Mix Design, Modelling and Analysis of Low Carbon Concrete

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Happy birthday Trond!

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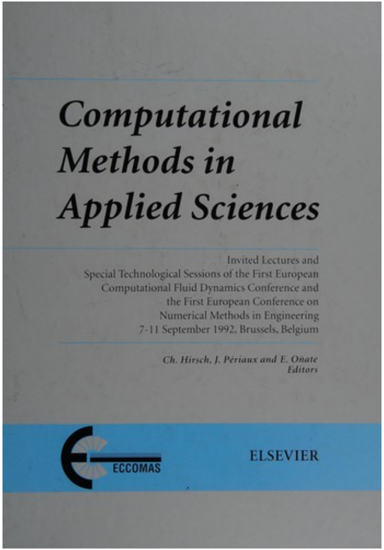


33 years friendship!

Motivation

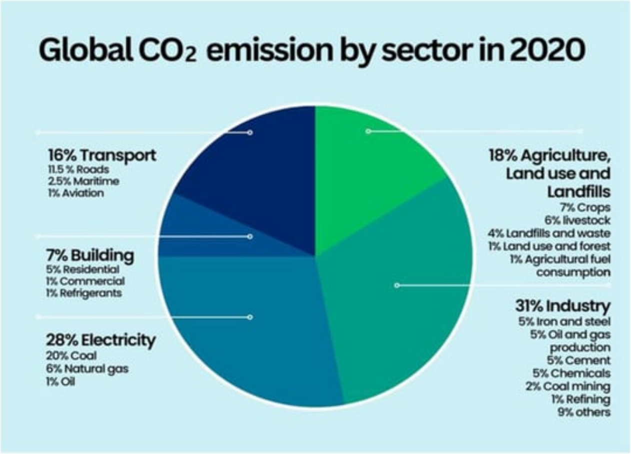
Concrete - what it is?

Mixture of

Cement	20 % (mass)
Water	10 %
Aggregates	70 %

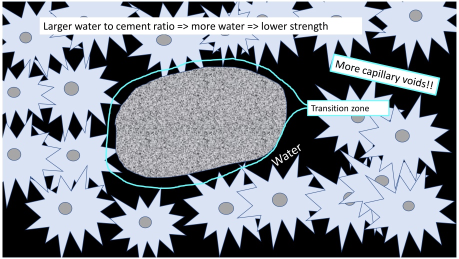
Production of 1 t of Portland Cement (PC) consumes 4 GJ of energy and emits 0.85 t of CO_2.

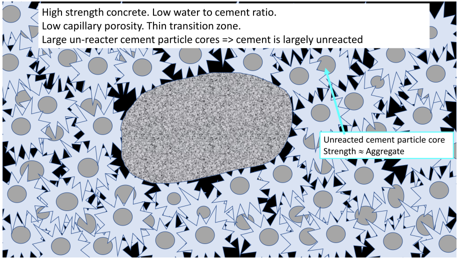
Current estimates of world cement manufacture are of the order of $1.7 \cdot 10^9$ t/year, about 1 m^3 per person (2004).

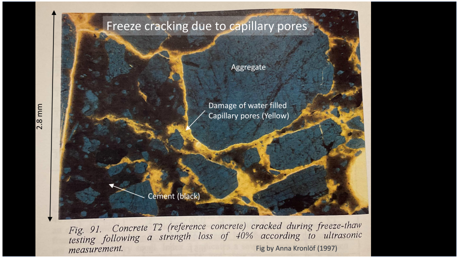


Issa Zadeh, S.B.; et al. Scope of the Literature on Efforts to Reduce the Carbon Footprint of Seaports. *Sustainability* 2023, 15, 8558. https://doi.org/10.3390/su15118558

More on concrete







Figs by Anna Kronlöf.

Towards Sustainable Carbon Free Concrete Construction (ConSus)

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Participants:

- Oulu University
- VTT Technical Research Centre of Finland Ltd.
- Tampere University

Goal: To develop low CO_2 binders with strength and ductility comparable (or better) than Portland cement (PC) and computational methodology to analyse the behaviour of different concrete types.

