Comparison of pore network model with macro models and experiments

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Introduction. Drying of porous media is a process with micro-macro interactions in a structured medium or a particle system. During drying moisture is removed from inside a wet porous sample. The choice of the process as well as process parameters, such as temperature (pressure, air velocity), and the characteristic properties of the wetted porous medium to be dried (porosity, tortuosity, connectivity of the void space, pore size distribution; contact angle, surface tension, liquid viscosity of the liquid phase) define the order of emptying of liquid filled pores (on the micro-scale) and thus impact on the macro-scale product quality after drying. The correlation between the drying result and pore-scale phenomena can be described with discrete pore network models which have a physical base and account for mass, energy and impulse balances in individual micro pores.

Problem Definition

Pore network models are a strong tool to simulate, understand and describe drying of porous media. However, solving the set of mass balances of gas and liquid phase for each pore is very time consuming, thus simulation at the sample scale with available computing technology is impossible.

Objectives

- Experimental validation of the results obtained from 2-dimensional pore network simulations.
- Parameterization of empirical macroscopic and continuous models by Monte Carlo simulation with 2- and 3-dimensional pore network models.
- Simulation of drying on the sample scale.

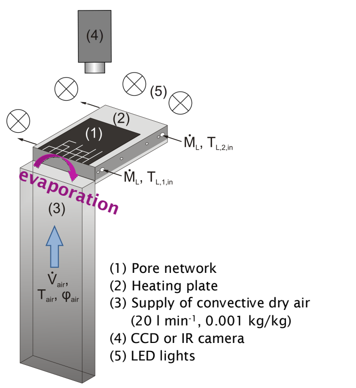
Cooperation

- Florian Schulz, ISUT, FVST, OvGU (contact angle measurements).
- Stephan Baer, ISUT, FVST, OvGU (measurements with infrared camera).
- Yujing Wang, IVT, FVST, OvGU (liquid film modeling and experimental validation)

Drying Experiments

Experimental set-up

- Network dried by one open side.
- Horizontal orientation: → **no gravity**.

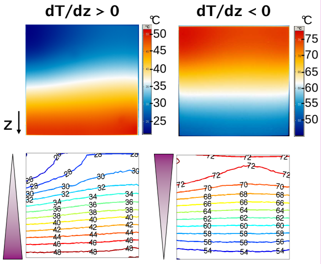


(1) Pore network
(2) Heating plate
(3) Supply of convective dry air (20 l min^{-1}, 0.001 kg/kg)
(4) CCD or IR camera
(5) LED lights

Imposed temperature gradients

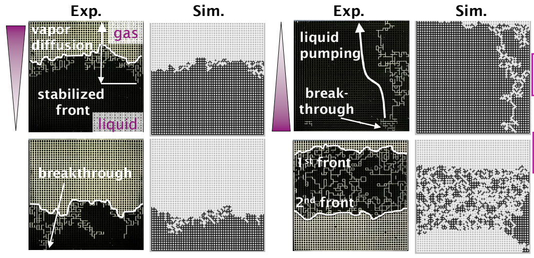
- Monitored once with infrared measurement (S. Baer, ISUT).
- Reference measurement by thermocouples in metal plate.
- Stationary temperature field during experiments.

positive gradient $dT/dz > 0$ — **negative gradient** $dT/dz < 0$



Experimental vs simulation results

T = 74 … 53 °C, T_{air} = 25.2 °C — **T = 27 … 49 °C, T_{air} = 25.6 °C**



Vapor Diffusion

$$\dot{M}_{v,ij} = \pi r_{ij}^2 \frac{\delta(T_{ij})}{L} \frac{\tilde{M}_v P}{\tilde{R} T_{ij}} \cdot \ln\left(\frac{P - P_{v,i}}{P - P_{v,j}}\right)$$

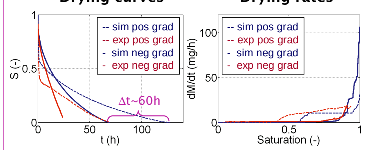
Capillarity

$$P_{w,ij} = P - \frac{2\sigma(T_{ij})}{r_{ij}} \qquad r_{ij} = 2\frac{r_{ij,1} \cdot r_{ij,2}}{r_{ij,1} + r_{ij,2}}$$

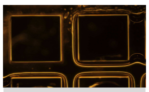
Boundary Condition

$$\dot{M}_{w,ij} = \dot{M}_{v,ij}$$

Drying curves — **Drying rates**



Role of thick capillary liquid films



Liquid Films in Pore Network. (Ref. M. Prat, IMFT)

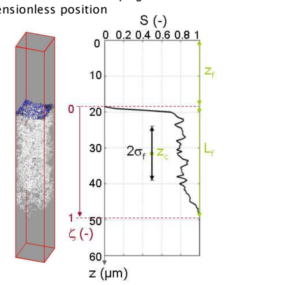
- Connected liquid phase in 2-phase zone.
- Enhanced mass transfer.
- → Drying front at overall higher position.
- → Increased drying rate.
- → Shorter drying time, lower energy effort.

