COMSOL CONFERENCE 2018 LAUSANNE

Alternative implementation of a porous media model for simulating drying of heated concrete

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Motivation

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 increase due to evaporation and dehydration
  - Thermal stresses

Introduction (1)

- Porous medium, partially saturated
- Gas (air+vapor) and liquid phase
- Heat and moisture transfer
- Vapor sources: evaporation and dehydration
- Mechanical stresses not considered

- Single classical formulation for concrete in literature (presented in previous COMSOL conference)
  - Uses capillary pressure as primary variable
  - Vapor pressure from phase equilibrium

} undefined for $S=0$ and for $T>T_{cr}$ (374°C)

Introduction (2)

- Different implementations for other applications
  - Food drying
  - Oil and gas exploration
  - Compressible / incompressible phases
  - With or without phase change
- Alternative formulation
  - Non-equilibrium: evaporation rate from deviation of vapor pressure from equilibrium pressure
- Use weak form interface

Conservation equations

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

- Gas conservation $\rho_g = \rho_a + \rho_v$

$$\frac{\partial}{\partial t}\left(\phi(1-S)\rho_g\right) + \nabla \cdot \left(\rho_g \mathbf{v}_g\right) = \dot{m}_{\text{evap}} + \dot{m}_{\text{dehyd}}$$

- Vapor mass fraction $\omega_v = \rho_v / \rho_g$

$$\phi(1-S)\rho_g \frac{\partial \omega_v}{\partial t} + \nabla \cdot \mathbf{j}_v + \underbrace{\rho_g \mathbf{v}_g}_{\text{convection}} \cdot \nabla \omega_v = (1-\omega_v)(\dot{m}_{\text{dehyd}} + \dot{m}_{\text{evap}})$$

- Liquid conservation

$$\frac{\partial}{\partial t}\left(\phi S \rho_l\right) + \nabla \cdot \left(\rho_l \mathbf{v}_l\right) = -\dot{m}_{\text{evap}}$$

- Energy conservation

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

Dependent variables and BC

Dependent variables	Conservative Flux	Dirichlet BC → dependent variable Neumann BC → conservative flux	
p_g	$\rho_g \mathbf{v}_g$	$p_g = p_g^{amb}$	
$\omega_v = \rho_v / \rho_g$	$\mathbf{j}_v = -\rho_g D_{eff} \nabla \omega_v$	$-\mathbf{n} \cdot \mathbf{j}_v = 0$	constant mixture
S	$\rho_l \mathbf{v}_l$	$-\mathbf{n} \cdot (\rho_l \mathbf{v}_l) = -K_0^l \left\langle p_l - p_g^{amb} \right\rangle^+$	outflow
T	$-k_{\text{eff}} \nabla T$	$-\mathbf{n} \cdot \left(-k_{\text{eff}} \nabla T\right) = h_T \left(T_{ext} - T\right) + \varepsilon\sigma\left(T_{\text{ext}}^4 - T^4\right)$	

- Choice of primary variables and equations influences formulation of BCs

Capillary effects

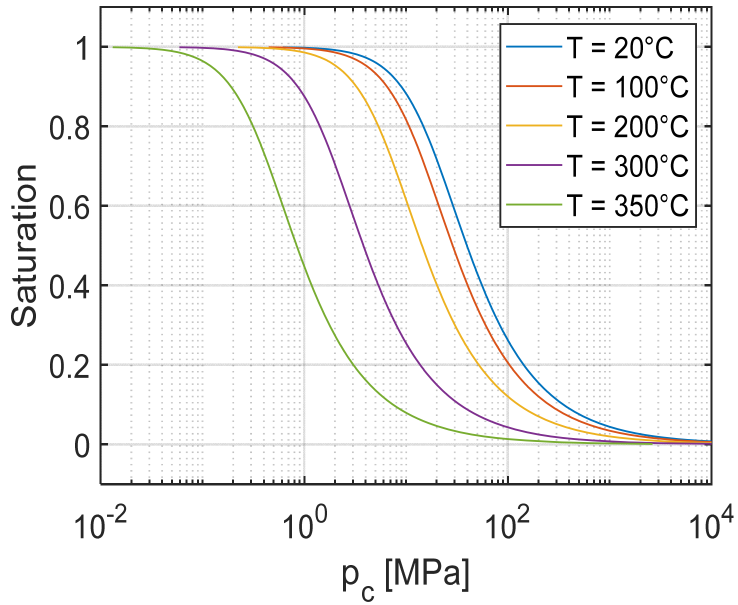
(1) Capillary pressure $p_c = p_g - p_l$

