Constitutive Modeling and Numerical Simulation of Casting Materials

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Abstract. The need of increasing productivity, quality and control of casting process requires the understanding of the effects of the process variables in the casting model. This is the reason why in the program VULCAN we tried to reproduce via numerical simulations the complete casting process considering filling, solidification and cooling phases. To do that, it was necessary to provide a mathematical model that accounts for both thermal and mechanical constitutive and boundary assumptions. Moreover an accurate definition of the interfacial heat transfer between the solidifying casting and the mould was essential in producing a reliable casting model. In fact, either solidification or temperature evolution strongly depend on the heat exchange at the contact interface. This exchange is affected by the insulating effect of the air-gap due to the thermal shrinkage of the casting part during solidification and cooling phases. The aim of this work is to show the advances in the simulation of casting processes providing the detailed formulation of the constitutive equations and evolution laws assumed for the casting material taking into account the transformations in the material behavior during the solidification according to the phase changes.
1 Introduction

The solution of coupled problems considered consists of an up-to-date finite element numerical model for fully coupled thermomechanical systems, focusing in the simulation of solidification processes of industrial metal parts. The formulation of the governing equations is consistently derived within a thermodynamic context. The proposed constitutive model is defined by a *thermo-viscoplastic* free energy function which includes contribution for *phase change*. A continuous transition between the initial fluid-like and the final solid-like behavior of the part is modelled by considering an improved J2-thermo-viscoplastic model. Thus, an elasto-viscoplastic response suitable for solid-like behavior degenerates into a purely viscous model according to the solid fraction function capturing the liquid-like behavior. Either nonlinear kinematic and isotropic hardening due to plastic deformation or thermal softening of the yield stress due to the temperature evolution is assumed. Phase change contribution is taken into account assuming both latent heat release and shrinkage effects during phase change. Fractional step method arising from an operator split of the governing differential equations is considered. Within the time discrete setting, the additive operator splits lead to a *product formula algorithm* and to a *staggered solution scheme* of the coupled problem.

2 Local governing equations

The local system of partial differential equations governing the coupled thermo-mechanical problem is defined by the momentum and energy balance equations, restricted by the inequalities arising from the second law of thermodynamics. This system is supplemented by suitable constitutive equations and prescribed boundary and initial conditions.

2.1 General form of the local balance laws

Let \( \Omega \in \mathbb{R}^{\text{dim}} \) be the set with smooth boundary \( \partial \Omega \) of a continuum body \( \beta \) in the space dimension \( \mathbb{R}^{\text{dim}} \). Let \([0,T]\) be the time interval of interest.

The local form of the *balance of momentum equation* also known as *Cauchy’s equation of motion* is given by

\[
\nabla \cdot \sigma + b = \rho_o \frac{dv}{dt}
\]

(1)

where \( \sigma \) is the Cauchy stress tensor, \( \nabla \cdot (\mathbf{v}) \) is the reference divergence operator, \( b \) is the vector of forces per unit of volume, \( \rho_o \) is the density in the reference configuration and \( \mathbf{v} \) is the velocity field.

The *balance of energy* equation can be written as

\[
\dot{E} = \sigma : \dot{\varepsilon} - \nabla \cdot \mathbf{Q} + R
\]

(2)

so that the increase of the internal energy \( \dot{E} \) per unit of volume consists of three parts: the stress power \( \sigma : \dot{\varepsilon} \) which represents the mechanical work done by the external forces not converted into kinetic energy, the heat supplied by the internal sources per unit of volume \( R \), and the term
which is the heat provided by the flow of thermal energy through the boundary into the system. The balance of energy equation is the local form for the First law of Thermodynamics. The Second law of Thermodynamics limits the direction of the energy transformations and it postulates that there exists a state function called entropy $S$ so that

$$D = \Theta \dot{S} - R + \Theta \cdot \nabla \cdot \left( \frac{Q}{\Theta} \right) \geq 0$$

(3)

where $D \geq 0$ is a thermomechanical variable usually referred as thermomechanical dissipation. A stronger format for the previous equation (3) is given by the following relations

$$D_{int} = \Theta \dot{S} - R + \nabla \cdot Q \geq 0$$

(4)

$$D_{cond} = -\frac{Q \nabla \Theta}{\Theta} \geq 0$$

(5)

where $D_{int}$ and $D_{cond}$ are the internal dissipation and the dissipation by conduction, respectively. Equation (4) is known in the literature as the Clausius-Plank equation. Taking into account the balance of energy equation (2) the following format for the Clausius-Plank equation is also available

$$D_{int} = \Theta \dot{S} - \dot{E} + \sigma : \dot{\varepsilon} \geq 0$$

(6)

