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

Lorenzo Fiore

Supervisors: Andrea Piccolroaz and Séverine Romero Baivier

Workshop to celebrate 150 years since the formation of Wales' first university

June 7–9, 2023, Aberystwyth, Wales, UK

VESUVIUS

UNIVERSITÀ DI TRENTO

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 955944 – RE-FRACTURE2.

RE-FRACTURE2 ITN EID PROJECT

Case study: the ladle shroud

Figure 1: 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

Design tool: the theory of plasticity

For isotropic materials:

Elastic theory - Linear equations

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right) \qquad \text{COMPATIBILITY}$$

$$\boldsymbol{\sigma} = \mathbb{D}\left[\boldsymbol{\varepsilon}\right] \qquad \text{CONSTITUTIVE EQ}$$

Plastic theory - Incremental equations

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

$$\boldsymbol{\sigma} = \mathbb{D}\left[\boldsymbol{\varepsilon}_e\right] \qquad \text{CONSTITUTIVE EQ}$$

$$F(\boldsymbol{\sigma}, \boldsymbol{A}) = 0 \qquad \text{YIELD SURFACE}$$

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\gamma}\ \boldsymbol{N}(\boldsymbol{\sigma}, \boldsymbol{A}) \qquad \text{PLASTIC FLOW}$$

$$\dot{\boldsymbol{\alpha}} = \dot{\gamma}\ \boldsymbol{H} \qquad \text{HARDENING LAW}$$

$$F \leq 0 \quad \dot{\gamma} \geq 0 \quad F\dot{\gamma} = 0 \qquad \text{LOADING CONDITION}$$

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

Elastic potential

Simple elastic potential

$$\varepsilon = \varepsilon_e + \varepsilon_p$$

$$\boldsymbol{\sigma} = \frac{\partial W(T,\varepsilon)}{\partial \varepsilon_e}$$

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

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

- The elastic potential has the simplest expression compatible with thermodynamics
- The Young modulus is considered as piece-wise linear expression
- The Poisson coefficient is considered as a constant value

Yield surface in the Haigh–Westergaard stress space

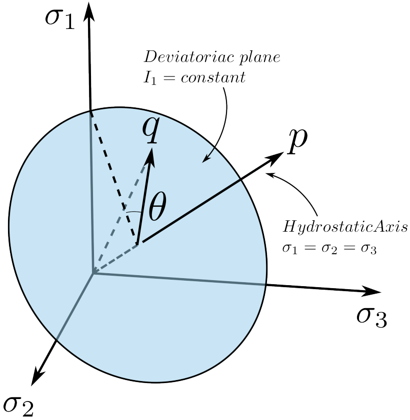


Figure 2: Haigh Westergaard stress space representation

Stress space coordinates

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

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

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

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

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

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

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

Bigoni-Piccolroaz yield criterion

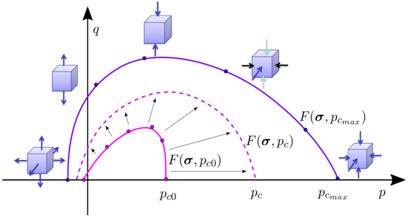


Figure 3: Meridian section view of a BP yield surface. The figure shows an example of evolution during non isotropic hardening. Liberally taken from the PhD thesis of Ing. Massimo Penasa.

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

BP yield surface

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

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

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

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

Hardening laws for BP parameters

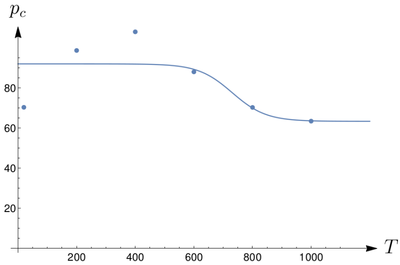
Mechanical [1]

$$p_c = p_{cT} + \frac{k_{1T}}{1 + \delta_T \ \bar{\varepsilon}_p} \ \bar{\varepsilon}_p$$

$$c = \Omega \ p_c$$

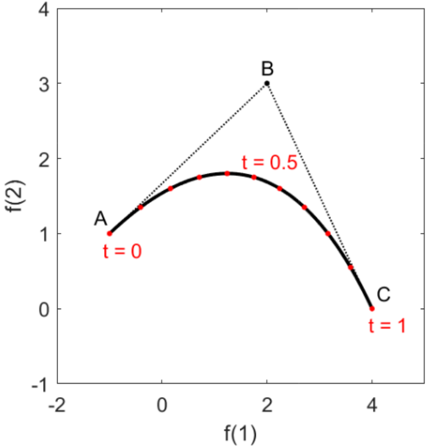
- p_c is related to the resistance to hydrostatic compression
- c is related to the resistance to hydrostatic tension
- $\bar{\varepsilon}_p$ is cumulated plastic deformation