About AAM mix design

For years, Portland cement (PC) has been partly replaced by industrial waste such as blast furnace slag (BFS) to reduce CO_2 emissions.

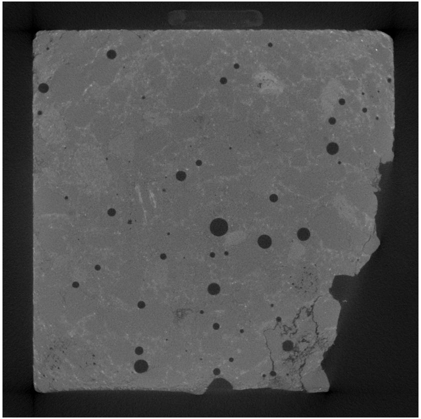
Iron and steel making industry generate more than 400 million tonnes of slags worldwide

Blast furnace is going to be replaced by electric arc furnace (EAF).

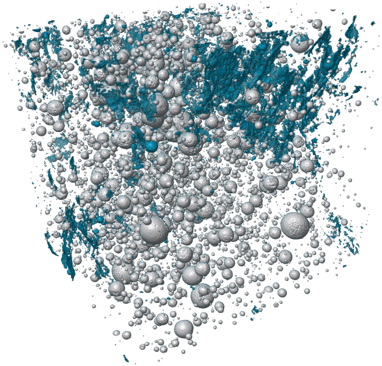
Alkali-Activated Materials (AAM), also called geopolymers, has been found to be a promising alternative for PC. AAMs are consisting of precursor and alkali-activator: Commonly used precursors are for example fly ash, slag, and metakaolin, and alkali-activators are sodium silicate and sodium hydroxide.

How Machine Learning (ML) can help in the thermodynamic modelling and optimisation of the physical tests?

Experiments - identifying damage due to loading



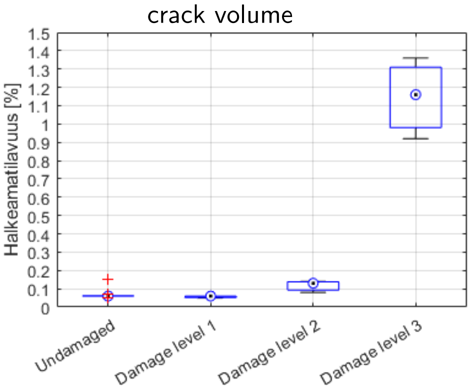
XCT scan of damaged specimen. Uniaxial compression at max. load.

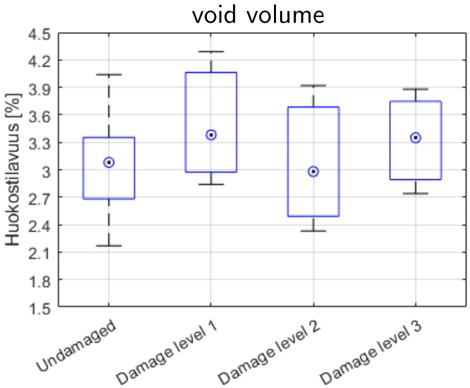


3D model of crack (blue) and void (grey) distribution.

How ML can help in the regocnition of the microstructure?

Identifying damage due to loading (cont'd)





level 1 $\approx 40\%$ of σ_c, level 2 at σ_c, level 3 in post peak region $\varepsilon \approx 1.2\varepsilon(\sigma_c)$.

Can ML guide the model development in constructing the evolution equations for damage?

