On the Constitutive Modeling of Thermoplastic Phase-change Problems

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Table of Contents

Abstract.
1. Introduction.
2. Procedures, Results and Discussion.
3. Conclusions.
   References.
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ABSTRACT- In this paper an up-to-date constitutive numerical model for the computational simulation of coupled thermoplastic frictional contact problems, focusing in solidification processes, is presented. The constitutive model incorporates a viscoelastic and phase-change straining behaviour. Fractional step methods, arising from isothermal and isentropic splits of the governing equations, have been used to solve the nonlinear coupled system of equations.

INTRODUCTION: In spite of important progresses achieved lately in computational mechanics, the large scale numerical simulation of coupled thermomechanical contact problems continues to be nowadays a very complex task due mainly to the highly nonlinear nature of the problem. In particular, phase-change problems introduce a new source of complexity due to the different phases involved in the analysis, the moving solidification front, the straining during phase-change and the constitutive modeling of the whole process. In this paper a constitutive model for coupled thermoplastic problems, including phase-change and frictional contact, is presented.

PROCEDURES, RESULTS AND DISCUSSION: The local system of partial differential equations governing the coupled thermomechanical initial boundary value problem is defined by the momentum and energy balance equations, restricted by the inequalities arising from the second law of the thermodynamics. This system must be supplemented by suitable constitutive equations. Additionally, one must supply suitable prescribed boundary and initial conditions, and consider the equilibrium equations at the contact interfaces. Micromechanically based phenomenological models of infinitesimal strain plasticity adopt a local additive decomposition of the strain tensor into elastic and plastic parts. Hardening mechanisms in the material are characterized by an additional set of phenomenological internal variables, collectively denoted here by $\xi_a$. Viscoelastic behaviour is introduced by considering an additional viscous internal variable $\alpha$. An additive split of the local entropy into elastic and plastic parts is adopted, where the plastic entropy is viewed as an additional internal variable arising as a result of dislocation and lattice defect motion. This additive split of the local entropy was adopted by Armero & Simo [1993]. The above considerations, motivates the following additive split of the infinitesimal strain tensor $\varepsilon := \varepsilon^e + \varepsilon^p$ and local entropy $H := H^e + H^p$ and the following set of microstructural internal variables $G := \{\varepsilon^p, H^p, \xi_a, \alpha\}$. The internal energy is assumed to take the functional form $E := \hat{E}(\varepsilon^e, H^e, \xi_a, \alpha)$ and, using the Legendre transformation $\Psi = E - \Theta H^e$, the free energy takes the functional form $\psi := \hat{\psi}(\varepsilon^e, \Theta, \xi_a, \alpha)$. Table 1 shows a particular expression of the free energy considered here, which includes small strains hyperelastic,
coupled thermoelastic, pure thermal and plastic hardening potentials. Note that latent heat and phase-change contributions have been considered within the pure thermal and coupled thermoelastic potentials, respectively. The material properties have been considered to be temperature dependent. Thermoplastic response has been modeled by a J2 temperature dependent plastic model, including hardening due to plastic deformation and thermal softening. A continuous transition between the initial fluid-like and the final solid-like behaviour of the part is modelled using the solid fraction. The mechanical deviatoric behaviour of the initial fluid-like phase of the part is modelled using a pure viscous model. Also, viscous-like induced strains due to the variation of the elastic modulus during the cooling process are considered.

Following the recent approach of Laursen [1998], a thermomechanical contact formulation is thermodynamically consistent derived following a parallel approach to the one of the bulk continua. Contact temperature $\Theta_c$ and contact entropy $H_c$ are introduced as new variables and energy balance at the contact interface is formulated. Frictional hardening mechanisms are characterized by a set of internal variables denoted as $\zeta_{cb}$. A local additive split of the tangential gap and the local contact entropy $\xi_c$ into elastic and plastic parts, is considered. The above considerations motivates the following additive split of the tangential gap $g_T^\alpha := g_T^{\alpha, e} + g_T^{\alpha, p}$ and contact entropy $H_c := H_c^e + H_c^p$ and the following set of contact internal variables $G_c := \{g_T^{\alpha, e}, H_c^e, H_c^p, \zeta_{cb}\}$. The contact internal energy is assumed to take the functional form $E_c := E_c(g_N, g_T^{\alpha, e}, H_c^e, \zeta_{cb})$ and, using the Legendre transformation $\Psi_c = E_c - \Theta_c H_c^e$, the free energy takes the functional form $\Psi_c := \hat{\Psi}_c(g_N, g_T^{\alpha, e}, \Theta_c, \zeta_{cb})$. Contact heat fluxes are assumed to take the form $Q_{c}^{(\alpha)} := h_c^{(\alpha)}(t_n, \Theta_c) g_T^{(\alpha)}$ where $h_c^{(\alpha)}(t_n, \Theta_c)$ is the heat transfer coefficient and $g_T^{(\alpha)} := \Theta^{(\alpha)} - \Theta_c$ is the thermal gap for contact surface $\alpha$.

The use of an operator split, applied to the coupled system of nonlinear ordinary differential equations, and a product formula algorithm, leads to a staggered solution algorithm in which each one of the subproblems defined by the partition is solved sequentially, within the framework of classical fractional step methods.