- The $p_c(T)$ law captures the changes in material behavior at a specific transition temperature [$\approx 600^\circ C$]
- The first approximation was the *atan* function



[1] *Poltronieri Piccolroaz Bigoni and Romero Baivier 2014* - "A Simple and Robust Elastoplastic Constitutive Model for Concrete."

Bézier curves



Parametric curve

$$\boldsymbol{B}^2(t) = \sum_{i=0}^{2} b_{i,n}(t)\ \boldsymbol{P}_i$$

$$b_{i,n}(t) = \binom{n}{i} t^i\ (1-t)^{n-1}$$

Interpolation with Bézier curves

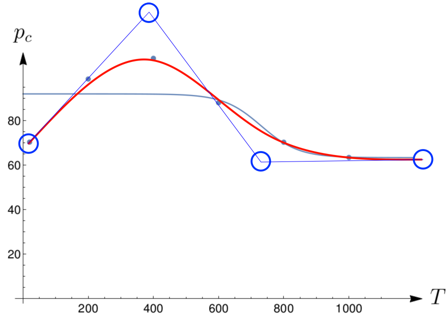
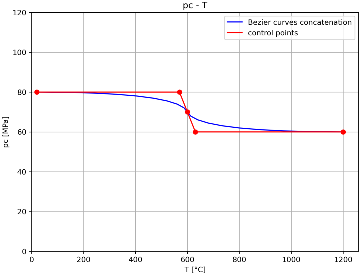
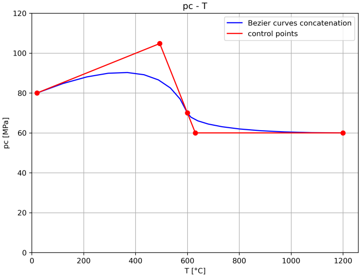


Figure 4: Interpolation of experimental data with a cubic Bézier.

- It's possible to control both position and tangent at first and last control point
- In the easiest case the tangent at both the first and last interpolation points can be horizontal thus **reproducing the behaviour of the arctan function at a comparable cost in terms of parameters to identify**
- Usign a 3^{rd} order Bézier curve there is no control on the intersection point at $T = T_c$

Interpolation with two quadratics Bézier curves





- Given:
  - pc0 @ T0
  - pcTmax @ Tmax
  - tangent @ pc0
  - tangent @ pcTmax
  - change of properties Temperature Tc
- In order to define a unique Bezier set of curves, define in a sensible way:
  - slope at Tc
  - intersection point on vertical for Tc
- Minimizing the least square distance of points from the curve

Industrial piece simulation

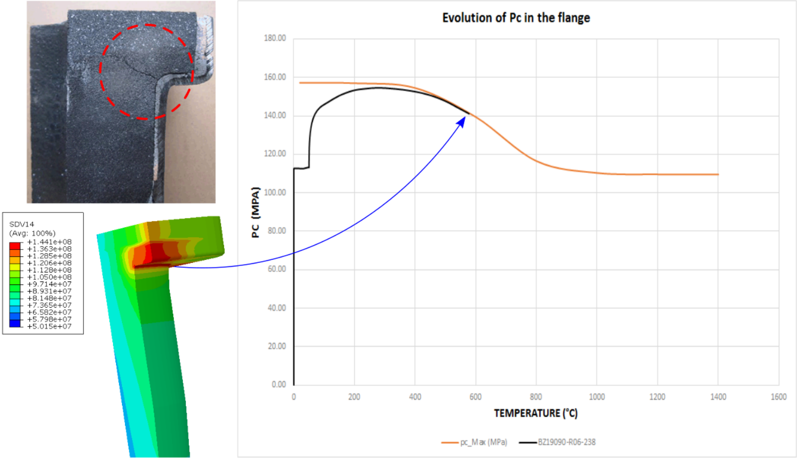
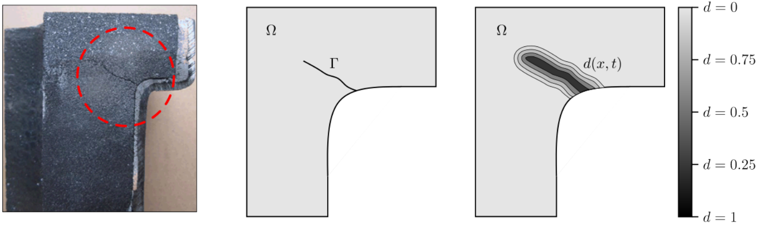