(2) Sorption isotherms (van Genuchten)
→ Description of porous medium

$$S = \left[1 + \left(\frac{p_c^{amb}}{a} \right)^{\frac{b}{b-1}} \right]^{-1/b} \qquad p_c = p_c^{amb} \left(\frac{T_{cr} - T}{T_{cr} - T_{amb}} \right)^N$$

(3) Vapor saturation pressure (Kelvin)

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



Connecting variables with capillary effects

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Classic		**Alternative**
$T \quad p_g \quad p_c$		$T \quad p_g \quad \omega_v \quad S$
$S(p_c, T)$ → (2)	S	← S
$p_v = p_v^{eq}(T, p_c)$ → (3)	p_v	← $p_v = \omega_v p_g M_g / M_w$
Vapor conservation Liquid conservation →	$\dot{m}_{evap}$	← (3,2) $\dot{m}_{evap} = \begin{cases} K_0 \left[p_v^{eq}(T, p_c) - p_v \right] & \text{if } p_c \text{ defined} \\ 0 & \text{else} \end{cases}$
$p_l = p_g - p_c$ → (1)	p_l	← (1,2) $p_l = \begin{cases} p_g - p_c & \text{if } p_c \text{ defined} \\ p_g & \text{else} \end{cases}$

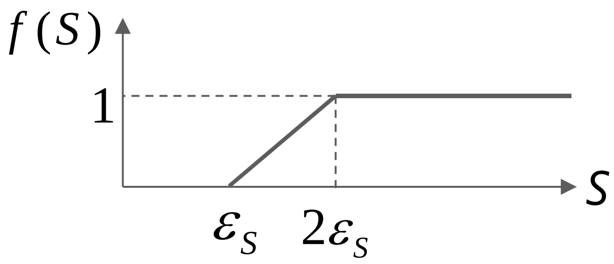
$p_c(S,T)$ defined if $S > 0$ and $T < T_{cr}$

(1) Capillary pressure (2) Sorption isotherm (3) Vapor saturation pressure

Regularization (1)

- Stop evaporation if S=0 or $T>T_{cr}$
- Only evaporation restricted, not condensation

$$\Delta p_v = \underbrace{\left\langle p_v^{eq} - p_v \right\rangle^+}_{\text{positive part evaporation}} \underbrace{\frac{\max(S-\varepsilon_S,0)}{\max(S-\varepsilon_S,\varepsilon_S)}}_{f(S)} + \underbrace{\left\langle p_v^{eq} - p_v \right\rangle^-}_{\text{negative part condesation}}$$



- Also restriction with temperature

$$\dot{m}_{evap} = K_0^{evap} \frac{M_w}{RT} \Delta p_v \frac{\max(T-T_{cr}-\varepsilon_T,0)}{\max(T-T_{cr}-\varepsilon_T,\varepsilon_T)}$$

Regularization (2)