→ Including film effects in the mathematical model (cooperation with Y. Wang, IVT).

Empirical Macroscopic Model

Definition of front width

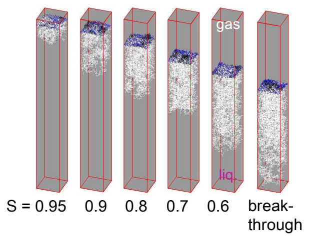
L_f = front width
σ_f = standard deviation of drying front
ζ = dimensionless position



3D drying simulation

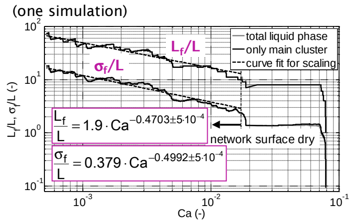
Network size
15x15x120

- liquid throats (S_{slice} < 0.6)
- gas throats (S_{slice} > 0.6)
- partially filled throats



Scaling of front width with Ca

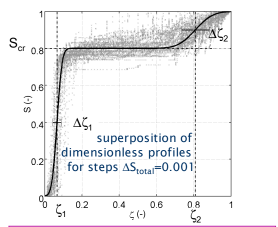
(one simulation)



$$\frac{L_f}{L} = 1.9 \cdot Ca^{-0.4703 \pm 5 \cdot 10^{-4}}$$

$$\frac{\sigma_f}{L} = 0.379 \cdot Ca^{-0.4992 \pm 5 \cdot 10^{-4}}$$

Averaged saturation profiles



$$S(\zeta) = \frac{S_{cr}}{\sqrt{2\pi}\Delta\zeta} \int_{-\infty}^{\zeta} \exp\left(-\frac{1}{2}\left(\frac{\zeta - \zeta}{\Delta\zeta}\right)^2\right) d\zeta + (1 - S_{cr}) \cdot \zeta$$

Access to drying rate curves

- Drying rate is estimated at position z_f, least advanced point of the front, (assuming a flat front):

$$\dot{m}_v = -\left(\frac{s}{\delta} + \frac{z_f L^2}{\delta \cdot \pi r_0^2}\right)^{-1} \frac{\tilde{M}_v P}{\tilde{R} T} \cdot \ln\left(1 - \frac{P_v^*}{P}\right)$$

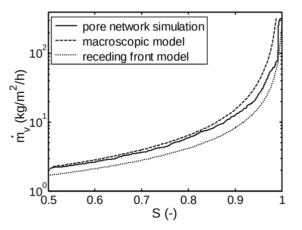
- With corresponding capillary number:

$$Ca = \frac{4 \nu_w L^3 \dot{m}_v}{\sigma \pi r_0^2 \sigma_0}$$

- The scaling law is applied to calculate the front width:

$$L_f = 1.9 \cdot Ca^{-0.4703 \pm 5 \cdot 10^{-4}} \cdot L$$

- Network saturation **S** follows from the master curve of saturation profiles **S(ζ)** in the interval from z_f to $z_f + L_f$.



The curve for a planar receding front (with L_f = 0) corresponds to the limit of infinite liquid viscosity and is estimated for $z_f = z_{max}$ (most advanced front position).

Outlook: Parameterization of 3D Continuous Drying Model

Continuous model of drying

- **One PDE for liquid and vapor transport:**

$$\frac{\partial}{\partial t}\left(S\psi\rho_w + (1-S)\psi\frac{\tilde{M}_v P_v}{\tilde{R}T}\right) = \frac{\partial}{\partial z}\left(D_{eff}\frac{\tilde{M}_v P}{\tilde{R}T}\frac{\partial \ln(P - P_v)}{\partial z} - \frac{K k_w}{\nu_w}\frac{\partial P_c}{\partial z}\right)$$

- Parameterization by Monte Carlo simulations with 3D pore networks.
- **Extraction of parameters from the fractal drying front zone**

→ account for fractal front structure in continuous model.

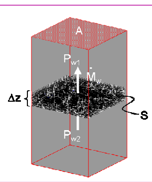
Effective parameters

- Absolute and relative liquid permeability, K(S=1) and $k_w(S)$.
- Absolute and relative diffusivity, $D_{eff}(S=0)$ and $D_{eff}(S)$.
- Capillary pressure curve $P_c(S)$.

$$K k_w(S) = \nu_w \frac{\dot{M}_w(S)}{A}\frac{\Delta z}{\Delta P_w}$$

$$D_{eff}(S) = \frac{\tilde{R}T}{\tilde{M}_v}\frac{\dot{M}_v(S)}{A}\frac{\Delta z}{\Delta P_v}$$

$$P_c^{min}(S)$$



- For a given slice saturation 0<S<1, impose a pressure gradient DP_w and calculate the resulting flow $\dot{M}_w$ to determine k_w.
- Compute K for totally saturated slice (S=1).
- Treat gas phase analoguously to find D_{eff} and D_{eff}(S=0).
- Determine the minimum capillary pressure of the (connected) main cluster inside the slice.

DFG-Graduate School 1554 “Micro-Macro-Interactions in Structured Media and Particle Systems”