Figure 5: Comparison between simulation results and real industrial piece (sub-entry nozzle) show that the yield function parameter p_c is a good indicator of the material resistance and can be used to predict crack initiation. Liberally taken from the PhD thesis of Ing. Massimo Penasa.

The phase field approach to fracture mechanics



Crack regularization

$$\int_{\Omega} G_c \; \Gamma(x,t) \; d\Gamma \approx \int_{\Omega} G_c \; \gamma(d, \nabla d) \; d\Omega$$

$$\gamma(d, \nabla d) = \frac{1}{2}\left(\frac{1}{l} d^2 + \frac{l}{2} |\nabla d|^2\right)$$

- The integral over a changing crack path is replaced by an integral over a given domain

Variational theory of brittle fracture

Energy integral [2]

$$W_{int} = \int_{\Omega} \psi_R(\varepsilon(\boldsymbol{u})) + g(d)\ \psi_D(\varepsilon(\boldsymbol{u}))dV + \int_{\Omega} G_c\ \gamma(d, \nabla d)$$

$$g(d) = (1-d)^2$$

- The elastic energy is splitted in two parts in order to account for traction-compression asymmetry
- A degradation function accounts for damage in material points
- The phase field fracture equation acts as an **additional physics** in the problem, alongside thermal and displacement

[2] *Francfort and Marigo 1998* - "Revisiting Brittle Fracture as an Energy Minimization Problem."

Local evolution equation

Ginzburg–Landau-type evolution equation [3]

$$\dot{d} = \frac{1}{\eta}\left\langle -\frac{\delta(\psi + G_c\gamma(d, \nabla d))}{\delta d}\right\rangle$$

$$\underbrace{\eta\dot{d}}_{\text{evolution}} = \underbrace{g'(d)\,\mathcal{H}}_{\text{driving}} \underbrace{-[d - l^2\Delta d]}_{\text{geometrical resistance}}$$

$$\mathcal{H} = \max_{s\in[0,t]}\{\psi_D(\varepsilon)/G_c\}$$

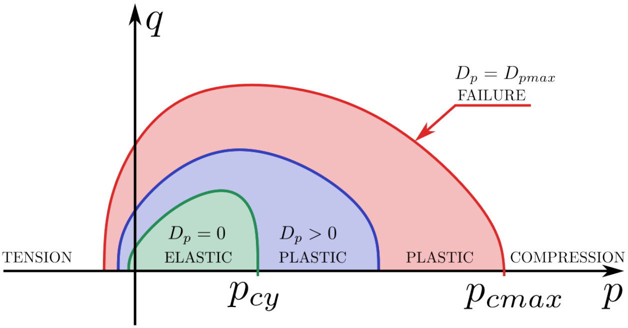
- Damage is considered as an **internal variable**, similarly to plastic strain and BP parameters
- The damage equation is not solved at the material point but on the whole domain

[3] *Miehe Welschinger and Hofacker 2010* - "Thermodynamically Consistent Phase-Field Models of Fracture: Variational Principles and Multi-Field FE Implementations."

Fracture driving force for refractories

Plasticity term

$$\mathcal{H} = \max_{s\in[0,t]} \left(\frac{2l}{G_c}\psi_D(\varepsilon) + \left\langle \left(\frac{p_c}{p_{cYIELD}} \right)^2 - 1 \right\rangle \right)$$



Preliminary results of ladle shroud section simulation