**Numerical Simulation:** Solidification of a cast iron brake component into a sand mould. This example deals with the numerical simulation of the solidification process of an industrial part, in this case, one of the components of the braking system of an automobile. Fig. 1 shows a view of the manufactured part. Assumed starting conditions in the numerical simulation of the casting process are given by a completely filled mould with iron in liquid state at uniform temperature. The initial temperatures of the iron part and the sand mould were 1420°C and 20°C, respectively. Only gravitational forces have been assumed. All the material properties for the cast iron and the sand have been assumed to be temperature dependent. The cast iron used for the part presents a liquid-solid phase change between 1145°C and 1155°C, and a solid-solid phase change between 750°C and 800°C. Both phase changes have been accounted for in the numerical simulation. The finite element mesh for the cast iron part consists of 6300 4-noded tetrahedral elements while 26630 tetrahedral elements have been used for the sand mould.
Table 1: J2-Thermoplastic Constitutive Model. Free Energy Function.

<table>
<thead>
<tr>
<th>Free energy function</th>
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</thead>
<tbody>
<tr>
<td>( \hat{\psi}(\epsilon^e, \xi, \Theta, \alpha) = \hat{W}(\epsilon^e, \Theta, \alpha) + \hat{M}(\epsilon^e, \Theta, \alpha) + \hat{T}(\Theta) + \hat{K}(\xi, \Theta) )</td>
</tr>
</tbody>
</table>

i. **Linear hyperelastic response** \((\mu(\Theta) > 0, \kappa(\Theta) > 0)\),

\[
\hat{W}(\epsilon^e, \Theta, \alpha) = \hat{W}(\text{dev}[\epsilon^e - \alpha], \Theta) + \hat{U}(\text{tr}[\epsilon^e - \alpha], \Theta)
\]

\[
\hat{W}(\text{dev}[\epsilon^e - \alpha], \Theta) = \mu(\Theta) \text{dev}^2[\epsilon^e - \alpha],
\]

\[
\hat{U}(\text{tr}[\epsilon^e - \alpha], \Theta) = \frac{1}{2} \kappa(\Theta) \text{tr}^2[\epsilon^e - \alpha],
\]

with \( \mu(\Theta) = \hat{\mu}(\Theta)/f_s(\Theta) \) where \( f_s(\Theta) \in [0, 1] \).

ii. **Thermoelastic coupling**

\[
\hat{M}(\epsilon^e, \Theta, \alpha) = -\kappa(\Theta) \text{[[\hat{\epsilon}(\Theta) - \hat{\epsilon}(\Theta_0)]] tr[\epsilon^e - \alpha]},
\]

where

\[
\hat{\epsilon}(\Theta) := 3\alpha(\Theta)(\Theta - \Theta_{ref}) + \epsilon^{ps}(\Theta),
\]

\[
\epsilon^{ps}(\Theta) := \sum_{p=1}^{n_p} \frac{\Delta V_p}{V_{p0}} \hat{f}_p(\Theta).
\]

iii. **Thermal contribution** \((c_s(\Theta) > 0)\),

IF \((c_s(\Theta) = \text{constant} \ \text{AND} \ \Omega(\Theta) = 0)\) THEN

\[
\hat{T}(\Theta) = \rho c_s \left[ (\Theta - \Theta_0) - \Theta \log(\Theta/\Theta_0) \right],
\]

ELSE

\[
\hat{T}(\Theta) = \int_{\Theta_0}^{\Theta} \hat{T}_{\Theta}(\Theta) d\Theta, \quad \hat{T}_{\Theta}(\Theta) = -\int_{\Theta_0}^{\Theta} \left[ \rho c_s(\Theta) + \Omega'(\Theta) \right] \frac{d\Theta}{\Theta},
\]

END IF

iv. **Hardening potential**

\[
\hat{K}(\xi, \Theta) = \frac{1}{2} h(\Theta) \xi^2 - [y_0(\Theta) - y_{\infty}(\Theta)] \hat{H}(\xi),
\]

where \( \hat{H}(\xi) := \begin{cases} \xi - [1 - \exp(-\delta\xi)]/\delta, & \text{if } \delta \neq 0; \\ 0, & \text{if } \delta = 0. \end{cases} \)

Fig. 2a shows the temperature evolution at points A, B and C, located at the casting center, at the casting surface and at the mould surface, respectively (see Fig. 1). A typical temperature plateau due to the release of latent heat during solidification can be observed at the casting center point A, up to a 150 sec., approximately. The smoother solid-solid phase change can also be observed for this point, between 600 sec. and 950 sec., approximately. Fig. 2b shows the evolution of the mechanical gap that develop between the part
and the mould at points C, D and E (see Fig. 1) as the part contracts due to the temperature drop. It is remarkable that the gap at point D grows quite significantly, reaching an amplitude close to 2 mm.

Fig. 1. Solidification of a brake component. Geometry of the part.

Fig. 2. Solidification of a brake component. (a) Temperature evolution at the casting center A, casting surface B and mould surface C. (b) Gap evolution at points C, D and E.

CONCLUSIONS: A constitutive numerical model for the analysis of coupled thermomechanical problems, involving frictional contact and thermal multiphase change phenomena, has been presented. The model has been successfully applied to the numerical simulation of industrial solidification processes.

REFERENCES: