COMSOL CONFERENCE 2016 MUNICH

COMSOL Implementation of a Porous Media Model for Simulating Pressure Development in Heated Concrete

B. Weber[1], D. Dauti[2], and S. Dal Pont[2]

[1]Empa, Swiss Federal Laboratories for Material Science and Technology, Dübendorf
[2]Laboratoire 3SR, University Grenoble Alpes, Grenoble, France

Motivation: concrete spalling

Photo CSTB

- When exposed to high temperatures (fire), concrete can spall.
- Spalling: violent detachment of flakes
- Severe damage in tunnels after fire
- Presumable causes:
  - Pore pressure
  - Thermal stresses

→ Simulate pore pressure development

Thermo-hydro model

- Porous medium
- Gas (air+vapor) and liquid phase, partially saturated
- Heat transfer
- Moisture transfer

- Implemented with weak form interface (no physics interfaces)
  - Comparison with other implementations
  - Explore different formulations

Conservation equations

- General form of conservation equation

$$\frac{\partial}{\partial t} density + \nabla \cdot flux = source$$

- Air

$$\frac{\partial}{\partial t}(\phi(1-S)\rho_a) + \nabla \cdot (\rho_a \mathbf{v}_a) = 0$$

- Water species (vapor+liquid water, evaporation does not appear)

$$\frac{\partial}{\partial t}\phi\left(S\rho_l + (1-S)\rho_v\right) + \nabla \cdot \left(\rho_v \mathbf{v}_v + \rho_l \mathbf{v}_l\right) = \dot{m}_{\mathrm{dehyd}}$$

- Energy

$$\rho c_p \frac{\partial T}{\partial t} + \nabla \cdot (\underbrace{-k_{\mathrm{eff}} \nabla T}_{\text{heat conduction}}) + (\underbrace{\rho_v c_{pv} \mathbf{v}_v + \rho_a c_{pa} \mathbf{v}_a}_{\text{advective heat flux}}) \cdot \nabla T = -\dot{m}_{\mathrm{dehyd}} \Delta h_{\mathrm{dehyd}} - \dot{m}_{\mathrm{evap}} \Delta h_{\mathrm{evap}}$$

Variables

- Variables
  - Temperature
  - Mass densities (air, vapor, liquid)
  - Mass flux (air, vapor, liquid)
  - Saturation (liquid, gas)

- Three equations → 3 dependent variables
  - Temperature
  - Gas pressure
  - Variable for water content
    - Capillary pressure (used here)
    - Vapor pressure (used as alternative)
    - Saturation

- Need constitutive equations

Constitutive equations: mass density and flux

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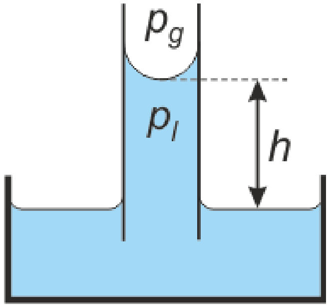
- Ideal gas law $\rho_a = \frac{p_a M_a}{RT}$ $\rho_v = \frac{p_v M_v}{RT}$
- Dalton's law $p_g = p_a + p_v$
- Darcy's law $\mathbf{v}_g = -\frac{\kappa_{rg} K}{\mu_g} \nabla p_g$ $\mathbf{v}_l = -\frac{\kappa_{rl} K}{\mu_l} \nabla p_l$
- Fick's law
- Incompressible water $\rho_l(T)$

Intrinsic permeability
Relative permeability

Capillary effects: vapor-liquid equilibrium

$$h = \frac{p_c}{\rho_l g}$$



- Surface tension in interface (meniscus)