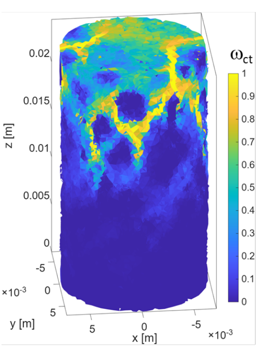
On concrete's mechanical behaviour

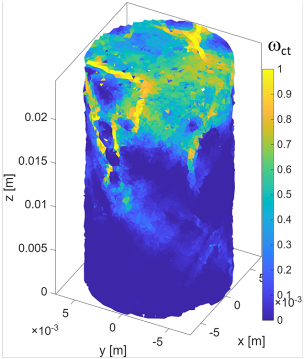
- The non-linear behaviour of quasi-brittle materials, like concrete and rock under loading is mainly due to damage and micro-cracking rather than plastic deformation.
- Damage of quasi-brittle materials can be modelled using scalar, vector or higher order damage tensors.
- Failure in tension is mainly due to the growth of the most critical micro-crack.
- Failure in compression can be seen as a cooperative action of a distributed microcrack array.

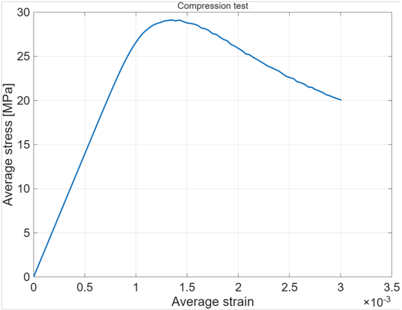
http://mps-il.com

Mesoscopic model, uniaxial compression

Two phase material, aggregate + cement paste, consistency viscoplastic DP two-surface model with Rankine tenson cut-off for both phases. Isotropic damage with separate tensile and compressive components. 400 000 linear tetrahedra.







$$\omega_{ct} = 1 - (1-\omega_c)(1-\omega_t)$$

What is the best way to reconstruct the FE mesh from microstructure? Sensitivity analysis?

Macroscopic models

Our approach for macroscale model is to use CDM to imitate

Ottosen's Failure function

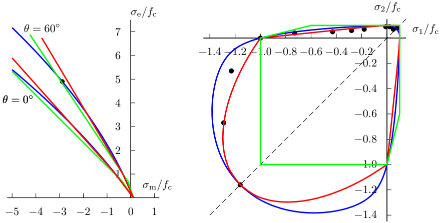
$$A\frac{J_2}{\sigma_c} + \Lambda\sqrt{J_2} + BI_1 - \sigma_\mathrm{c} = 0$$

$$\Lambda = \begin{cases} k_1 \cos[\frac{1}{3}\arccos(k_2\cos 3\theta)] & \text{if} \quad \cos 3\theta \geqslant 0 \\ k_1 \cos[\frac{1}{3}\pi - \frac{1}{3}\arccos(-k_2\cos 3\theta)] & \text{if} \quad \cos 3\theta \leq 0 \end{cases}$$

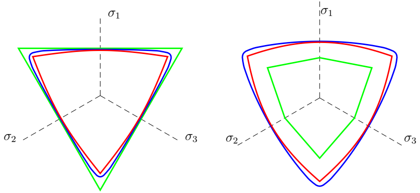
$$\cos 3\theta = \frac{3\sqrt{3}}{2}\frac{J_3}{J_2^{3/2}}$$

σ_c: the uniaxial compressive strength
$I_1 = \mathrm{tr}\boldsymbol{\sigma}$: the first invariant of the stress tensor
$J_2 = \frac{1}{2}\boldsymbol{s} : \boldsymbol{s}$, $J_3 = \det \boldsymbol{s} = \frac{1}{3}\mathrm{tr}\boldsymbol{s}^3$: deviatoric invariants
A, B, k_1, k_2: material constants

Meridian plane & plane stress



Deviatoric plane



$\pi -$ plane $\qquad\qquad$ $\sigma_\mathrm{m} = -f_\mathrm{c}$

Green line = Mohr-Coulomb with tension cut-off
Blue line = Ottosen's model
Red line = Barcelona model, Lubliner et al.

