COUPLED THERMOMECHANICAL BEHAVIOUR FOR METAL CASTING FE ANALYSIS

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Abstract. The aim of this work is to show the necessity of a coupled thermo-mechanical analysis for the simulation of foundry processes. The solution of such a problem consists of an up-to-date finite element numerical model for fully coupled thermo-mechanical systems. The formulation of the governing equations is consistently derived within a thermodynamic context. The proposed constitutive model is defined by a thermo-visco-plastic free energy function. A continuous transition between the initial fluid-like and the final solid-like behaviour of the part is modelled by considering an improved J2-thermo-viscoplastic model. Thus, an elasto-visco-plastic response suitable for solid-like behaviour degenerates into a purely viscous model according to the solid fraction function capturing the liquid-like behaviour [1-5]. A stabilization technique based on the orthogonal sub-grid scale method is introduced as a convenient framework to deal with the complex behaviour of the casting metal during the solidification process [6-11]. Within this formulation it is possible to properly deal with the incompressibility behaviour of either the casting material during the initial liquid phase or the isochoric viscoplastic strain evolution. 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. Computational simulations show the good performance of the model.

1 INTRODUCTION. MOTIVATION AND GOALS

The numerical formulation of coupled thermo-mechanical solidification processes has been one of the research topics of great interest over the last years. Also, during the last decade, a growing interest on this and related topics has been shown by many industrial companies, such as automotive and aeronautical, motivated by the need to get high-quality final products and to reduce manufacturing costs. However, and despite the enormous progress achieved in computational mechanics, the large-scale numerical simulation of these problems continues to be nowadays a very complex task. This is mainly due to the highly non-linear nature of the problem, involving non-linear constitutive behavior, liquid-solid phase-change, non-linear thermal and mechanical boundary conditions and thermo-mechanical contact interaction,
The aim of this work is to show the necessity of a coupled thermo-mechanical analysis for the simulation of casting processes. Up to now, mostly purely thermal simulation have been considered to study the evolution of the solidification and cooling phenomena. This is mainly due to the fact that a (purely) thermal analysis is easier and less costly, and therefore more convenient for large scale industrial simulations. Moreover, it must be pointed out that in the case of sand die casting thermal results are not so much affected by the mechanical behavior due to the low conductivity and stiffness of the sand. However, an accurate modeling of stresses and deformations during the solidification and cooling phases of the part is essential to capture the accurate thermal pattern in casting processes, particularly when a metallic mold is used. In fact, the thermal deformation of both part and mold modify the original interfacial heat transfer among all the casting tools involved in the process. The relationship between heat transfer coefficients and air-gap has been closely observed [12]. Hence, an accurate prediction of air-gap widths by coupling the thermal simulation with a mechanical analysis is essential to produce a reliable casting model. On the other hand, it must be observed that the mechanical interaction between part and mold induced by the thermal deformations and contact pressure leads to a modification of the final shape and residual stresses of the casting system. An accurate study of the thermal stresses induced during the casting process can prevent mold fissures and an excessive amount of accumulated residual stresses in the part, results that cannot be captured with a purely thermal simulation.

This paper presents an up-to-date finite element numerical tool for the simulation of foundry processes. A fully coupled thermo-mechanical formulation including phase change phenomena is considered [1-5]. The mathematical framework to account for both thermal and mechanical constitutive and boundary assumptions is introduced. The proposed constitutive model is consistently derived from a thermo-elasto-viscoplastic free energy function. Mechanical and thermal material properties are assumed to be temperature-dependent. A continuum transition from the initial fluid-like to the final solid-like behavior of the part is modeled considering a temperature dependent viscoplastic-surface evolution. Phase-change contribution is taken into account assuming both latent-heat release and shrinkage effects. Moreover, an accurate definition of the interfacial heat transfer between the solidifying casting and the mold, essential in producing a reliable casting model, has been considered. In fact, both the solidification process and the temperature evolution strongly depend on the heat exchange at the contact interface. This exchange is affected by the insulating effects of the air-gap due to the thermal shrinkage of the casting part during the solidification and cooling phases. The need for a so closely coupled formulation is the reason why the coupled thermo-mechanical finite element code VULCAN, developed by the authors, is presented as an accurate, efficient and robust numerical tool, allowing the numerical simulation of solidification and cooling processes for the casting industry.