- van Genuchten not invertible for S=0

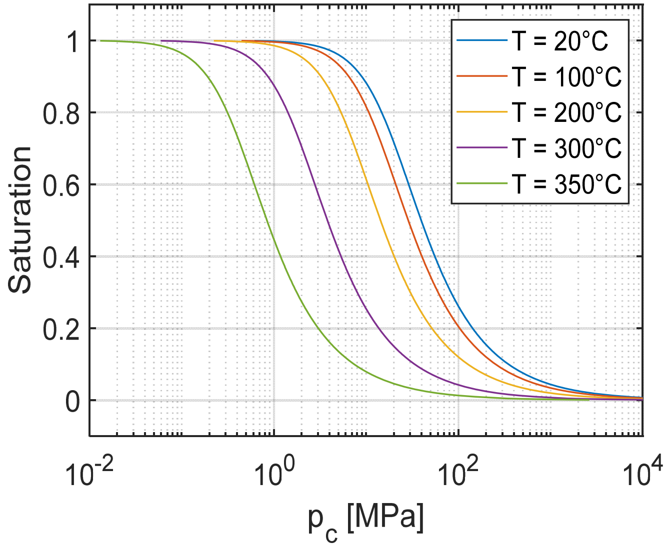
$$p_c^{amb} = a\left(S^{-b} - 1\right)^{(1-1/b)}$$

- Relative liquid permeability also undefined for S=0

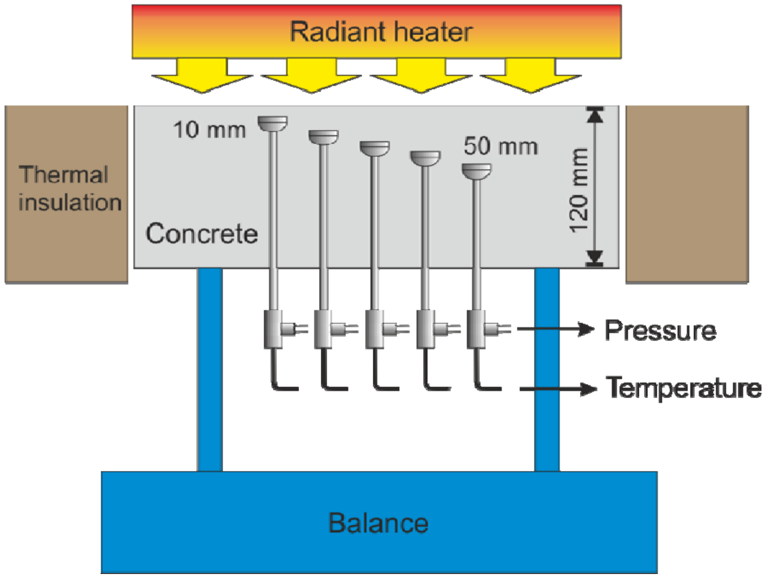
$$\kappa_{rl} = \sqrt{S}\left[1-\left(1-S^{b}\right)^{1/b}\right]^2$$

- For relative permeability and saturation use

$$S_{reg} = \max(S, \varepsilon_s)$$



Experiment

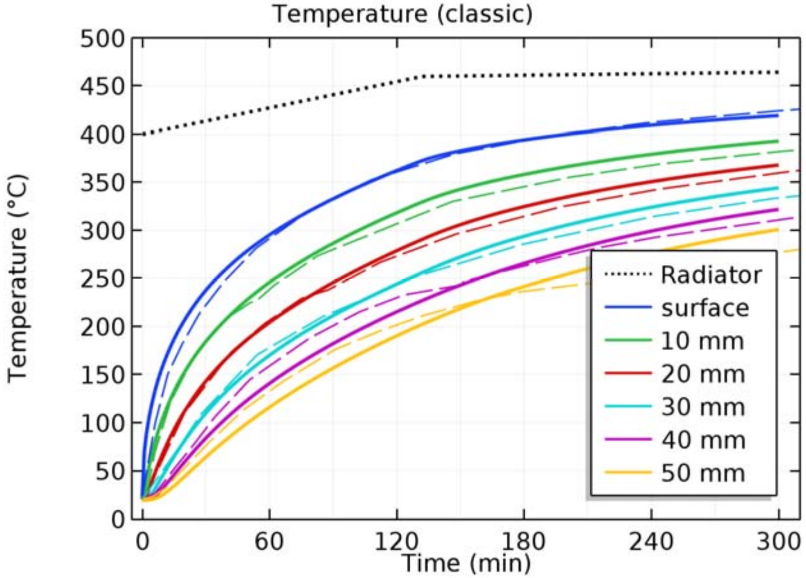


- 12-cm-thick concrete slab 30 x 30 cm^2
- Pressure and temperature sensors
- Heated with radiator from top during several hours
- Not all material parameters are provided in the paper: others from literature or by calibration.

