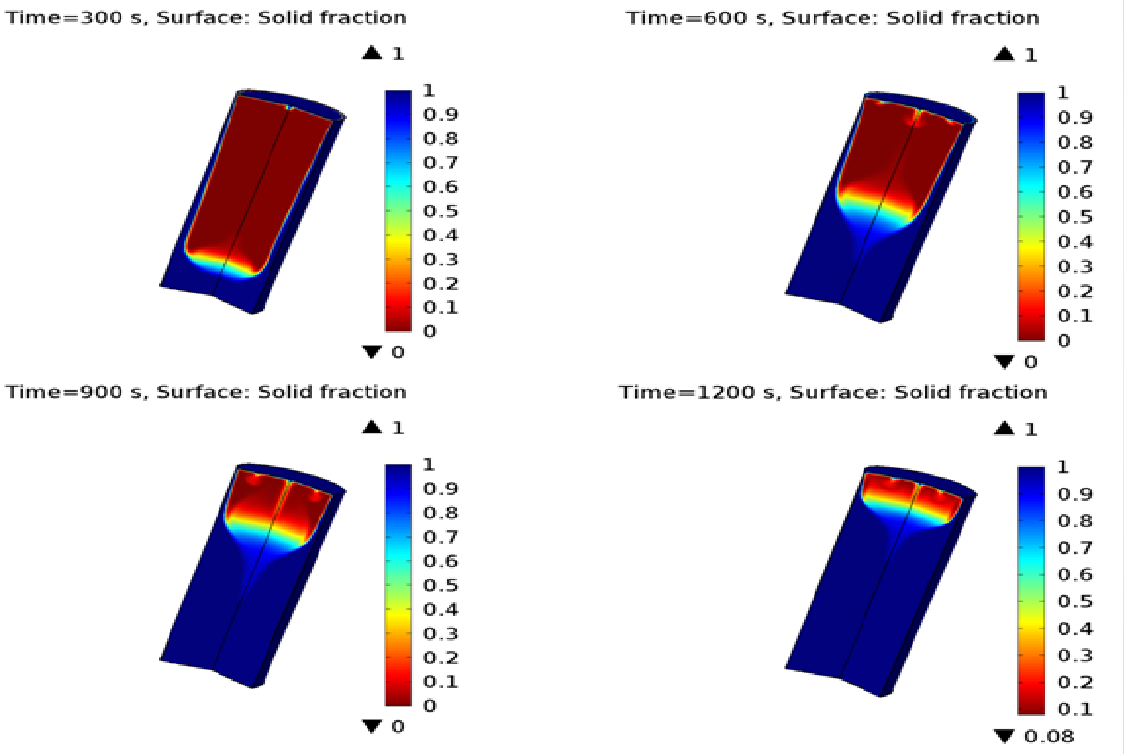

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- solidification front rising and from the sides: main mode is upward solidification.
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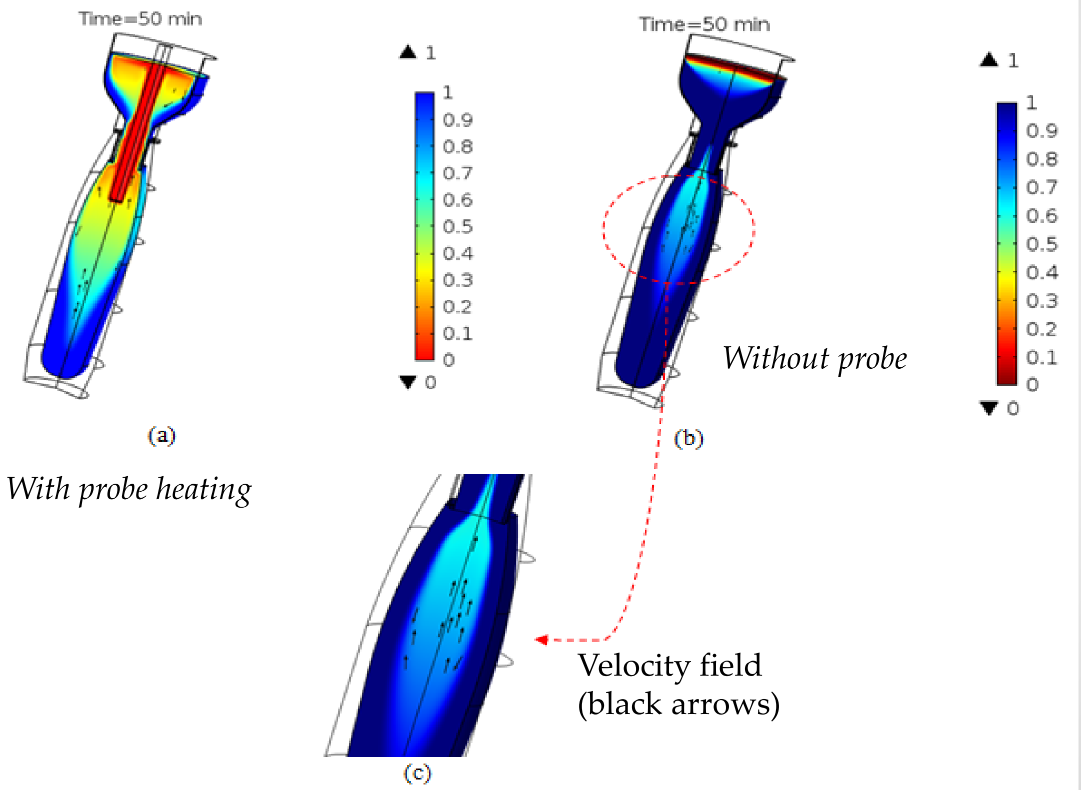
Comparison of temperature profiles between numerical and experimental results

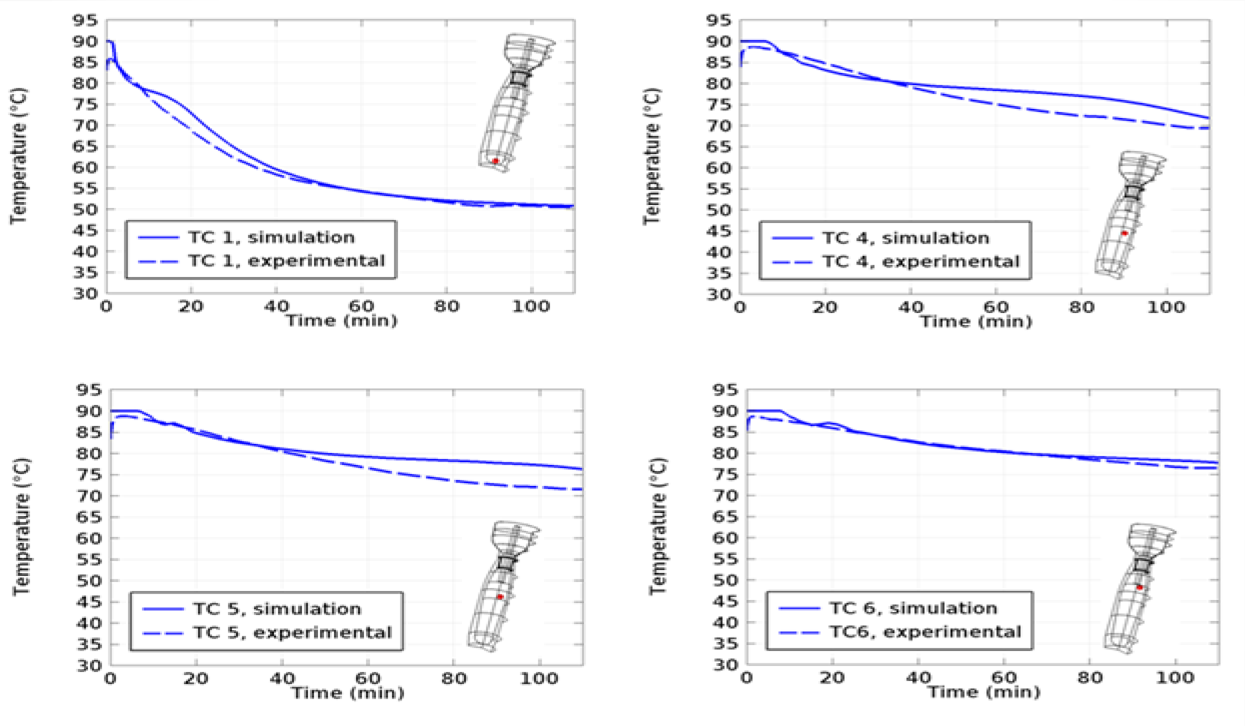
Importance of probe heating :

- Under same conditions for (a) and (b)
- Long convection cell along axis breaks up in the case of (b) ,leaving behind a melt pocket, which is a potential site for void formation under shrinkage.
- Zoomed region (c) shows convection pattern in melt pocket (black arrows).

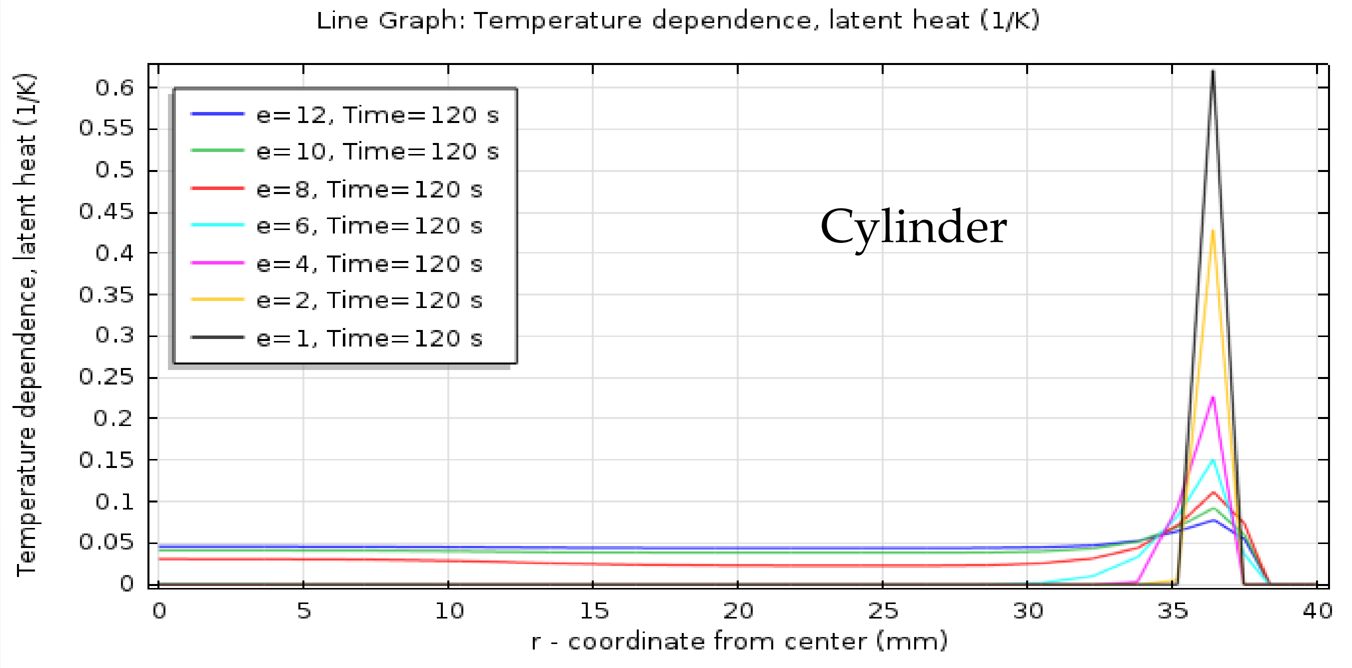
Solidification level (1 completely solid) at 50 min

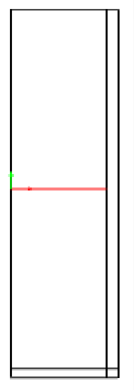


Comparison with experimental results:



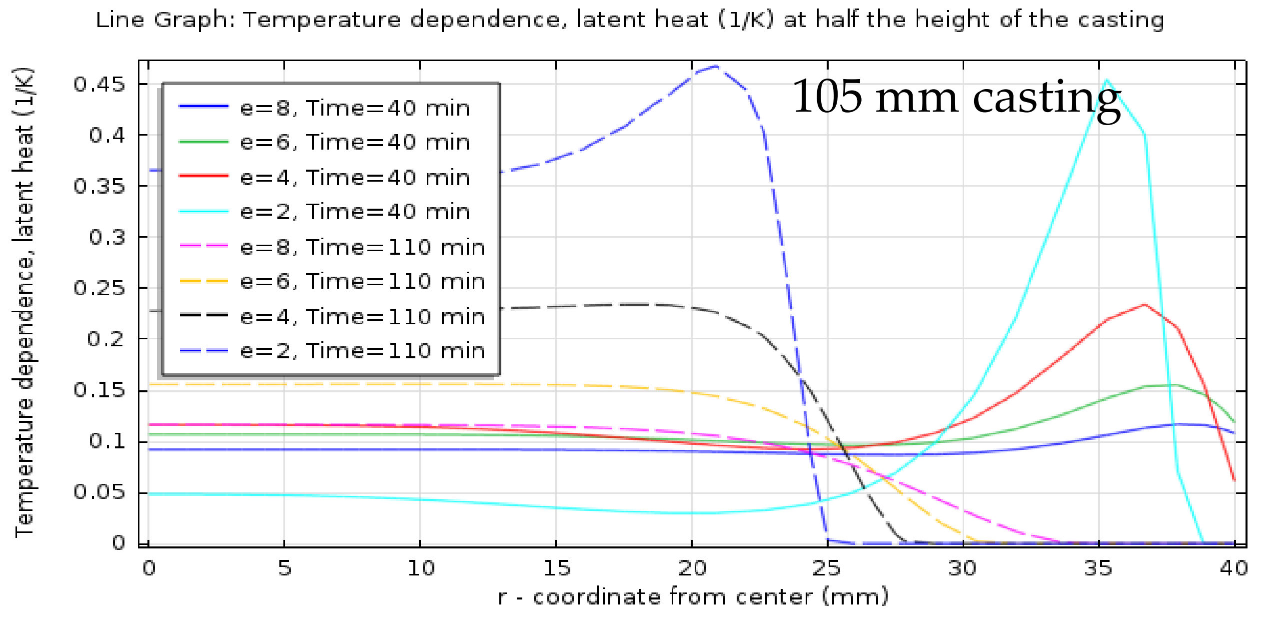
- Cooling conditions : water bath (50 °C), probe heating (95 °C), ambient air (18 °C)

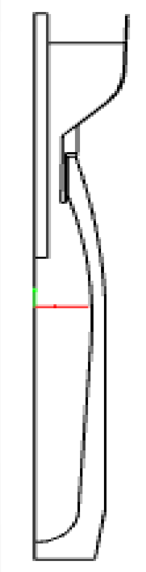




The smaller the half-interval ε , the steeper is the transition due to latent heat .

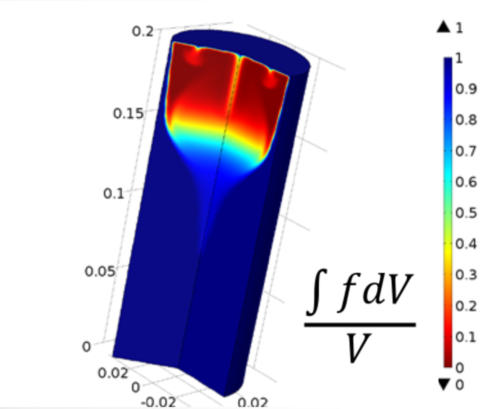
Importance of half-temperature interval ε :