$$p_c = \frac{2\sigma}{r}$$

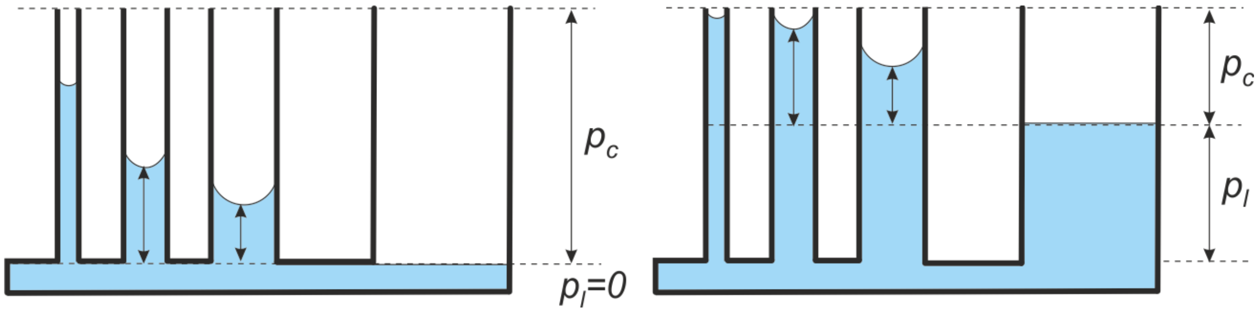
- Surface tension gives rise to pressure difference between gas and liquid water = capillary pressure

$$p_c = p_g - p_l$$

- Vapor-liquid equilibrium (Kelvin equation)

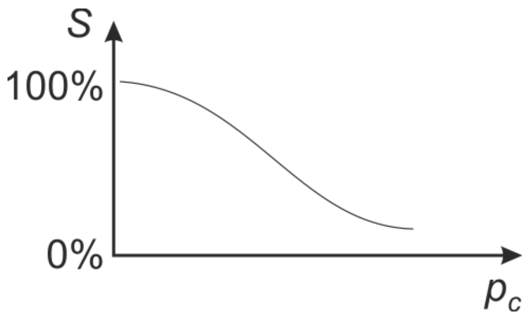
$$p_v = p_{sat}(T) \cdot \exp\left(\frac{-p_c M_w}{\rho_l RT}\right)$$

Capillary effects: Saturation



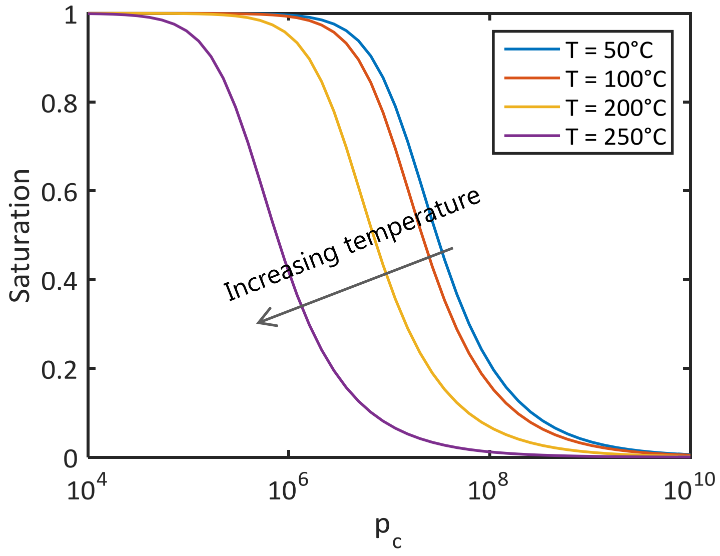
Bundle of capillary tubes

- Saturation $S(p_c)$ where $p_c = p_g - p_l$ (global)
- Relative height in each tube depends only on radius
- If global water pressure (reservoir level) is increased
  - Global p_c decreases
  - Saturation increases