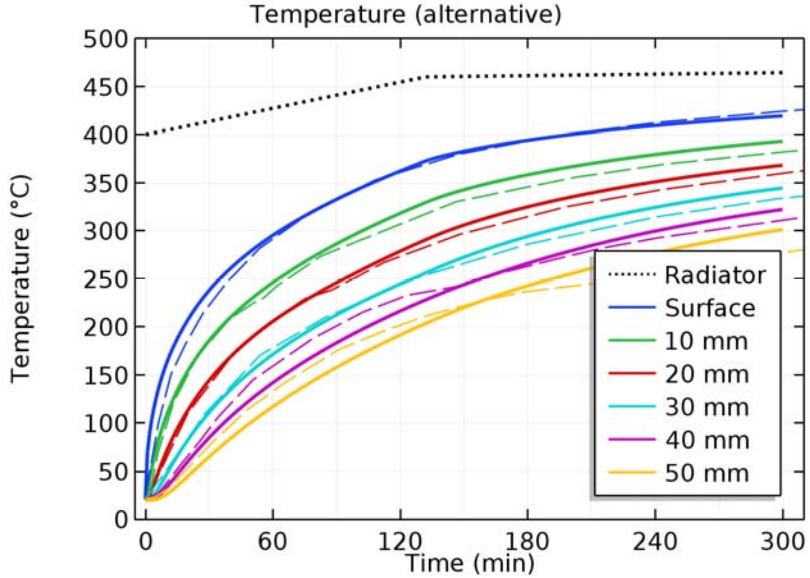
Kalifa, et al., Spalling and pore pressure in HPC at high temperatures, *Cement and concrete research*, **30**, 1915-1927 (2000).