2 FORMULATION OF THE COUPLED THERMOMECHANICAL PROBLEM

The local system of partial differential equations governing the (quasi-static) coupled thermo-mechanical problem is defined by the energy and momentum balance equations,
restricted by the inequalities arising from the second law of the thermodynamics. The local
form of these equations can be written as:

\[ \Theta \dot{S} = -\nabla \cdot \mathbf{q} + R + D_{\text{int}} \]
\[ \nabla \cdot \sigma + \mathbf{b} = 0 \]

where \( \Theta \) is the temperature field, \( S \) the specific entropy, \( \mathbf{q} \) the heat flux per unit surface, \( R \) the
prescribed heat sources per unit of volume, \( D_{\text{int}} \) the internal dissipation per unit of volume, \( \sigma \)
is the stress tensor and \( \mathbf{b} \) the prescribed body forces per unit of volume. Specific entropy and
stress tensor must be defined by suitable constitutive equations restricted by the inequality
arising from the second law of the thermodynamics, given by:

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

where \( \varepsilon \) is the infinitesimal strain tensor and \( E \) is the internal energy per unit of volume.

2.1 Formulation of the thermal problem

The thermal solution, i.e. the temperature and solidification evolution, is obtained by an
enthalpy formulation of the balance of energy equation, which can be rewritten as a function
of the enthalpy \( H \) as:

\[ \dot{H} = -\nabla \cdot \mathbf{q} + R + D_{\text{mech}} - H^{\text{ep}} \]

where \( D_{\text{mech}} \) and \( H^{\text{ep}} \) are the mechanical dissipation and the elasto-plastic heating,
respectively, defined as:

\[ D_{\text{mech}} = \sigma : \dot{\varepsilon}^{\text{ep}} \geq 0 \]
\[ H^{\text{ep}} = -\Theta_{\text{ref}} \frac{\partial \sigma}{\partial \Theta} : \dot{\varepsilon}^{\text{ep}} \]

where \( \Theta_{\text{ref}} \) is a reference temperature while \( \varepsilon^{\text{e}} \) and \( \varepsilon^{\text{ep}} \) are the elastic and inelastic
components of the total strain tensor \( \varepsilon \), respectively. Both terms are usually negligible in case
of casting simulations if compared with the much higher heat flux generated by the thermal
gradient between the part and the mold.

Enthalpy rate \( \dot{H} \) can be defined as a function of the temperature field as:

\[ \dot{H}(\Theta) = C(\Theta) (\dot{\Theta} + \dot{L}(\Theta)) \]

where \( C = C(\Theta) \) is the (temperature dependent) heat capacity coefficient and \( \dot{L}(\Theta) \) is the rate
of latent heat released during the solidification process. Let \( \Theta_L \) and \( \Theta_S \) be the liquidus and
solidus temperature, respectively. Introducing the solid fraction function \( f_S(\Theta) \) as:

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

a convenient form to compute \( \dot{L}(\Theta) \) is the following:
\[ \dot{L}(\Theta) = -L \frac{df_\Sigma(\Theta)}{d\Theta} \Theta \]  

(7)

where \( L \) is the total amount of latent heat to be released during the phase-change [1-5].

The heat flux \( q \) is computed as a function of the temperature field through the Fourier’s law as:

\[ q = -k \nabla \Theta \]  

(8)

where \( k = k(\Theta) \) is the (temperature dependent) heat conductivity.

