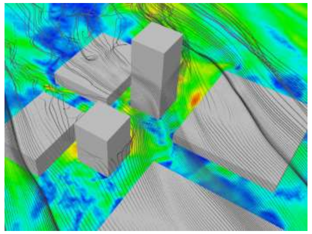
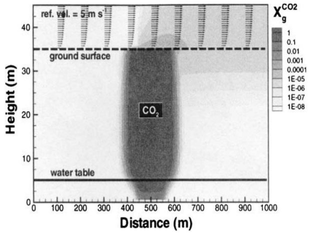
# Introduction

## Motivation

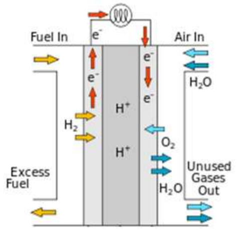


http://www.project-simba.eu

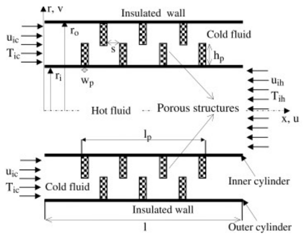



Oldenburg and Unger 2004

- urban climate
- $CO_2$ leakage
- atomic waste storage, …

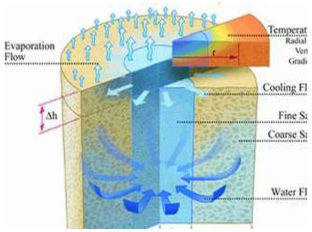



www.en.wikipedia.org

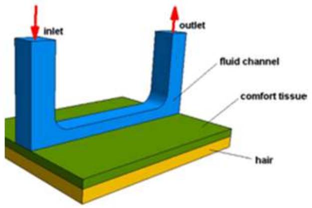



Targui and Kahalerra 2008

- fuel cells
- heat exchanger
- oil filters, …




www.step.ethz.ch

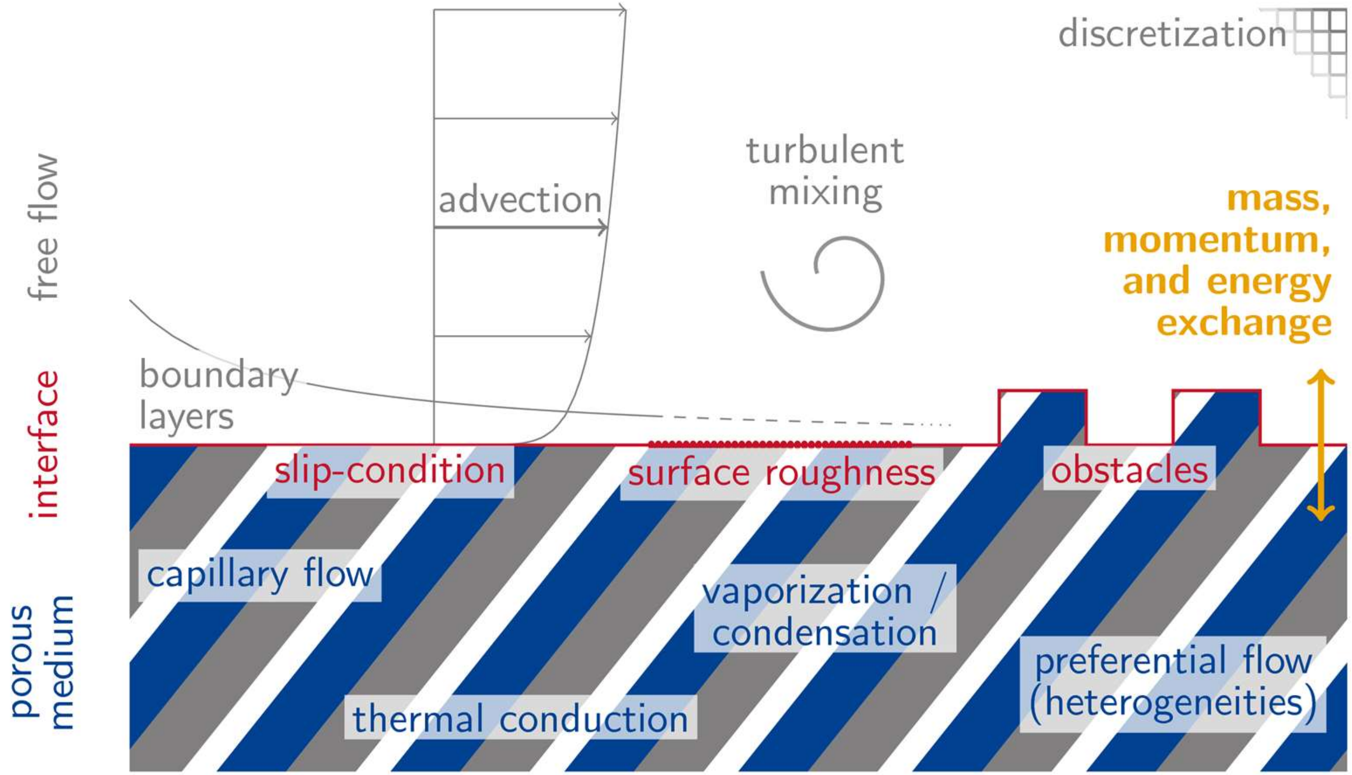



Cimolin and Discaciatti 2013

- soil water evaporation
- evaporative cooling
- soil salinization, …

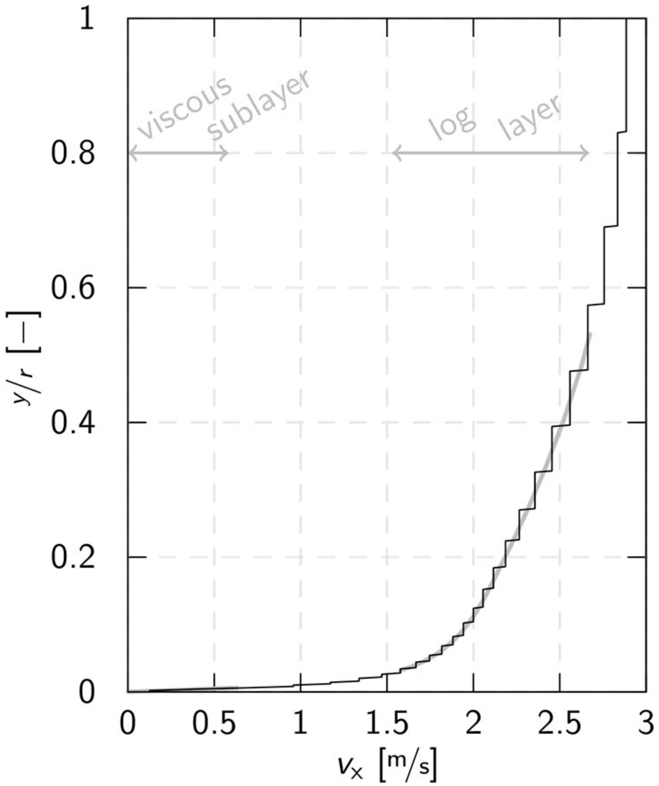
# Introduction

## Processes and Properties



# Introduction

## Spatial Resolution of Processes



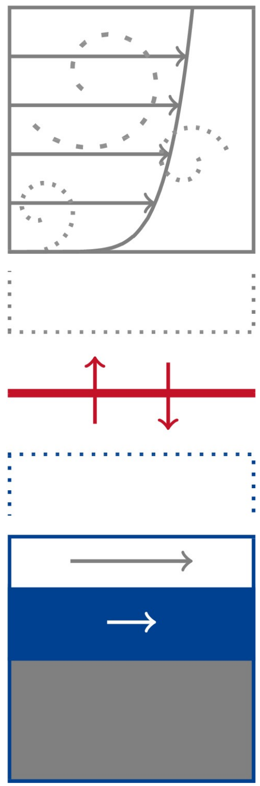
# Model

## Two-Domain/ Sharp-Interface Concept

- Stokes/ Navier-Stokes/ RANS
- 1 phase, n-components, non-isothermal

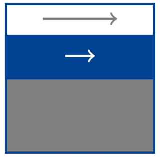
- no thickness, no storage
- local thermodynamic equilibrium
- continuity of fluxes
- continuity of state variables

- Darcy/ Forchheimer/ Richards
- m-phases, n-components, non-isothermal



# Model

## Porous Medium – Equations



- total mass balance

$$\sum_{\alpha\in\{\mathrm{l},\mathrm{g}\}} \left( \underbrace{\phi \frac{\partial \left(\varrho_{\mathrm{mol},\alpha} S_\alpha\right)}{\partial t}}_{\text{storage}} + \underbrace{\nabla \cdot \left(\varrho_{\mathrm{mol},\alpha} \mathbf{v}_\alpha\right)}_{\text{advection}} \right) = 0$$

- component mass balance