Thus, the first order system of local equations that govern the coupled thermo-mechanical problem is the following

$$\dot{\mathbf{u}} = \mathbf{v}$$

(7)

$$\rho_b \dot{\mathbf{v}} = \nabla \cdot \sigma + \mathbf{b}$$

(8)

$$\Theta \dot{S} = R - \nabla \cdot Q + D_{int}$$

(9)

restricted by the inequalities arising from the second law of thermodynamics

$$D = D_{int} + D_{cond} \geq 0$$

(10)

$$D_{int} = \Theta \dot{S} - \dot{E} + \sigma : \dot{\varepsilon} \geq 0$$

(11)

$$D_{cond} = -\frac{Q \nabla \Theta}{\Theta} \geq 0$$

(12)
2.2 Additive decomposition

Let’s assume an *additive decomposition* of the total strain tensor $\varepsilon$ into its *elastic* and *inelastic* parts $\varepsilon^E$ and $\varepsilon^I$, respectively, that is

$$\varepsilon = \varepsilon^E + \varepsilon^I$$

(13)

where the elastic strain tensor $\varepsilon^E$ is given by the sum of the effective elastic deformation plus the thermal deformation, $\varepsilon^e$ and $\varepsilon^\theta$, respectively, so that

$$\varepsilon^E = \varepsilon^e + \varepsilon^\theta$$

(14)

while the inelastic strain tensor takes care of viscoplastic effects

$$\varepsilon^I = \varepsilon^{vp}$$

(15)

Another hypothesis is the split of total entropy $S$ into its *elastic* and *inelastic* part, $S^E$ and $S^I$, respectively, as

$$S = S^E + S^I$$

(16)

It is now possible to write in a new format the energy equation (4) using the elastic entropy $S^E$ as the state variable

$$\Theta \dot{S}^E = R - \nabla \cdot Q + D_{\text{mech}}$$

(17)

where the decomposition of the internal dissipation $D_{\text{int}}$ into *mechanical* and *thermal* part, $D_{\text{mech}}$ and $D_{\text{ther}}$, respectively, is assumed

$$D_{\text{int}} = D_{\text{mech}} + D_{\text{ther}} \geq 0$$

(18)

so that the thermal dissipation results in

$$D_{\text{ther}} = \Theta \dot{S}^I \geq 0$$

(19)

Taking care of previous assumptions, the first order system of local equations that governs the coupled thermo-mechanical problem is the following [6], [1], [2]

$$\dot{\mathbf{u}} = \mathbf{v}$$

(20)

$$\rho_o \dot{\mathbf{v}} = \nabla \cdot \mathbf{\sigma} + \mathbf{b}$$

(21)

$$\Theta \dot{S}^E = R - \nabla \cdot Q + D_{\text{mech}}$$

(22)

restricted by the following inequalities
\[ D = D_{\text{mech}} + D_{\text{ther}} + D_{\text{cond}} \geq 0 \] (23)

\[ D_{\text{mech}} = \Theta \dot{S}^E - \dot{E} + \sigma : \dot{\varepsilon} \geq 0 \] (24)
\[ D_{\text{ther}} = \Theta \dot{S}^f \] (25)
\[ D_{\text{cond}} = -\frac{Q \nabla \Theta}{\Theta} \geq 0 \] (26)

together with the boundary conditions

\[ \mathbf{u} = \mathbf{u}_0 \quad \text{on} \quad \partial \Omega_u \times [0, T] \]
\[ \sigma \cdot \mathbf{n} = \mathbf{t} \quad \text{on} \quad \partial \Omega_t \times [0, T] \]
\[ \Theta = \Theta_0 \quad \text{on} \quad \partial \Omega_\Theta \times [0, T] \]
\[ \mathbf{Q} \cdot \mathbf{n} = \mathbf{q}_n \quad \text{on} \quad \partial \Omega_q \times [0, T] \] (27)

and the initial conditions

\[ \mathbf{u} = \mathbf{u}_o \quad \text{in} \quad \Omega \times [0] \]
\[ \mathbf{v} = \mathbf{v}_o \quad \text{in} \quad \Omega \times [0] \]
\[ \Theta = \Theta_o \quad \text{in} \quad \Omega \times [0] \] (28)

### 3 Constitutive equations

Let \( \Psi (\varepsilon^E, \alpha^I, \Theta) \) be the Helmholtz free energy function (per unit reference volume) obtained from the internal energy \( E (S^E, \varepsilon^E, \alpha^I) \) by the Legendre transform as

\[ \Psi = \Theta S^E \] (29)

where \( \alpha^I \) is a set of generic internal variable that defines the material behavior. If we compute the rate of the free energy function and we make use of equation (24) it is possible to write

\[ \dot{\Psi} = \sigma : \dot{\varepsilon} - \dot{\Theta} S^E - D_{\text{mech}} \] (30)