Temperature

Classic



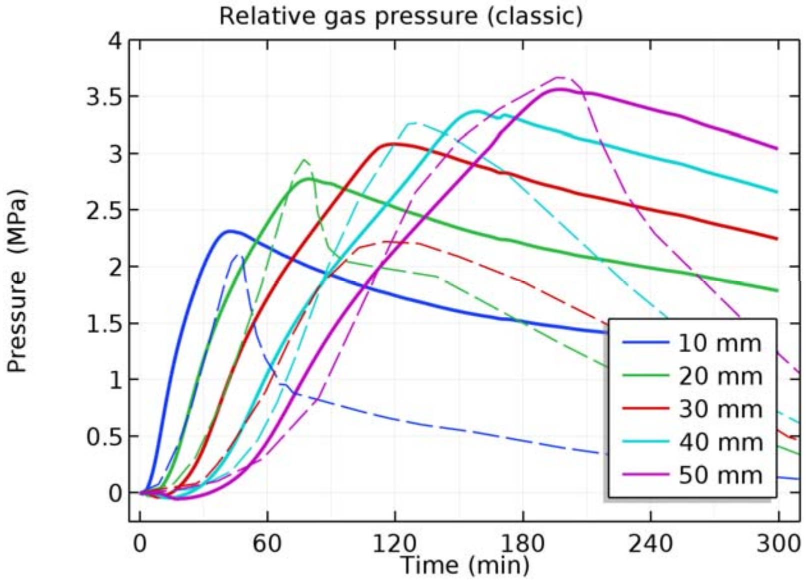
Alternative



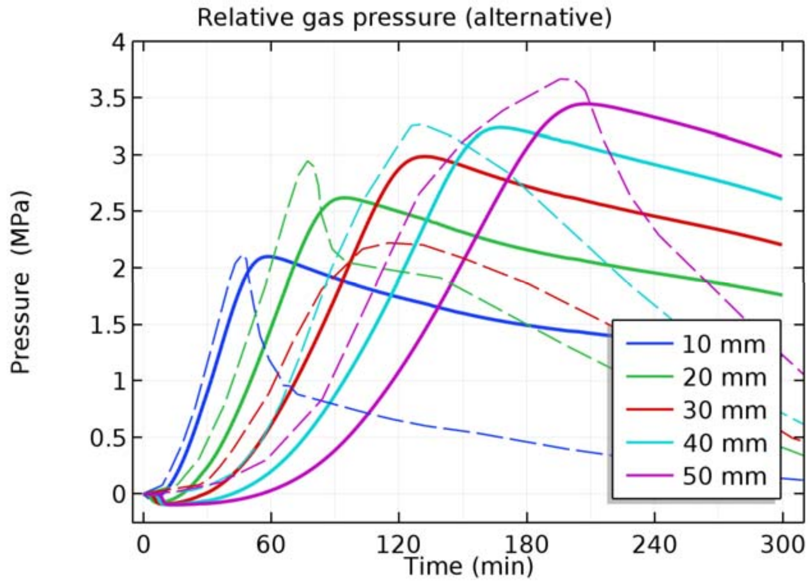
- Identical results

Pore pressure

Classic



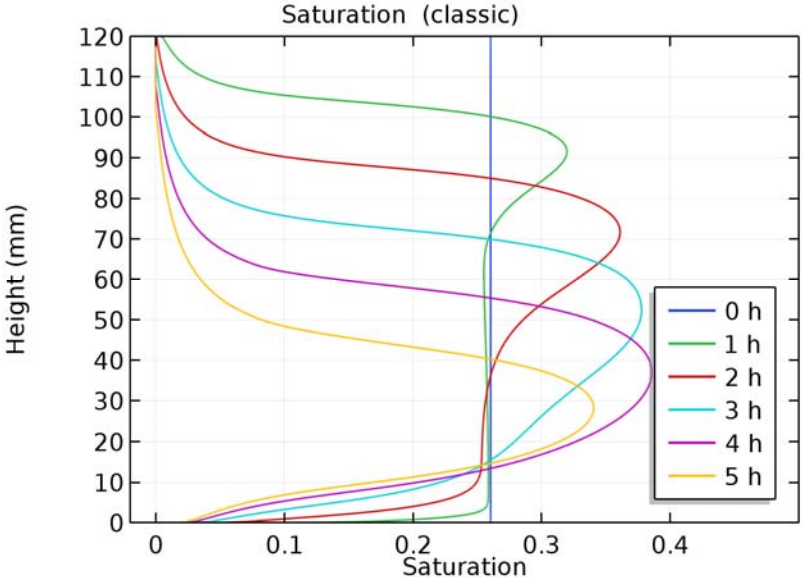
Alternative



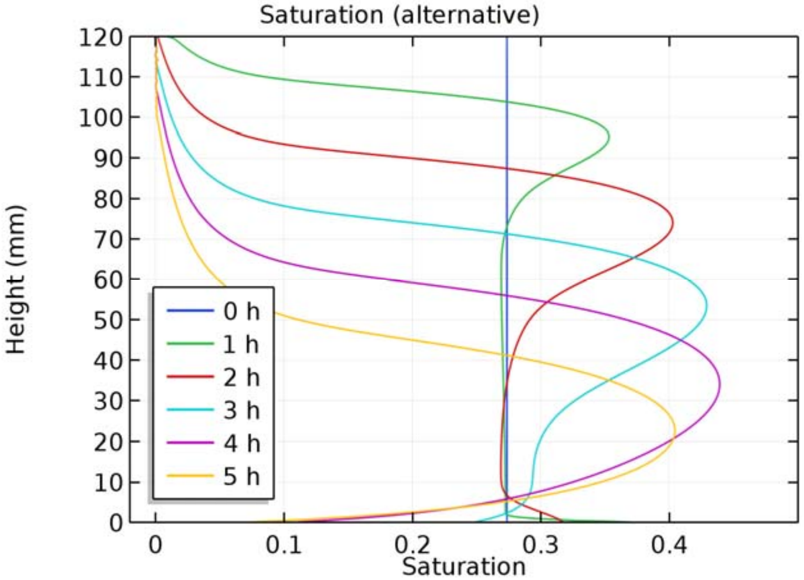
- Similar profiles
- Better shape at beginning