Thermodynamic formulation

Two potential functions

$$\psi^{\mathrm{c}} = \psi^{\mathrm{c}}(S), \quad S = (\boldsymbol{\sigma}, \boldsymbol{D}, \kappa) \qquad \text{Specific Gibbs free energy}$$

$$\gamma = \rho_0 \dot{\psi}^{\mathrm{c}} - \dot{\boldsymbol{\sigma}} : \boldsymbol{\varepsilon}, \quad \gamma \geqslant 0 \qquad \text{Clausius-Duhem inequality}$$

$$\varphi(W; S), \quad W = (\boldsymbol{Y}, K) \qquad \text{Dissipation potential}$$

$$\gamma \equiv \boldsymbol{B}_Y : \boldsymbol{Y} + B_K K$$

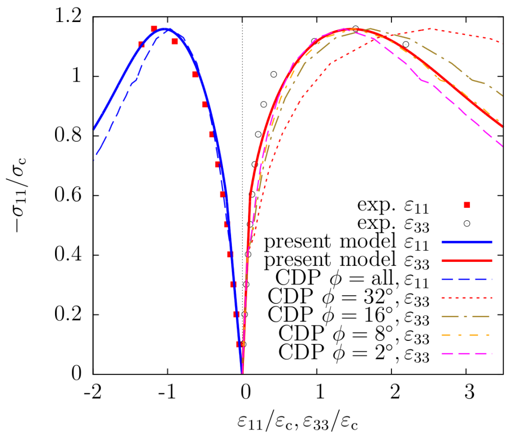
$$\text{Define} \quad \boldsymbol{Y} = \rho_0 \frac{\partial \psi^c}{\partial \boldsymbol{D}}, \quad K = -\rho_0 \frac{\partial \psi^c}{\partial \kappa}$$

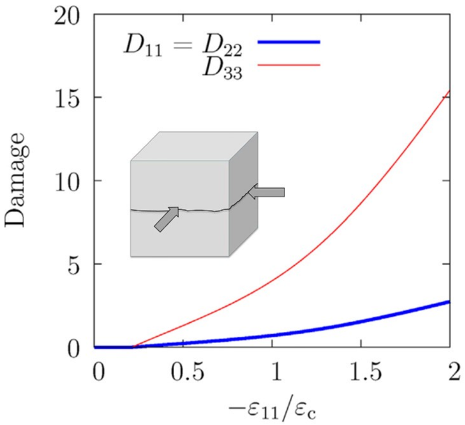
$$\left(\rho_0 \frac{\partial \psi^c}{\partial \boldsymbol{\sigma}} - \boldsymbol{\varepsilon}\right) : \dot{\boldsymbol{\sigma}} + \left(\dot{\boldsymbol{D}} - \boldsymbol{B}_Y\right) : \boldsymbol{Y} + (-\dot{\kappa} - B_K)K = 0 \quad \forall \text{ admissible } \dot{\boldsymbol{\sigma}}, \boldsymbol{Y}, K$$

$$\Rightarrow \quad \boldsymbol{\varepsilon} = \rho_0 \frac{\partial \psi^c}{\partial \boldsymbol{\sigma}}, \quad \dot{\boldsymbol{D}} = \boldsymbol{B}_Y, \quad \dot{\kappa} = -B_K$$

Handshaking with micro-/meso-scale models? Can ML help in constructing the potential functions?

Equibiaxial compression test





(lhs) Stress-strain behaviour in equibiaxial compression ($\sigma_{11} = \sigma_{22}$) with experimental results from Kupfer et al. 1969. The Abaqus CDP model responses are shown for four values of the dilatation angle. Notice that different dilatation angle gives the best fit to experimental data in comparison to unconfined uniaxial compression for the CDP model.

(rhs) Damage-strain behaviour, damage is the largest in the 33-direction, i.e. the fracture mode corresponds splitting along the compressive plane illustrated.

Conclusions and future work

- Experimental data closer to computation.
- Better tools for coarsening/upscaling.
- International collaboration for open data needed.
- What are the most efficient numerical methods for materials fracturing simulations?
- Are ML, DL, EML, etc. GOOD, BAD or OGLY?

Acknowledgements

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Thank You!