If we differentiate the free energy function with respect to the state variables we obtain

\[ \dot{\Psi} = \frac{\partial \Psi}{\partial \varepsilon^E} : \dot{\varepsilon}^E + \frac{\partial \Psi}{\partial \alpha^I} : \dot{\alpha}^I + \frac{\partial \Psi}{\partial \Theta} \dot{\Theta} \]

\[ = \frac{\partial \Psi}{\partial \varepsilon^E} : \dot{\varepsilon}^E - \frac{\partial \Psi}{\partial \varepsilon^E} : \varepsilon^I + \frac{\partial \Psi}{\partial \alpha^I} : \dot{\alpha}^I + \frac{\partial \Psi}{\partial \Theta} \dot{\Theta} \] (31)

From equations (30) and (31) it is possible to obtain the following inequality

\[ D_{\text{mech}} = \left( \sigma \frac{\partial \Psi}{\partial \varepsilon^E} \right) : \dot{\varepsilon}^E - \left( S^E + \frac{\partial \Psi}{\partial \Theta} \right) \dot{\Theta} + \frac{\partial \Psi}{\partial \varepsilon^E} : \dot{\varepsilon}^I - \frac{\partial \Psi}{\partial \alpha^I} : \dot{\alpha}^I \geq 0 \] (32)

Applying Coleman’s method, we obtain the definition of the constitutive equations as
\begin{align}
\sigma &= \frac{\partial \Psi (\varepsilon^E, \alpha^I, \Theta)}{\partial \varepsilon^E} \\
S^E &= -\frac{\partial \Psi (\varepsilon^E, \alpha^I, \Theta)}{\partial \Theta}
\end{align}

(33)

(34)

where the internal dissipation is given by

\[ D_{\text{mech}} = \sigma : \dot{\varepsilon}^I + \beta^I : \dot{\alpha}^I \geq 0 \]

(35)

being for definition

\[ \beta^I = -\frac{\partial \Psi (\varepsilon^E, \alpha^I, \Theta)}{\partial \alpha^I} \]

(36)

Equation (35) is known in the literature as the reduced equation of dissipation.

### 3.1 Definition of the free energy function

We have seen how it is possible to formulate and obtain the constitutive equation that govern the thermo-mechanical problem starting from the definition of the potential \( \Psi (\varepsilon^E, \Theta, \alpha^I) \). A possible choice of the set of internal variables to particularize the free energy function to the case of thermo-viscoplastic behavior is given by \( \alpha^I = [\xi, \zeta] \), that is the isotropic and kinematic hardening variables, respectively. Thus, a possible format of the free energy function \( \Psi = \Psi (\varepsilon^E, \Theta, \zeta, \xi) \) is given as the sum of following contributions

\[ \Psi = \Psi (\varepsilon^E, \Theta, \zeta, \xi) = W (\varepsilon^E) + T (\Theta) + M (\varepsilon^E, \Theta) + K (\zeta, \xi) \]

(37)

where \( W (\varepsilon^E) \), \( M (\varepsilon^E, \Theta) \), \( T (\Theta) \) and \( K (\zeta, \xi) \) are the elastic stored energy, the coupling potential, the thermal potential including phase change contribution and the plastic hardening potential, respectively. The expressions chosen here for these terms are the following

\[ W (\varepsilon^E) = \frac{1}{2} k \operatorname{tr}^2 (\varepsilon^E) + G \operatorname{dev}^2 (\varepsilon^E) \]

(38)

\[ M (\varepsilon^E, \Theta) = -k' \varepsilon^E (\Theta) \varepsilon^E : 1 \]

(39)

\[ T (\Theta) = -\int_{\Theta_0}^{\Theta} d\tilde{\Theta} \int_{\Theta_0}^{\tilde{\Theta}} C_v \frac{dL}{d\Theta} d\tilde{\Theta} \]

(40)

\[ K (\zeta, \xi) = f_s [\sigma_\infty - \sigma_o] \left[ \xi - \frac{1 - \exp(-\delta \xi)}{\delta} \right] \\
+ \frac{1}{2} f_s H \xi^2 + \frac{1}{3} f_s K \| \xi \|^2 \]

(41)

where \( k \) is the bulk \( G \) the shear modulus, \( \alpha \) the thermal volumetric-change coefficient, \( \Theta_0 \) the initial temperature field, \( C_v \) the heat capacity at constant volume (not including the phase change contribution), \( \sigma_o \) the initial flow stress, \( \sigma_\infty \) the saturation hardening limit, \( H \) the linear isotropic...
hardening coefficient, \( K \) the linear kinematic hardening coefficient, and finally \( 1 = \delta_{ij} e_i \otimes e_j \) the rank-two symmetric unit tensor.

Note that thermal potential \( T(\Theta) \) incorporates the contribution coming from the phase change. This contribution concerns the latent heat released in the temperature range between the liquidus and solidus temperature that can be defined as the product between the total amount of latent heat \( L \) and a particular function \( f_S \) that controls the heat flow during the phase change process, so that

\[
L(\Theta) = L \cdot f_S(\Theta)
\]

\( L(\Theta) \) is the so called latent heat function. In case of a single phase change \( f_S(\Theta) \) represents the solid-fraction function so that the latent heat will be released (or absorbed) depending on the fraction of solid existing in the considered volume. This function takes the form

\[
f_S(\Theta) = \begin{cases} 
0 & \text{if } \Theta \geq \Theta_L \\
0 \leq f_S(\Theta) \leq 1 & \text{if } \Theta_S < \Theta < \Theta_L \\
1 & \text{if } \Theta \leq \Theta_S
\end{cases}
\]

where \( \Theta_L \) and \( \Theta_S \) are the liquid and solid temperature, respectively.

Term \( e^\Theta(\Theta) \) is the volumetric thermal deformation and it is defined as

\[
e^\Theta(\Theta) = \begin{cases} 
0 & \text{if } \Theta \geq \Theta_L \\
e^{pc}(\Theta) & \text{if } \Theta_S < \Theta < \Theta_L \\
\hat{c}^\Theta(\Theta) & \text{if } \Theta \leq \Theta_S
\end{cases}
\]

where \( e^{pc}(\Theta) \) is the thermal shrinkage during phase change while \( \hat{c}^\Theta(\Theta) \) is the thermal deformation during cooling phase, respectively defined as

\[
e^{pc}(\Theta) = \frac{\Delta V}{V_0} f_S(\Theta)
\]

\[
\hat{c}^\Theta(\Theta) = 3 \left[ \alpha(\Theta)(\Theta - \Theta_{ref}) - \alpha(\Theta_S)(\Theta_S - \Theta_{ref}) \right]
\]

being \( V_0 \) is the volume at the initial temperature and \( \Delta V \) the total volume change observed during the phase change; \( \Theta_{ref} \) is the environment temperature during the experimental evaluation of the dilatation coefficient \( \alpha(\Theta) \).

This given, the constitutive equations that govern the coupled problem result in

\[
\sigma = \frac{\partial \Psi}{\partial \varepsilon^E} = k \left[ \text{tr} \left( \varepsilon^E \right) - e^\Theta(\Theta) \right] 1 + 2G \text{ dev} \left( \varepsilon^E \right) \\
= k e^\varepsilon 1 + 2G \text{ dev} \left( \varepsilon^E \right)
\]

\[
S^E = -\frac{\partial \Psi}{\partial \Theta} = \int_{\Theta_o}^{\Theta} \frac{C_v}{\Theta} d\hat{\Theta} - M_\Theta + \int_{\Theta_o}^{\Theta} \frac{dL/\Theta}{\hat{\Theta}} d\hat{\Theta}
\]
It is possible to identify two different contributions to the elastic entropy function, respectively given by

\[ S^e = \int_{\Theta_0}^{\Theta} \frac{C_{ii}}{\Theta} d\Theta - M_{\Theta} \]  \hspace{1cm} (49)

\[ S^{pe} = \int_{\Theta_0}^{\Theta} \frac{dL_i}{\Theta} d\Theta \]  \hspace{1cm} (50)

Thus, the total entropy function is now given by the sum of following contributions

\[ S = S^E + S^I = S^e + S^{pe} + S^I \]  \hspace{1cm} (51)

The mechanical dissipation is obtained as

\[ D_{mech} = \sigma : \dot{\varepsilon}^{vp} + q\dot{\zeta} + q : \dot{\zeta} \geq 0 \]  \hspace{1cm} (52)

where the state variables \( q \) and \( q \) are defined as the derivatives of the free energy function with respect to \( \varepsilon \) and \( \zeta \), respectively, so that

\[ q = -\frac{\partial \Psi}{\partial \varepsilon} = -f_S \left[ \sigma_{\infty} - \sigma_0 \right] \left[ 1 - \exp \left( -\delta \varepsilon \right) \right] - f_S \ H \varepsilon \]  \hspace{1cm} (53)

\[ q = -\frac{\partial \Psi}{\partial \zeta} = -\frac{2}{3} f_S \ K \zeta \]  \hspace{1cm} (54)

Finally, let us introduce in this section the Fourier's law as the constitutive law that governs the heat flux, so that

\[ Q = -k(\Theta) \nabla \Theta \]  \hspace{1cm} (55)

where \( k(\Theta) = k(\Theta) \ 1 \) is the conductivity tensor.