Saturation profile

Classic



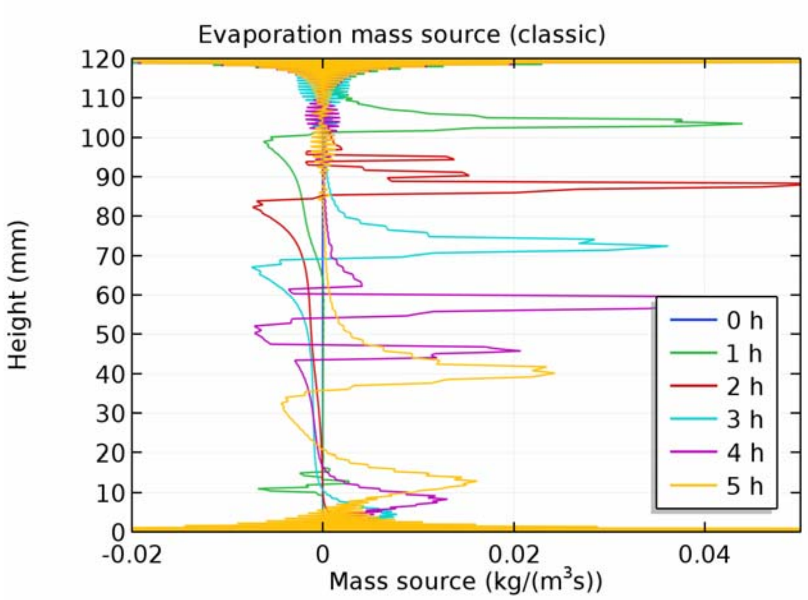
Alternative



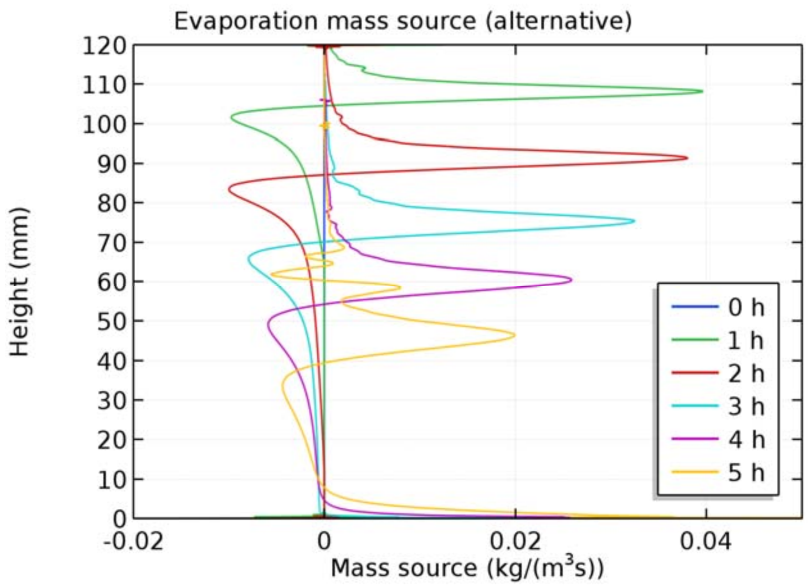
- Very similar
- Different at boundaries