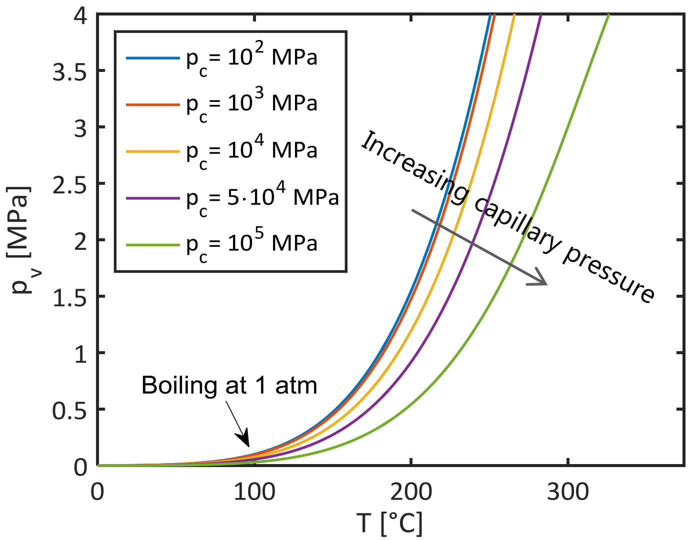


Properties related to capillary pressure

- Saturation(van Genuchten)

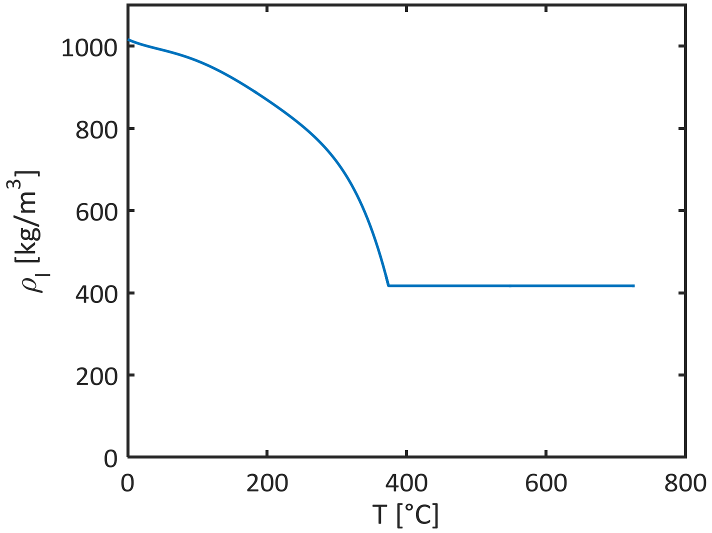


- Vapor pressure (Kelvin)



Limitations of model

- Density of liquid water



- Density is used in Kelvin's equation

$$p_v = p_{sat}(T) \cdot \exp\left(\frac{-p_c M_w}{\rho_l R T}\right)$$

- Liquid water density undefined above critical temperature (374°C)
- As a workaround, we kept the water density constant beyond the critical density.

Example: weak form for air conservation

$$\frac{\partial}{\partial t}\left(\phi(1-S)\rho_a\right)+\nabla\cdot\left(\rho_a\mathbf{v}_a\right)=0$$

PDE for air

Weak form

$$0=-\int_{\Omega}\tilde{p}_g\frac{\partial}{\partial t}\left(\phi(1-S)\rho_a\right)\mathrm{d}\Omega$$

−test(pg)*d(phi*(1-S)*rho_a,t)

$$+\int_{\Omega}\nabla\tilde{p}_g\cdot\left(\rho_a\mathbf{v}_a\right)\mathrm{d}\Omega$$

test(pgx)*flux_ax+test(pgy)*flux_ay (2D)

$$+\int_{\Sigma}\tilde{p}_g\underbrace{\left(\rho_a\mathbf{v}_a\right)\cdot\mathbf{n}}_{\text{air outflow}}\mathrm{d}\Sigma$$

Boundary condition

Automatic recursive variable substitution

$$\frac{\partial}{\partial t}\left(\phi(1-S)\rho_a\right)$$

d(phi*(1-S)*rho_a,t)

Derivative with resp. to t

phi= phi0+Aphi*(T-Tamb)