Let \( \Omega \) be the integration domain with smooth boundaries \( \partial \Omega \). Let \( \delta \Theta \) be the test function associated to the temperature field \( \Theta \). Denoting by \( \langle ; ; \rangle \) the inner product in \( L^2(\Omega) \), the weak form associated to the energy balance equation takes the following expression [1-5]:

\[ \langle C \dot{\Theta} + \dot{L}, \delta \Theta \rangle + \langle k \nabla \Theta, \nabla \delta \Theta \rangle = \langle \delta \Theta, \delta \Theta \rangle_{\partial \Omega} - \langle q_{\text{cond}} + q_{\text{conv}} + q_{\text{rad}}, \delta \Theta \rangle_{\partial \Omega} \]  

(9)

where \( \bar{q} \) is the prescribed normal heat flux on the boundary and \( q_{\text{cond}}, q_{\text{conv}}, q_{\text{rad}} \) are the conduction, convection and radiation heat fluxes at the contact interfaces of the casting tools.

The last term of the weak form defined above is probably the most important one, and drives the solidification and cooling evolution. It is possible to observe either experimentally [12] or numerically [1-5] that a reliable solidification model highly depends on the appropriate definition of the thermo-mechanical heat transfer at the contact interface.

Starting from the radiation heat flux, and assuming that only small deformations of the casting tools can occur, \( q_{\text{rad}} \) can be computed as a direct function of the surface temperatures \( \Theta_c \) and \( \Theta_m \) of the two bodies in contact and their emissivities \( \varepsilon_c \) and \( \varepsilon_m \) as:

\[ q_{\text{rad}} = \frac{\sigma_u (\Theta_c^4 - \Theta_m^4)}{(1/\varepsilon_c + 1/\varepsilon_m - 1)} \]  

(10)

On the other hand, heat conduction through the contact surface, \( q_{\text{cond}} \), can be assumed to be proportional to the thermal gap \( g_\Theta \) between the contact surfaces, in the form:

\[ q_{\text{cond}} = h_{\text{cond}} g_\Theta \]  

(11)

In this case the surfaces of the two bodies are in contact that is no macroscopical air-gap is formed due to the thermal shrinkage of the casting during the cooling phase. As a consequence, the model assumes that a thermal resistance, \( R_{\text{cond}} \), only arises as a result of the air (gasses) trapped between the mold and the casting surfaces, due to the roughness values measured on those surfaces. In addition, the thermal resistance due to the mold coating can be also considered. As a result, the total thermal resistance \( R_{\text{cond}} \), can be computed as [12]:

\[ R_{\text{cond}} = 0.5 \frac{R_c}{k_g} + \frac{\delta_c}{k_c} \]  

(12)

where \( R_c = \sqrt{R_{z,\text{cast}}^2 + R_{z,\text{mold}}^2} \) is the mean peak-to-valley height of the rough surfaces, \( \delta_c \) is the effective thickness of the coating and \( k_g \) 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 \( h_{\text{cond}} \) can be defined using the following expression:

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

(13)

where \( H_e \) is the Vickers hardness and \( 0.6 \leq n \leq 1.0 \) a constant exponent.

Finally, heat convection between the two bodies arises when they separate from each other due to thermal shrinkage. Heat convection \( q_{\text{conv}} \) has been assumed to be a function of coefficient \( h_{\text{conv}} \) depending on the air-gap, \( g_N \), multiplied by the thermal gap \( g_\Theta \), in the form [13]:

\[
q_{\text{conv}} = h_{\text{conv}}(g_N) g_\Theta
\]

(14)

In this case, the heat transfer coefficient \( h_{\text{conv}} \) is defined by the inverse of the thermal resistances of both air-gap and coating as:

\[
h_{\text{conv}} = \frac{1}{\max(g_N/R_e) + \delta_e/k_e}
\]

(15)

Observe that both heat conduction and heat convection coefficients depend on mechanical quantities such as the contact pressure or the air-gap induced by the actual deformation of the casting tools. As a consequence, the solidification and cooling processes are driven by a heat exchange at the contact interfaces that is non-uniform and that in general cannot be expressed as a direct function of the temperature field. This is the main reason why a fully coupled thermo-mechanical simulation is required.