### 4 Evolution laws

The basic idea is to try to formulate a model the closest as possible to the experimental observation. The main difficulty is the very different behavior of the liquid phase compared with the solid phase. The liquid phase is characterized by a purely viscous behavior so that both the elastic and the plastic deformation must be neglected. On the other hand, when the material is solid a standard elastic-viscoplastic behavior should be taken into account. Let us consider a visco-plastic potential \( \Phi (s, q, q, \Theta) \) to deal with von Mises yield criterion with an isotropic and kinematic hardening combined with a thermal softening effect, defined as

\[ \Phi (s, q, q, \Theta) = \|s - q\| - R(q, \Theta) \leq 0 \]  \hspace{1cm} (56)
where \( s = \text{dev}(\sigma) \) is the deviatoric part of the stress tensor and \( R(q, \Theta) \) is the radius of the yield surface given by

\[
R(q, \Theta) = f_s(\Theta) \sqrt{\frac{2}{3} [\sigma_0(\Theta) - q]} \tag{57}
\]

According to the principle of maximum plastic dissipation, the evolution laws for the plastic variables can be obtained as

\[
\dot{\varepsilon}^{vp} = \gamma \frac{\partial \Phi(s, q, q, \Theta)}{\partial s} = \gamma \mathbf{n} \tag{58}
\]

\[
\dot{\varepsilon} = \gamma \frac{\partial \Phi(s, q, q, \Theta)}{\partial q} = -\gamma \mathbf{n} \tag{59}
\]

\[
\dot{\varepsilon} = \gamma \frac{\partial \Phi(s, q, q, \Theta)}{\partial q} = \gamma \sqrt{\frac{2}{3}} \tag{60}
\]

where \( \mathbf{n} \) is the unit normal to the yield surface and \( \gamma \) is the viscoplastic parameter, respectively given by

\[
\mathbf{n} = \frac{s - q}{\|s - q\|} \tag{61}
\]

\[
\gamma = \frac{1}{\eta(\Theta)} \langle \Phi(s, q, q, \Theta) \rangle^n \tag{62}
\]

being \( \eta(\Theta) \) and \( n \) the visco-plastic parameters associated to the model.

Note that if \( \Theta \geq \Theta_L \) the viscoplastic potential \( \Phi(s, q, \Theta) \) degenerate in a purely-viscous potential

\[
\Phi(s, q, q) \rightarrow \Phi(s) = \|s\| \tag{63}
\]

The evolution of the plastic multiplier transforms into

\[
\gamma = \frac{1}{\eta(\Theta)} \langle \Phi(s) \rangle \rightarrow \gamma = \frac{1}{\eta(\Theta)} \|s\| \tag{64}
\]

Therefore, it is possible to obtain a purely viscous relation between the deviator of the stress tensor \( s \) and the rate of visco-plastic strain \( \dot{\varepsilon}^{vp} \), governed by the viscous parameter \( \eta \)

\[
s = \eta(\Theta) \dot{\varepsilon}^{vp} \tag{65}
\]

In this condition, if the value of the viscous parameter \( \eta \) is enough small compared with the shear modulus \( G \), then the total deformation will be essentially visco-plastic, to say irreversible very close to the experimental observation.
Finally, observe that the evolution law of the inelastic entropy variable $S^I$ can be obtained by analogy as
\[
\dot{S}^I = \gamma^{vp} \frac{\partial \Phi}{\partial \Theta} = -\gamma^{vp} \sqrt{\frac{2}{3} \frac{d \sigma_0 (\Theta)}{d \Theta}}
\]
and if we introduce this result into the expression of thermal dissipation (19) then
\[
D_{\text{ther}} = -\gamma^{vp} \sqrt{\frac{2}{3} \frac{d \sigma_0 (\Theta)}{d \Theta}} \Theta \geq 0
\] (66)
leading to the restriction
\[
\frac{d \sigma_0 (\Theta)}{d \Theta} \leq 0
\] (67)
that is, only thermal softening is allowed.