S(pc,T)

rho_a= Ma/(R_const*T)*pa *Ideal gas*

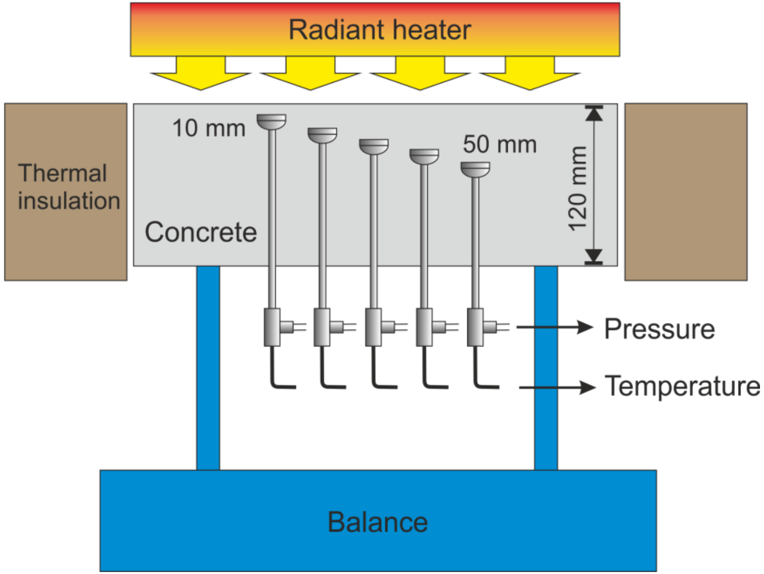
pa= pg-pv *Dalton in this form!*

pv= psat(T)*exp(-pc/rho_l*Mw/R_const/T) *Kelvin*

rho_l= c_1+c_2*T+c_3*T^2+...

- Dependent variables T, pg, pc on the right-hand side
- Avoid circular variable definitions

Experiment form literature

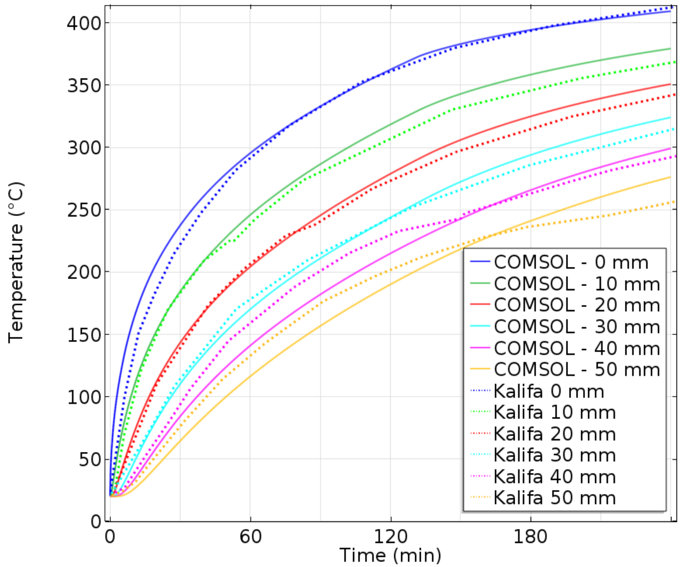


- 12-cm-thick concrete slab 30 x 30 cm^2
- Pressure and temperature sensors
- Heated with radiator from top during several hours
- Not all material parameters are provided in the paper: others from literature or by calibration.

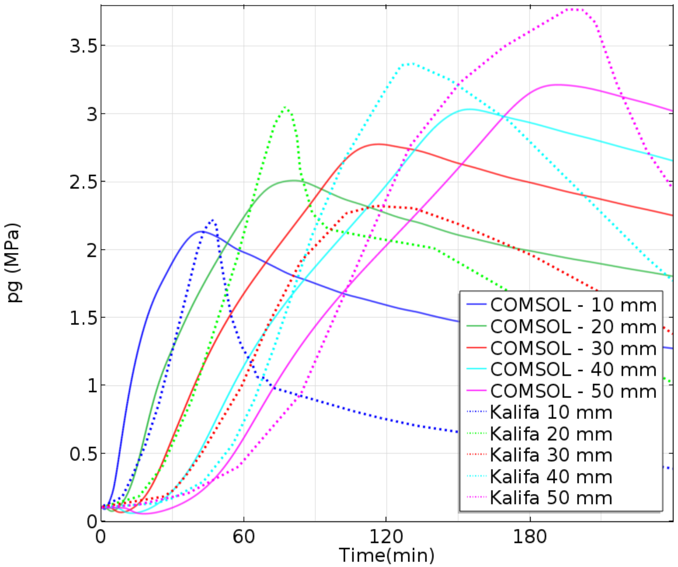
Kalifa, et al., Spalling and pore pressure in HPC at high temperatures, *Cement and concrete research*, **30**, 1915-1927 (2000).

