

Development of thermoplastic constitutive models for refractory ceramics in wide temperature range

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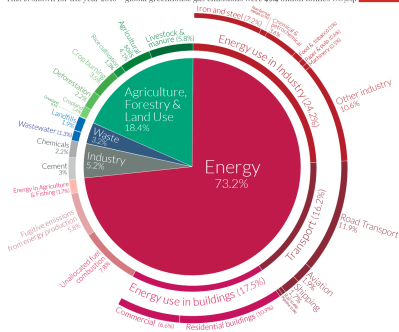


Motivation

Global greenhouse gas emissions by sector

This is shown for the year 2016 – global greenhouse gas emissions were 49.4 billion tonnes CO₂eq.

Our World
in Data



OurWorldinData.org – Research and data to make progress against the world's largest problems.
Source: Climate Watch, the World Resources Institute (2020).
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Figure 1: Global greenhouse gas emissions in the latest breakdown of global emissions by sector, published by Climate Watch and the World Resources Institute for the year 2016. Reference www.ourworldindata.org

- Steel is a **key resource** for a large variety of industries
- Steel production is one of the most polluting industry. Main pollution sources are:
 - the production of energy needed to melt the metal
 - the disposal of equipment for the handling of molten metal
- This industry is in constant need of **improvements in the design of devices and processes**

Case study: the ladle shroud



Figure 2: Ladle shroud in operation. Picture liberally taken from the Vesuvius website: www.vesuvius.com

- The ladle shroud is a refractory tube used for the movement of the molten steel.
- Its main function is to avoid chemical interaction of the molten metal with the atmosphere.
- Ladle shrouds are usually not preheated before operation so they have to be able to withstand:
 - high temperature gradient
 - high thermal shock

Ladle shroud design

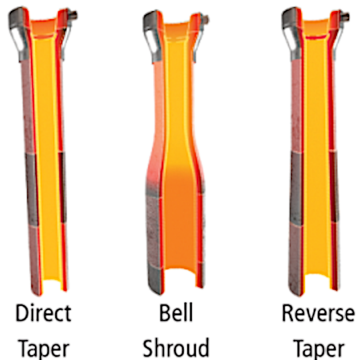


Figure 3: Ladle shroud design. Picture liberally taken from the Vesuvius website: www.vesuvius.com

- The ladle shroud is a critical component
- Design goals are:
 - maximize operation time
 - minimize crack initiation and propagation
 - reach zero failure during operation
- Physical phenomena to take into account:
 - insurgence of irreversible plastic deformation
 - change of material behavior during operation
 - insurgence of local instabilities (cracks)

Design tool: the theory of plasticity

For isotropic materials:

Elastic theory - Linear equations

$$\begin{aligned}\boldsymbol{\varepsilon} &= \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) && \text{COMPATIBILITY} \\ \boldsymbol{\sigma} &= \mathbb{D} [\boldsymbol{\varepsilon}] && \text{CONSTITUTIVE EQ}\end{aligned}$$

Plastic theory - Incremental equations

$$\begin{aligned}\boldsymbol{\varepsilon} &= \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p && \text{STRAIN DECOMPOSITION} \\ \boldsymbol{\sigma} &= \mathbb{D} [\boldsymbol{\varepsilon}_e] && \text{CONSTITUTIVE EQ} \\ F(\boldsymbol{\sigma}, \mathbf{A}) &= 0 && \text{YIELD SURFACE} \\ \dot{\boldsymbol{\varepsilon}}_p &= \dot{\gamma} \mathbf{N}(\boldsymbol{\sigma}, \mathbf{A}) && \text{PLASTIC FLOW} \\ \dot{\boldsymbol{\alpha}} &= \dot{\gamma} \mathbf{H} && \text{HARDENING LAW} \\ F \leq 0 \quad \dot{\gamma} \geq 0 \quad F\dot{\gamma} &= 0 && \text{LOADING CONDITION}\end{aligned}$$

- Plastic deformation is non-conservative
- The current state of a system depends on the whole system history
- The describing equations must be incremental

Design tool: the theory of thermo-plasticity

For isotropic materials:

Thermal coupling equations

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p + \boldsymbol{\varepsilon}_T \quad \text{STRAIN DECOMPOSITION}$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{\varepsilon}, T) \quad \text{CONSTITUTIVE EQ}$$

$$\boldsymbol{\varepsilon}_T = k_T (T - T_0) \mathbf{I} \quad \text{THERMAL EXPANSION}$$

$$\mathbf{A} = \mathbf{A}(T) \quad \text{THERMAL SOFTENING}$$

$$D_{mech} = \chi \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}}_p \quad \text{PLASTIC HEATING}$$

- Coupling of the mechanical effects with the thermal ones:
 - Thermal expansion
 - Thermal plastic softening
 - Plastic heating
- The problem can be solved as
 - **Decoupled:** the mechanical heating is neglected, the thermal problem is first solved and then used as input for the mechanical one
 - **Coupled:** all the effects are taken into account

Yield surface in the Haigh–Westergaard stress space

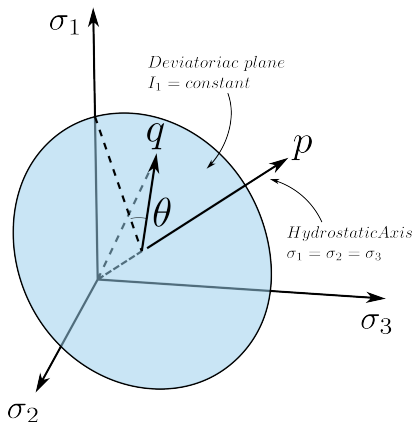


Figure 4: Haigh Westergaard stress space representation

Stress space coordinates

$$\mathbf{s} = \boldsymbol{\sigma} - \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) \mathbf{I}$$

$$J_2 = \frac{1}{2} (\mathbf{s} \cdot \mathbf{s})$$

$$J_3 = \det(\mathbf{s})$$

$$p = -\frac{1}{3} \text{tr}(\boldsymbol{\sigma})$$

$$q = \sqrt{3} J_2$$

$$\cos(3\theta) = \frac{3\sqrt{3}}{2} \frac{J_3}{J_2^{3/2}}$$

$$F(\boldsymbol{\sigma}) = F(p, q, \theta)$$

Bigoni-Piccolroaz yield criterion

- Suited for granular, pressure sensitive, materials
- Great flexibility, thus good interpolation of experimental data

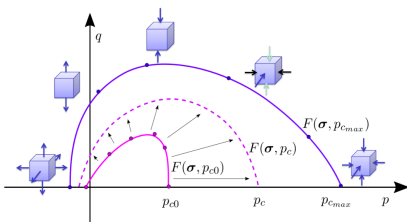


Figure 5: Meridian section view of a BP yield surface. The figure shows an example of evolution during non isotropic hardening. Liberally taken from the PhD thesis of Ing. Massimo Penasa.

BP yield surface

$$F(\sigma) = F(p, q, \theta) = f(p) + \frac{q}{g(\theta)}$$

$$\Phi = \frac{p + c}{p_c + c}$$

$$f(p) = \begin{cases} -Mp_c \sqrt{(\Phi - \Phi^m) [2(1 - \alpha)\Phi + \alpha]} \\ +\infty & \Phi \notin [0; 1] \end{cases}$$

$$g(\theta)^{-1} = \cos \left[\beta \frac{\pi}{6} - \frac{1}{3} \arccos(\gamma \cos(3\theta)) \right]$$

Bigoni-Piccolroaz yield surface

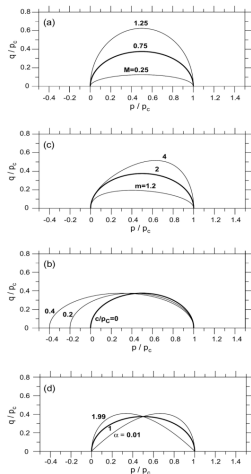


Figure 6: Meridian section flexibility.

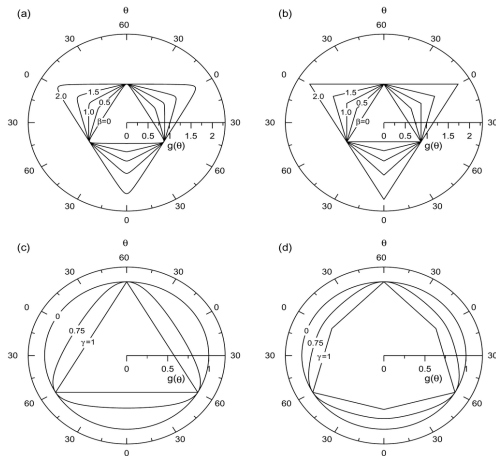


Figure 7: Deviatoric section flexibility

Source: D. Bigoni, A. Piccolroaz, "Yield criteria for quasibrittle and frictional materials," International Journal of Solids and Structures, 2004.