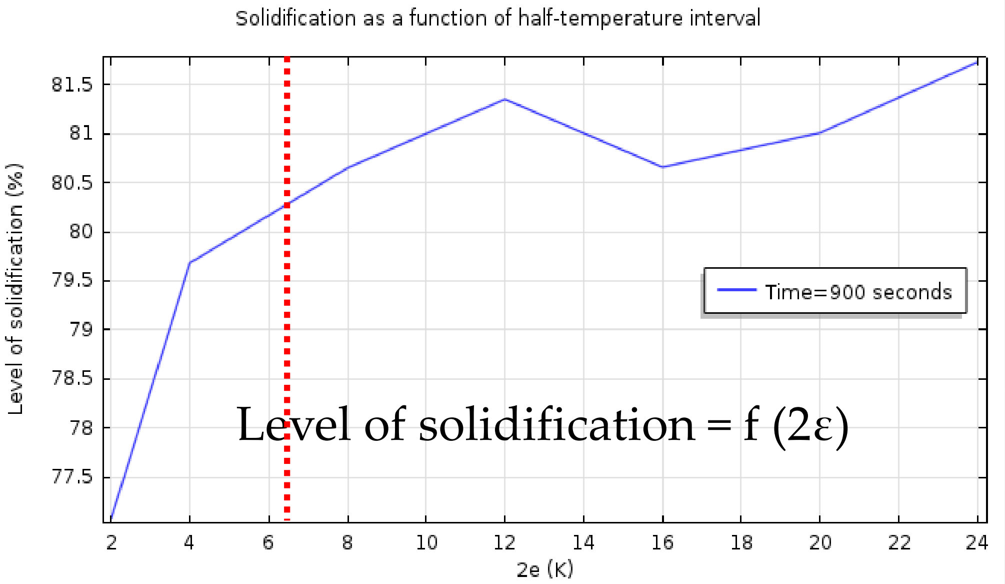


Interval length gives an idea of the size of the solidification front.

Importance of half-temperature interval ε :



$$\frac{\int f\,dV}{V}$$



There is an advantage in ramping down ε to the actual value (if known). However, in doing so, the mesh resolution must be increased as steeper gradients are encountered in an already very non-linear problem. Hence, a compromise has to be made between the right temperature interval for the mushy zone and the mesh resolution.

Difficulties encountered in heat transfer with phase change modeling:

- Extra care is needed in smoothing functions when using temperature dependent properties such as density , Cp and k.

- This is often insufficient and it is best practice to use a single value for the solid and a single one for the liquid, wherever possible and making sure there is minimal impact on the physics of the process (e.g. the thermal conductivity in the case of composition B explosives)

- It is essential to properly characterize or at least have a good idea of the quality of heat transfer (convective heat transfer coefficients).

Solver configurations: - solidification process is a highly non-linear problem, especially when thermal stresses are integrated to the model:

- Parametric sweeping (e.g. on temperature half-interval or mushy zone constant C) can help to approach the right solution.

- Specify lower relative/absolute error tolerances to ensure each intermediate solution converges enough.

- Adaptive meshing can also be an option to efficiently track the solidification front.

- In transient simulations, small time steps are often required initially to capture all the different boundary conditions involved. In some cases, the boundary conditions are themselves time-dependent (e.g. varying water bath temperature) .

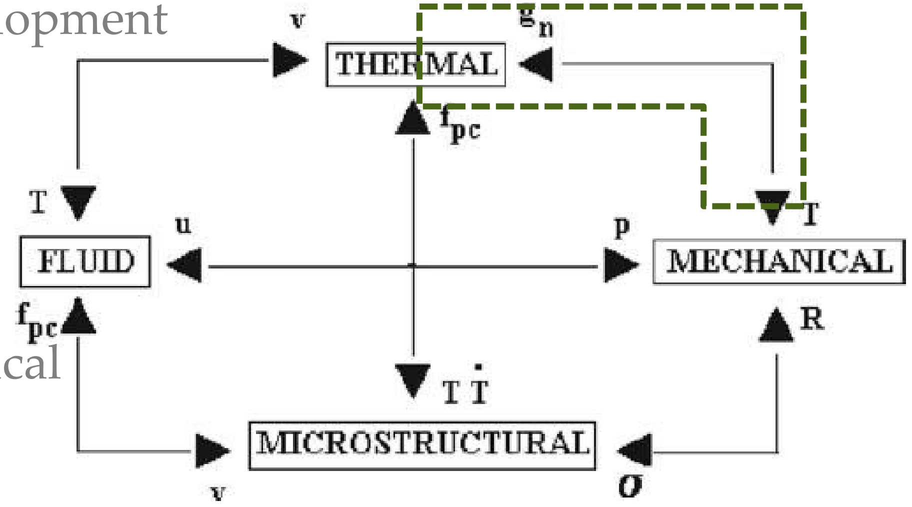
- The purpose of this work is to build up a comprehensive numerical model to optimize melt-casting of an explosive charge.
- A simulation for the cooling process and the phase change has been coupled to a structural analysis of the part.
- Verified & validated approach (via a benchmark problem and experimental data).

Thank you !

Example: A multiphysics approach = **Interdependent fields**

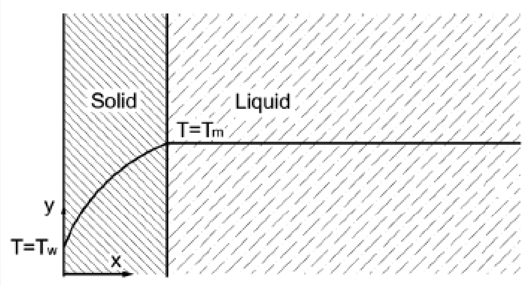
Thermal stress development in solidified shell

Thermo-mechanical problem (TM)

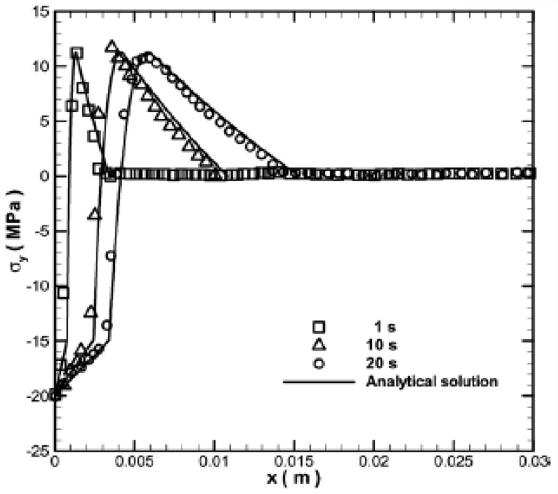


Interdependent fields for the analysis of solidification problems (Cruchaga et al., 2004)

- Verification problem: Elasto-plastic thermal stresses in an unconstrained solidifying body (Weiner & Boley, 1963)
  - o Benchmark problem to validate coupled model
  - o Based on Neumann problem for solidification