Evaporation mass profile

Classic



Alternative



- Globally similar
- Classic more noisy

Evaporation mass profile, classic formulation

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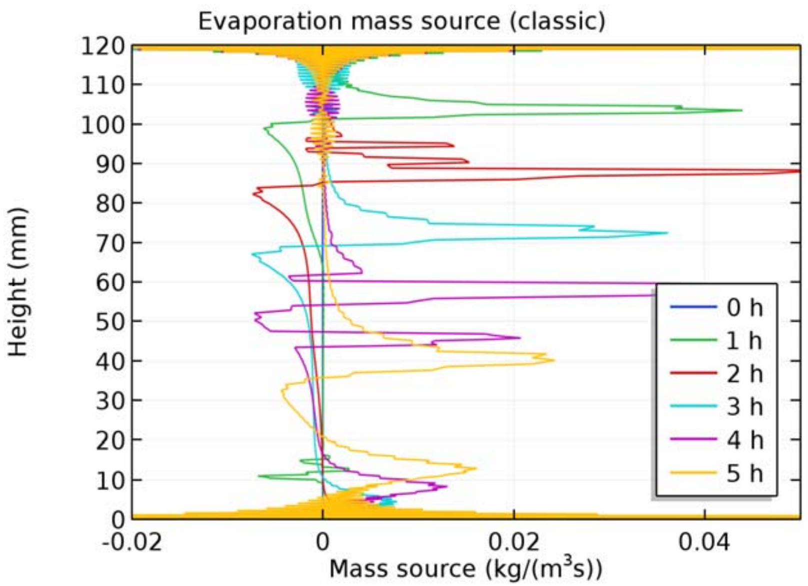
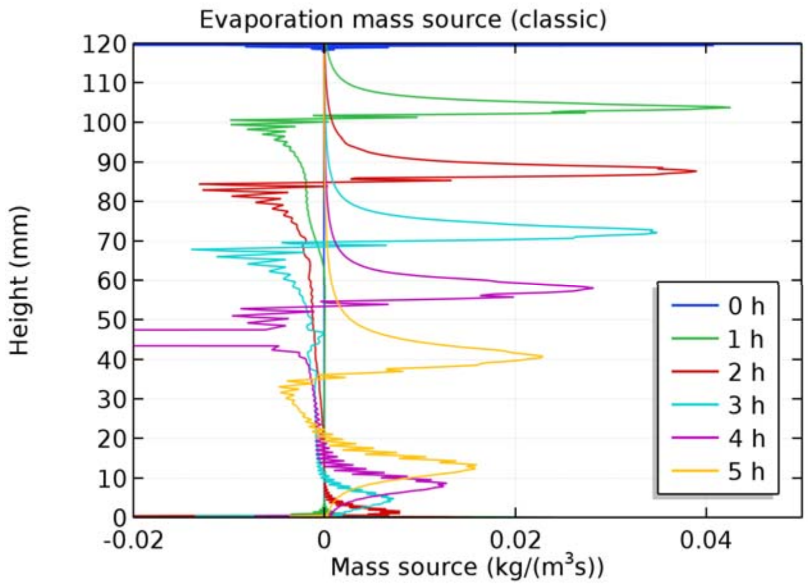
Postprocessing with vapor conservation



Postprocessing with liquid conservation



- Simulation and postprocessing with evaporation mass from vapor or liquid conservation equation
- Results depend mainly on postprocessing not on simulation

Discussion

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Classic

- Similar pressure and saturation
- Noisy evaporation mass
- Difficult interpretation for $T>T_{cr}$
- Faster execution time (70 s)
- Numerical tweaks necessary

Alternative

- Similar pressure and saturation
- Smooth evaporations mass
- Correct physics for $T>T_{cr}$
- Slower execution time (130 s)
- Additional primary variable and regularization

Conclusions

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- Alternative formulation to avoid nonphysical details of classical model, in particular, avoid capillary pressure as primary variable, since not physical when S=0 or $T>T_{cr}$
- Use non-equilibrium formulation: evaporation proportional to pressure difference (equilibrium pressure – actual pressure)
- Extra effort, but more rational physics
- Similar pressure and saturation, since relevant processes occur below T_{cr}
- Relatively easy to make major model changes and try different formulations with Equation-Based Modeling