Comparison with experiment

Temperature



Gas pressure

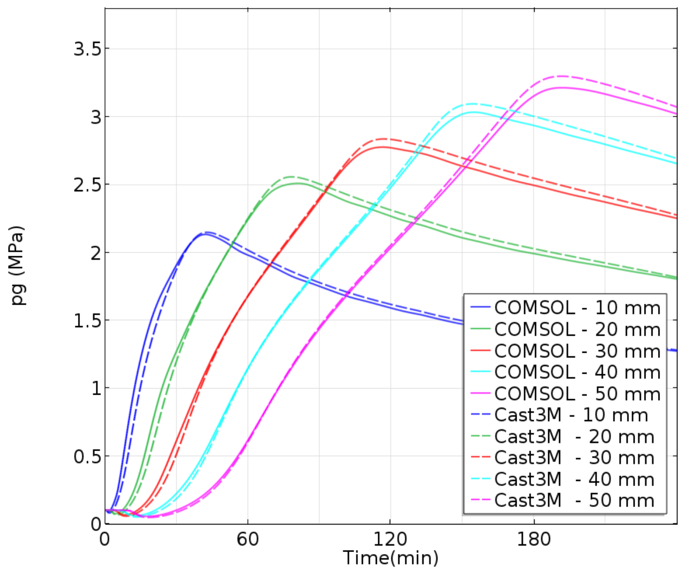


Material properties and calibration

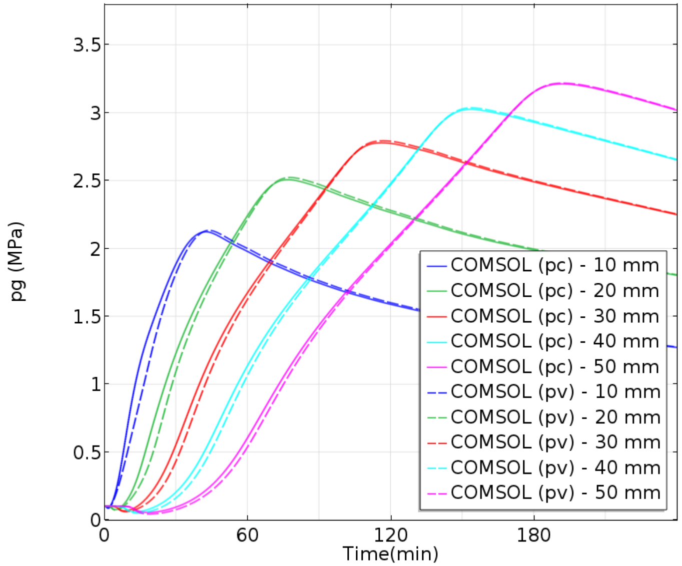
- Temperature (fitting)
  - Radiator temperature
  - Heat transfer coefficients
- Permeability (main tuning parameter)
  - Nominal value (tuning)
  - Evolution with temperature (cracking)
- Saturation law (main uncertainty)
  - Standard curve at room temperature (van Genuchten)
  - Temperature dependence: no data >100°C

Comparison with other implementations

Cast3M



pv instead of pc



- Similar computing time with fixed time step.
- COMSOL with variable time step 6-7 times faster, but curves not as smooth
- COMSOL with pv instead of pc does not significantly change computing time

Summary and conclusions

- Used Weak Form interface to implement a model for heat and mass transfer in heated concrete.
- Automatic variable substitution makes COMSOL very powerful for implementing complex problems.
- Model was also used to verify the implementation with Cast3M.
- Model was able to reproduce data from experiments.
- Calibration is needed for missing material properties (and model deficiencies).