Material model

$$W(T, \varepsilon) = \frac{\lambda(T)}{2} \text{tr}(\varepsilon^2) + \mu(T) \varepsilon^2$$

Temperature dependent elastic potential

$$E(T) = \sum_{i=0}^n d_i T^i$$

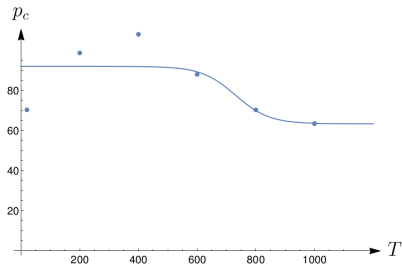
Young modulus polynomial approximation

$$p_c = p_{cT} + \frac{k_1 T}{1 + \delta_T P(\varepsilon_p)} P(\varepsilon_p)$$

Mechanical hardening

$$c = \Omega p_{cT}$$

Mechanical hardening



Thermal hardening. Liberally taken from the PhD thesis of Ing. Massimo Penasa.

Implementation instrument: AceGen

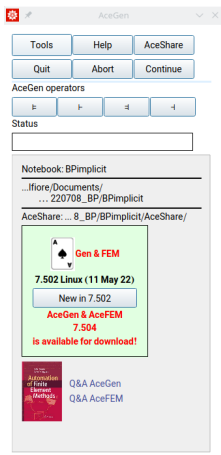


Figure 8: AceGen command palette. For more info visit: symech.fgg.uni-lj.si

- AceGen is a software development package built on top of Mathematica
- AceGen converts symbolic expressions into optimized subroutines for commercial Finite Element programs, ie Abaqus
- Its main features are automatic differentiation and stochastic optimization
- Automatic differentiation is particularly important since the most demanding task in the coding of material behavior is the computation of the **consistent tangent operator**

Industrial piece simulation

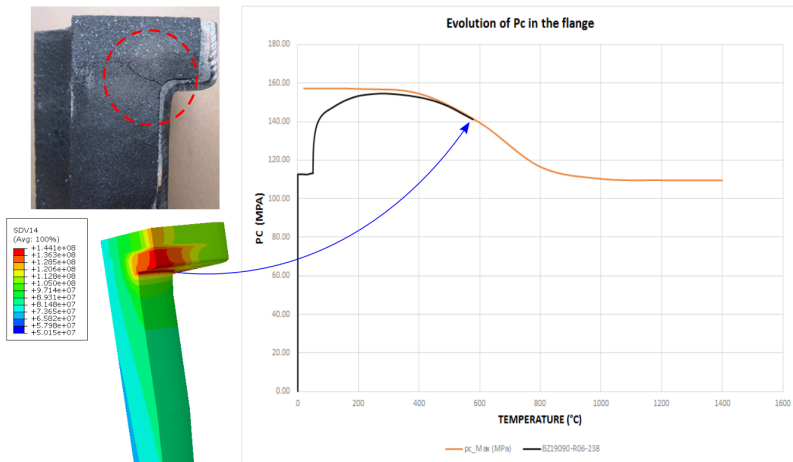


Figure 9: Comparison between simulation results and real industrial piece (sub-entry nozzle) show that the yield function parameter p_c is a good indicator of the material resistance and can be used to predict crack initiation. Liberally taken from the PhD thesis of Ing. Massimo Penasa.

Current problems and room for improvement

Present issues

- There is room of improvement for the simplification of parameter space
- Hardening laws can be improved to represent all refractories in use
- Refractory devices like the ladle shroud show **a transient behavior (thermal shock)**. Rate-dependent laws must be investigated and implemented.

Possible solutions

- Investigate physical meaning of the yield function parameters through additional experiments
- Change hardening laws on experimental results
- Introduce viscosity to model material creep and validate the model on experimental results

Thanks for your attention