5 Equivalent forms of the energy equation

Starting from the entropy form of the balance of energy equation given by
\[
\Theta \dot{S} = R - \nabla \cdot Q + D_{\text{int}}
\] (68)
and taking into account the additive decomposition of the entropy function (51) it is also possible to consider the following equivalent system of equations
\[
\Theta \dot{S}^e = R - \nabla \cdot Q + D_{\text{mech}} - \dot{L}
\] (69)
\[
\Theta \dot{S}^{pe} = \dot{L}
\] (70)
\[
\Theta \dot{S}^I = D_{\text{ther}}
\] (71)
showing the local evolution of the different contributions of the entropy function. Applying the chain rule to the elastic entropy function then it results
\[
\Theta \dot{S}^e = C (\Theta) \dot{\Theta} + H^{ep}
\] (72)
thus, equation (69) can be written as
\[
C (\Theta) \dot{\Theta} = R - \nabla \cdot Q + D_{\text{mech}} - \dot{L} - H^{ep}
\] (73)
where the following notation has been introduced
\[
C (\Theta) = \Theta \frac{\partial S^e}{\partial \Theta} = C_v - \Theta M_{\Theta \Theta}
\] (74)
\[
H^{ep} = \Theta \left[ \frac{\partial S^e}{\partial \varepsilon^E} : \varepsilon^E + \frac{\partial S^e}{\partial \xi} \right] = -\Theta \left[ \frac{\partial \sigma}{\partial \Theta} : \varepsilon^E - \frac{\partial q}{\partial \Theta} \varepsilon \right]
\] (75)
being \( C(\Theta) \) the heat capacity (not including the phase change contribution) and \( H^{ep} \) the structural elasto-plastic heating [6]. Finally, equation (73) can also be written in enthalpy form as
\[
\dot{H} = R - \nabla \cdot \mathbf{Q} + D_{\text{mech}} - H^{ep}
\] (76)
where the rate of the enthalpy function \( H \) is defined as
\[
\dot{H} = \left[ C(\Theta) + \frac{dL(\Theta)}{d\Theta} \right] \dot{\Theta}
\]

6 Formulation of the Contact Problem

In this section the main focus is the formulation and treatment of the contact problem recovering the same general structure used to describe the constitutive framework for the bulk continua.

6.1 Local contact governing equations

Let us extend the balance equations coming from the first and second laws of thermodynamics, to account for the contributions at the contact interfaces.

First, let us consider the balance of energy equation. If we denote with \( \dot{E}^s \) the time derivative of the total internal energy given by
\[
\dot{E}^s = \int_{\Omega} \dot{E} \, dV + \int_{\Gamma_c} \dot{E}_c \, dS
\] (77)
being \( \dot{E} \) the stored energy per unit volume in the bulk medium (see eq. 2) and \( \dot{E}_c \) the stored energy per unit area on the contact interface \( \Gamma_c \) defined as
\[
\dot{E}_c = t_N \dot{g}_N + Q_c
\] (78)
where \( g_N \) and \( t_N \) are the normal gap and normal contact pressure, respectively, and \( Q_c \) is the heat flux per unit of contact surface \( \Gamma_c \) supplied at the interface, assumed positive if they are flowing out of the bodies into the interface region.

Let us now consider the second law of thermodynamics. Suppose also in this case that the total entropy of the system \( S^s \) can be given by
\[
\dot{S}^s = \int_{\Omega} \dot{S} \, dV + \int_{\Gamma_c} \dot{S}_c \, dS
\] (79)
being \( \dot{S} \) the entropy per unit volume in the bulk media (see eq. 3) and \( \dot{S}_c \) the entropy per unit area on the contact interface \( \Gamma_c \) satisfying the following equation
\[
\Theta_c \dot{S}_c = Q_c
\] (80)
where \( \Theta_c \) is the contact interface temperature. Introducing this result into equation (78), the energy equation at the contact interface can be rewritten as
\[
\Theta_c \dot{S}_c - \dot{E}_c + t_N \dot{g}_N = 0
\] (81)
7 Contact Constitutive Equations

In what follows the contact free energy function is introduced. The constitutive equations of both contact pressure as well as the heat flux at the contact interface are obtained.

7.1 Mechanical contact model

Starting from the definition of the internal energy as a function of

\[ E_c = E_c (g_N, S_c) \]  \hspace{1cm} (82)

it is possible to define a free energy function \( \Psi_c \) via Legendre transformation as

\[ \Psi_c = E_c - \Theta_c S_c = \Psi_c (g_N, \Theta_c) \]  \hspace{1cm} (83)

Following a standard argument in thermodynamics, one may time differentiate equation (83) to obtain

\[ \dot{\Psi}_c = \dot{E}_c - \Theta_c \dot{S}_c - \dot{\Theta}_c S_c 
\]
\[ = \frac{\partial \Psi_c}{\partial g_N} \dot{g}_N + \frac{\partial \Psi_c}{\partial \Theta_c} \dot{\Theta}_c \]  \hspace{1cm} (84)

Taking into account the energy equation at the contact interface (81) then

\[ \left( t_N - \frac{\partial \Psi_c}{\partial g_N} \right) \dot{g}_N - \left( S_c + \frac{\partial \Psi_c}{\partial \Theta_c} \right) \dot{\Theta}_c = 0 \]  \hspace{1cm} (86)

which must hold for any \( \dot{g}_N \) and \( \dot{\Theta}_c \). Applying Coleman’s method, it results

\[ t_N = \frac{\partial \Psi_c}{\partial g_N} \]  \hspace{1cm} (87)

\[ S_c = - \frac{\partial \Psi_c}{\partial \Theta_c} \]  \hspace{1cm} (88)

Let us now particularize the contact free energy function to obtain the standard restrictions at the contact interface, assuming the following terms [3]

\[ \Psi_c (g_N, \Theta_c) = W_c (g_N) + T_c (\Theta_c) \]  \hspace{1cm} (89)

being \( W_c (g_N) \) and \( T_c (\Theta_c) \) are the stored energy due to the bodies interaction at the contact interface and the thermo-contact potential, respectively given by
\[ W_c(g_N) = \frac{1}{2} \varepsilon_N \langle g_N \rangle^2 \quad (90) \]
\[ T_c(\Theta_c) = C_{co} [ (\Theta_c - \Theta_o) - \Theta_c \log (\Theta_c / \Theta_o)] \quad (91) \]

where \( \Theta_o \) is the initial temperature field, \( C_{co} \) is the heat capacity associated with the contact interface and \( \varepsilon_N \) is the normal penalty parameter that provides a \textit{penalty regularization} of the contact constrains [8].

From this definition the constitutive equations that completely specify the thermomechanical contact framework result in

\[ t_N = \varepsilon_N \langle g_N \rangle \quad (92) \]
\[ S_c = C_{co} \log (\Theta_c / \Theta_o) \quad (93) \]

Equation (92) defines the normal contact pressure as

\[ t_N = \left\{ \begin{array}{ll} 0 & \text{if} \quad g_N \leq 0 \\ \varepsilon_N \, g_N & \text{if} \quad g_N > 0 \end{array} \right. \quad (94) \]

which are the regularization of the contact constraints of impenetrability and non-adhesion, respectively given in Khun-Tucker form as

\[ t_N \geq 0 \quad (95) \]
\[ g_N \leq 0 \quad (96) \]
\[ g_N \, t_N = 0 \quad (97) \]

### 7.2 Thermal contact model

An accurate knowledge of the interfacial heat transfer coefficient between the a solidifying casting and a die is essential in producing a reliable solidification model. Hence, to complete the thermomechanical contact model, reliable heat conduction and heat convection laws must be considered.

#### 7.2.1 Heat conduction model

Heat conduction through the contact surface \( Q_{c,\text{cond}} \) has been assumed to be a function of coefficient \( h_{\text{cond}} \) depending on of the normal contact pressure \( t_N \), multiplied by the thermal gap \( g_\Theta \) between the contact surfaces of the form

\[ Q_{c,\text{cond}} = h_{\text{cond}} (t_N) \, g_\Theta \quad (98) \]
In this case we assume that no macroscopical air gap is formed due to the thermal shrinkage of the casting during cooling phase. The model assumes that a thermal resistances \( R_{cond} \) arise as a result of the air trapped between the mould and the casting surfaces due to the roughness values measured on those surfaces. In addition, it must be also considered the thermal resistance due to the mould coating, so that

\[
R_{cond} = 0.5 \frac{R_z}{k_a} + \frac{\delta_c}{k_c}
\]

where \( R_z = \sqrt{R_{z,cast}^2 + R_{z,coast}^2} \) is the mean peak-to-valley height of the rough surfaces, \( \delta_c \) is the effective thickness of the coating and \( k_a \) and \( k_c \) are the thermal conductivity of the gas trapped and the coating, respectively.

Moreover, it is also possible to assume that the microscopical interaction between the contact surfaces depends on the normal contact pressure so that the heat conduction coefficient \( h_{cond} \) could be defined using the following expression

\[
h_{cond}(t_N) = \frac{1}{R_{cond}} \left( \frac{t_N}{H_e} \right)^\epsilon
\]

where \( H_e \) is the Vickers hardness and \( \epsilon \) a constant exponent [10].

### 7.2.2 Heat convection model

Heat convection between the two bodies arises when they separate from each other due to the thermal shrinkage effect. Heat convection flux \( Q_{c,conv} \) has been assumed to be a function of coefficient \( h_{conv} \) depending on the mechanical gap \( g_N \) multiplied by the thermal gap \( g_\theta \) of the form

\[
Q_{c,conv}^{(i)} = h_{conv}(g_N) g_\theta
\]

where in this case the heat transfer coefficient \( h_{conv} \) is defined via the inverse of the thermal resistances of both the air gap and the coating

\[
h_{conv} = \frac{1}{k_a \max(0, R_a) + \frac{\delta_c}{k_c}}
\]