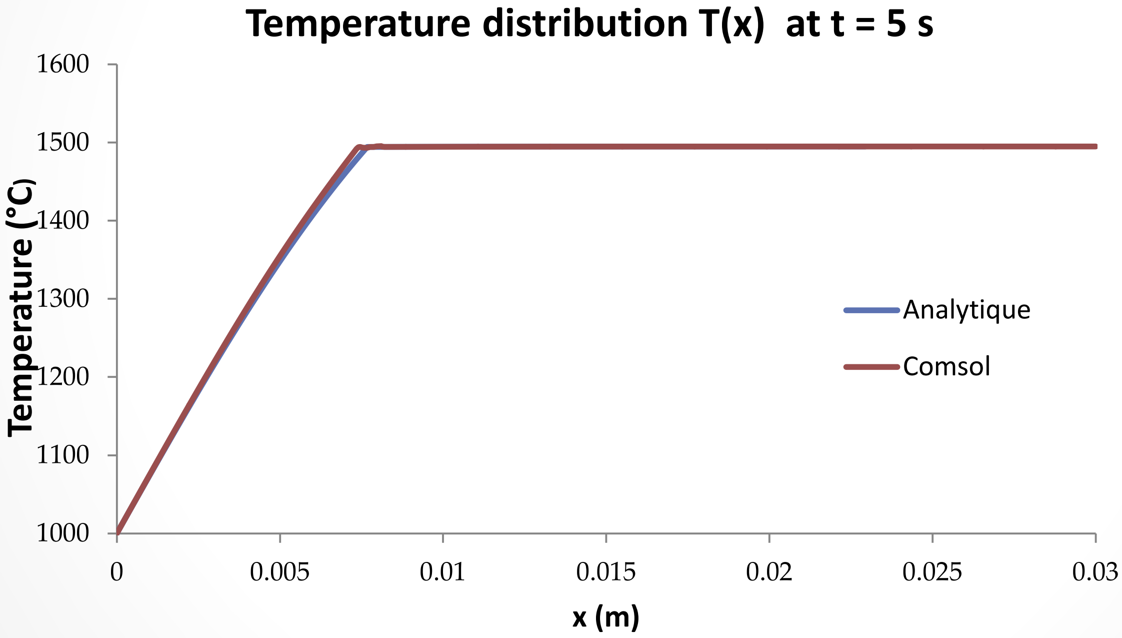


(Sun et al., 2007)



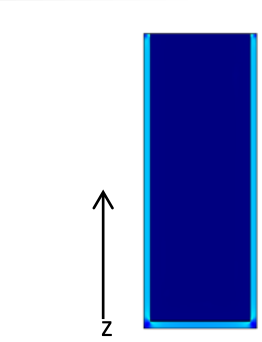
y- direction principal stresses (Sun et al., 2007)

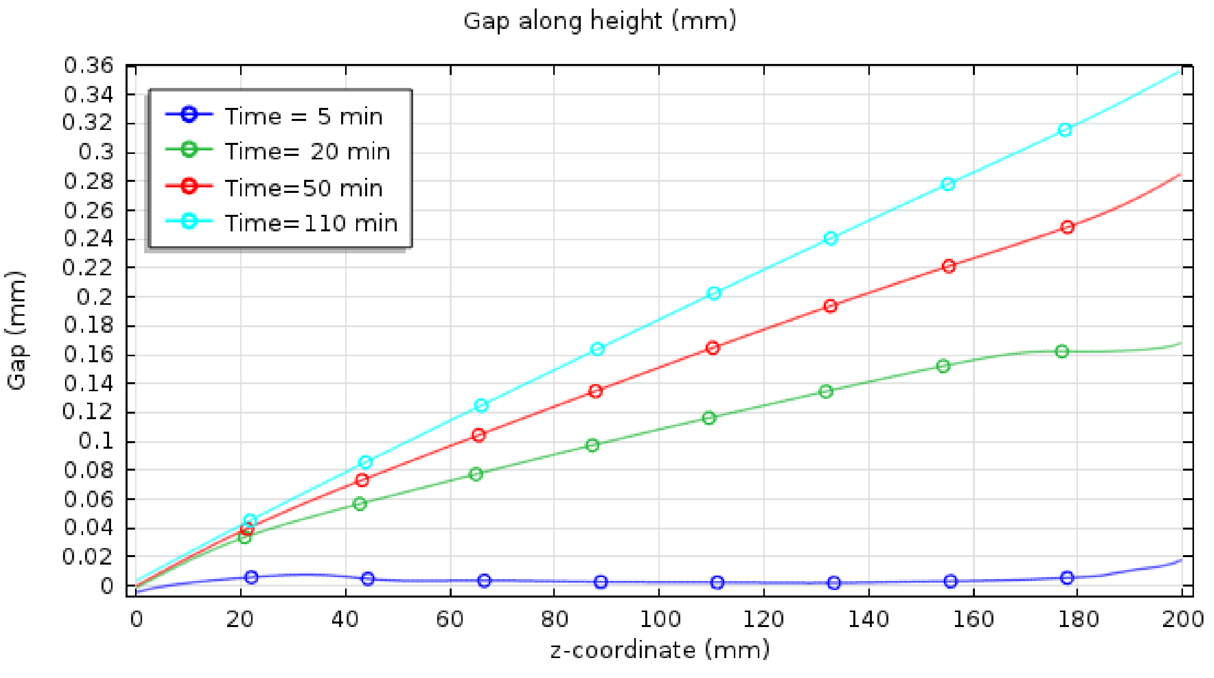
- Verification problem: Weiner & Boley Solution



Adhesion to the mold walls

- **Gap formation**





5.4 Adhesion to the mold walls

- **Gap formation**