2.2 Formulation of the mechanical problem

The mechanical model for the cast part and the mold material has been formulated to take into account many important features as thermal shrinkage of the cast during the phase-change, a smooth transition from the liquid-like to a solid-like behavior and the incompressibility constraint when the casting is still liquid, among others. To deal with these complex phenomena the mechanical model chosen is based on the recent developments of the authors in the fields of incompressibility in solid mechanics [6-11]. The mixed variational formulation proposed uses linear displacements and pressure interpolations, leading to robust and flexible triangular or tetrahedral elements suitable for large-scale computation of constrained media problems. An orthogonal sub-grid scale approach, introduced by Codina in the field of CFD [14-15], is assumed as an attractive alternative to circumvent the Babuska-Brezzi stability condition [16].

The strong form of the balance of momentum equation is stated introducing the hydrostatic pressure \( p \), as an independent unknown, additional to the displacement field, \( \mathbf{u} \), as:

\[
\begin{aligned}
\nabla \cdot \mathbf{s} + \nabla p + \mathbf{b} &= \mathbf{0} \\
\epsilon_{\text{vol}} &= \frac{p}{k}
\end{aligned}
\]

(16)
where $s = \text{dev}(\sigma)$ is the deviatoric part of the stress tensor $\sigma$ and $K = K(\Theta)$ is the (temperature dependent) bulk modulus that controls the material compressibility. The volumetric part of the elastic deformation $e_{vol}^\varepsilon$ is defined as:

$$e_{vol}^\varepsilon = tr(e^\varepsilon) = \nabla \cdot \mathbf{u} - e^\vartheta$$

where the thermal deformation $e^\vartheta$ is computed taking into account the shrinkage effects during liquid to solid phase-change as follows:

$$e^\vartheta(\Theta) = \begin{cases} 
0 & \text{if } \Theta > \Theta_L \\
e(\Theta) & \text{if } \Theta_L \leq \Theta \leq \Theta_S \\
\dot{e}^\vartheta(\Theta) & \text{if } \Theta \leq \Theta_S
\end{cases}$$

(18)

where $e(\Theta)$ and $\dot{e}(\Theta)$ are the thermal shrinkage during phase-change and the thermal deformation during cooling phase, respectively defined as:

$$e(\Theta) = \frac{\Delta V}{V_0} f_s(\Theta)$$

$$\dot{e}(\Theta) = 3[\alpha(\Theta)(\Theta - \Theta_{ref}) - 3\alpha(\Theta_S)(\Theta_S - \Theta_{ref})]$$

(19)

being $\alpha(\Theta)$ the (temperature dependent) dilatation coefficient, $V_0$ the reference volume at the initial casting temperature and $\Delta V$ the total volume change experimentally observed during the phase change.

As a result of the stabilized formulation proposed by the authors in [6-11], the weak form of the balance of momentum equation accounting for the incompressibility behavior is the following:

$$\left\{ \begin{array}{c} \langle \nabla \cdot \mathbf{v}, s \rangle + \langle \nabla \cdot \mathbf{v}, p \rangle = \langle \mathbf{v}, \mathbf{b} \rangle + \langle \mathbf{v}, \mathbf{f} \rangle \\
\langle q, e_{vol}^\varepsilon \rangle - \langle q, \frac{p}{K} \rangle - \sum_{e=1}^{\text{Nelem}} \tau_v \langle \nabla q, \nabla p - \Pi \rangle = 0
\end{array} \right.$$ 

(20)

where $\Pi$ is the smooth projection of the pressure gradient onto the finite element space, computed at each time-step as:

$$\langle \eta, \Pi \rangle - \langle \eta, \nabla p \rangle = 0$$

(21)

Observe that in case of liquid-like behavior, $K \to \infty$ and $e^\vartheta = 0$, so that the second equation in (20) transforms into:

$$\langle q, \nabla \cdot u \rangle - \sum_{e=1}^{\text{Nelem}} \tau_v \langle \nabla q, \nabla p - \Pi \rangle = 0$$

(22)

which is the weak form associated to the equation of incompressibility, $\nabla \cdot \mathbf{u} = 0$, where a stabilization term has been considered according to the orthogonal sub-grid scale formulation.