### 8 Weak Form of the Governing Equations

Let \( \Omega \) be integration domain with smooth boundaries \( \partial \Omega \). Let \( \delta \eta \) be the test function associated to the displacement field \( u \). The weak form of the balance of momentum equation (1) in the hypothesis of a quasi-static process results in

\[
\langle \delta \eta, \nabla \cdot \sigma \rangle + \langle \delta \eta, b \rangle = 0
\]

where \( b \) is the vector of forces per unit of volume.
Applying the divergence theorem to the first term in the above equation yields
\[
\langle \delta \eta, \nabla \cdot \sigma \rangle = -\langle \nabla \left( \delta \eta \right), \sigma \rangle + \langle \delta \eta, \bar{t} \rangle_{\partial \Omega} + \langle \delta g_N, t_N \rangle_{\Gamma_c} \tag{102}
\]
where \( \bar{t} = \sigma \cdot \mathbf{n} \) is the prescribed surface traction. Expression for \( \delta g_N \) can be found in [7] and therefore will not be given here. Substituting into (101) the result is the standard format of the weak form of the balance of momentum equation given by
\[
\langle \nabla^t (\delta \eta), \sigma \rangle = G \tag{103}
\]
where \( G \) is the mechanical work due to the internal forces and the prescribed surface tractions, as
\[
G = \langle \delta \eta, b \rangle + \langle \delta \eta, \bar{t} \rangle_{\partial \Omega}
\]
Let \( \delta \vartheta \) be the test function associated to the temperature field \( \Theta \). Let choose the balance of energy equation in entalpy form given by equation (76) then the weak form associated results in
\[
\langle \delta \vartheta, \dot{H} \rangle = \langle \delta \vartheta, R \rangle - \langle \delta \vartheta, \nabla \cdot Q \rangle + \langle \delta \vartheta, D_{\text{mech}} \rangle - \langle \delta \vartheta, H^{\text{op}} \rangle \tag{104}
\]
Integrating by part the conductivity term in the previous equation
\[
\langle \delta \vartheta, \nabla \cdot Q \rangle = \langle \nabla (\delta \vartheta), k \nabla \Theta \rangle + \langle \delta \vartheta, \bar{q} \rangle_{\partial \Omega} + \langle \delta \vartheta, Q_c \rangle_{\Gamma_c} \tag{105}
\]
where \( \bar{q} = Q \cdot \mathbf{n} \) is the flux normal to the boundaries. Substituting the result in (104) then the weak form of the energy equation is the following
\[
\langle \delta \vartheta, \dot{H} \rangle + \langle \nabla (\delta \vartheta), k \nabla \Theta \rangle = G^\vartheta \tag{106}
\]
where \( G^\vartheta \) is the thermal work due to the internal sources, the mechanical dissipation and the prescribed heat flux, given by
\[
G^\vartheta = \langle \delta \vartheta, R \rangle + \langle \delta \vartheta, D_{\text{mech}} \rangle - \langle \delta \vartheta, H^{\text{op}} \rangle - \langle \delta \vartheta, \bar{q} \rangle_{\partial \Omega} - \langle \delta \vartheta, Q_c \rangle_{\Gamma_c} \tag{107}
\]

9 Numerical Simulations

The formulation presented is illustrated here with a numerical simulation. The goal is to demonstrate the good accuracy properties of the proposed formulation in the framework of infinitesimal strain thermal-plasticity for an industrial solidification example.

The computations are performed with the finite element code VULCAN developed by the authors, project supported by the International Center for Numerical Method in Engineering (C.I.M.N.E.). Newton-Raphson method, combined with a line-search optimization procedure, is used to solve the nonlinear system of equations arising from the spatial and temporal discretization of the weak form of the governing equations. Convergence of the incremental iterative solution procedure was monitored by requiring a tolerance of 0.1% in the residual based error norm.
The analysis is concerned with the solidification process of an aluminium (AlSi7Mg) specimen in a steel (X40CrMoV5) mould. Geometrical and material data, as well as experimental results, were provided by TEXID. Fig. 1 shows a view of the finite element mesh used, consisting in 246,600 tetrahedral elements.

Aluminium material behavior has been modelled by the fully coupled thermo-viscoplastic model, while the steel mould behavior has been modelled by an easier thermo-elastic model. The values of the material properties used in the numerical analysis are confidential (TEXID material database). The initial temperature is $650 \, ^\circ C$ for the part and $250 \, ^\circ C$ for the mould. The heat transfer coefficient takes into account the air-gap considering the shrinkage of the coating during the solidification.

The temperature distribution during solidification is shown in Fig. 2. Fig. 3 and Fig. 4 show the temperature and von Mises deviatoric stress distribution on sections x-y, respectively. In these figures it is also possible to observe the mechanical gap between the part and the mould responsible of a non-uniform heat flux at the contact interface.

10 Conclusions

The developments presented in this paper demonstrate that the approach advocated can be the proper strategy in the context of thermo-mechanical phase-change analysis. All the formulation
presented has been implemented and tested in the context of the finite element method. The computations have been performed with the finite element code VULCAN developed by the authors, project supported by the International Center for Numerical Method in Engineering (C.I.M.N.E.).

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References

Figure 3: Solidification of a suspension component: temperature distribution section x-y.


Figure 4: Solidification of a suspension component: Von mises deviatoric stress distribution: section x-y.