The mechanical model for the cast part and the mold material is consistently derived from a thermo-elasto-viscoplastic free-energy potential. Constitutive equations for the deviatoric part of the stress tensor $s$ together with the kinematic and isotropic hardening stress-like variables $q$ and $g$, respectively, are described by the following equations:
\[ s = 2G \text{dev}(\varepsilon - \varepsilon^{vp}) \]
\[ q = -f_s(\Theta)\frac{2}{3}K\xi \]  
\[ q = -f_s(\Theta)\left[\left[\sigma_\infty - \sigma_0\right]\left[1 - \exp(\delta\xi)\right] + H\xi\right] \]

where \( G = G(\Theta) \) is the (temperature dependent) shear modulus, \( K\xi \) and \( H \) are the coefficients of the linear kinematic and isotropic hardening laws and finally, \( \sigma_\infty = \sigma_\infty(\Theta) \) and \( \sigma_0 = \sigma_0(\Theta) \) are the (temperature dependent) saturation and initial flow stress parameters.

The viscoplastic strains \( \varepsilon^{vp} \) are derived, together with the evolution laws for the kinematic and isotropic strain hardening variable \( \xi \) and \( \xi \), according to the principle of maximum plastic dissipation as:

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

where \( n \) and \( \gamma \) are the unit normal to the yield surface and the viscoplastic multiplier, respectively. It is possible to observe that the model considers a temperature dependent J2-yield-surface \( \Phi(s,q,q,\Theta) \) defined as:

\[ \Phi(s,q,q,\Theta) = \|s - q\| - R(q,\Theta) \leq 0 \]

where \( R(q,\Theta) \) is the (temperature dependent) yield-surface radio defined as:

\[ R(q,\Theta) = f_s(\Theta)\left[\frac{2}{3}\left[\sigma_\infty(\Theta) - q\right]\right] \]

It must be pointed out that the yield-surface radio, as well as the hardening effects, gradually reduce as the temperature increase, vanishing when liquidus temperature is reached. As a result, a purely viscous Norton model is assumed when liquid-like behavior must be simulated. In this case, the deviatoric stress tensor is simply given by:

\[ s = \eta \dot{\varepsilon}^{vp} \]

3 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 coupled thermal-plasticity for an industrial casting analysis. Computations
are performed with the finite element code VULCAN developed by the authors at the International Center for Numerical Method in Engineering (CIMNE) in Barcelona, Spain, and commercialized by the software company QUANTECH ATZ [17]. 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 iron casting specimen in a sand mould. Figures 1 and 2 show different views of the geometry and finite element mesh used for the part. The full mesh, including the mold, consists of 237,126 tetrahedral elements. Figure 3 shows the distribution of solid fraction at time 500 s and Figure 4 shows the temperature distribution at 1100 s. Figure 5 shows J2 von Mises deviatoric stress distributions at different sections of the part. In these figures it is also possible to appreciate the air-gap between the part and the mold, responsible of a non-uniform heat flux at the contact interface.
Figure 2. Different views of the finite element mesh of the part
Figure 3. Solid fraction contour at time 500 s.

Figure 4. Temperatures distribution at time 1100 s.
Figure 5. Contours of J2 von Mises equivalent stress at different sections of the part
4 CONCLUDING REMARKS

A formulation for coupled thermo-mechanical problems has been presented. An enthalpy format of the balance of energy equation has been considered to control the latent-heat released during phase-change, leading to the accurate simulation of the temperature evolution during solidification and cooling processes. Stress analysis is essential to define both conduction and convection heat transfer at the contact interfaces. A particular J2 thermoplastic model has been considered. Temperature dependency of both mechanical properties and yield surface allows an to predict deformations and the final residual stresses of the casting tools involved. The model has been successfully applied to the numerical simulation of industrial foundry processes.

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REFERENCES