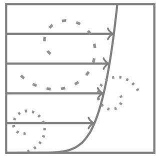
$$\sum_{\alpha\in\{\mathrm{l},\mathrm{g}\}} \left( \underbrace{\phi \frac{\partial \left(\varrho_{\mathrm{mol},\alpha} S_\alpha x_\alpha^\kappa\right)}{\partial t}}_{\text{storage}} + \underbrace{\nabla \cdot \left(\varrho_{\mathrm{mol},\alpha} x_\alpha^\kappa \mathbf{v}_\alpha\right)}_{\text{advection}} + \underbrace{\nabla \cdot \mathbf{j}_\alpha^{\kappa,\mathrm{pm}}}_{\text{diffusion}} \right) = 0$$

- energy balance

$$\sum_{\alpha\in\{\mathrm{l},\mathrm{g}\}} \left( \underbrace{\phi \frac{\partial \left(\varrho_\alpha S_\alpha u_\alpha\right)}{\partial t}}_{\text{storage (fluids)}} + \underbrace{\nabla \cdot \left(\varrho_\alpha h_\alpha \mathbf{v}_\alpha\right)}_{\text{advection}} \right) + \underbrace{\left(1 - \phi\right) \varrho_\mathrm{s} c_\mathrm{s} \frac{\partial T}{\partial t}}_{\text{storage (solid)}} - \underbrace{\nabla \cdot \left(\lambda^{\mathrm{pm}} \nabla T\right)}_{\text{conduction}} = 0$$

**Model**

## Free Flow – Reynolds-Averaged Navier-Stokes Equations



- total mass balance

$$\underset{\text{storage}}{\frac{\partial \varrho_{\mathrm{mol,g}}}{\partial t}} + \underset{\text{advection}}{\nabla \cdot \left(\varrho_{\mathrm{mol,g}} \bar{\mathbf{v}}_{\mathrm{g}}\right)} = 0$$

- momentum balance

$$\underset{\text{storage}}{\frac{\partial \left(\varrho_{\mathrm{g}} \bar{\mathbf{v}}_{\mathrm{g}}\right)}{\partial t}} + \underset{\text{inertia}}{\nabla \cdot \left(\varrho_{\mathrm{g}} \bar{\mathbf{v}}_{\mathrm{g}} \bar{\mathbf{v}}_{\mathrm{g}}^{\mathsf{T}}\right)} - \underset{\text{effective stress}}{\nabla \cdot \boldsymbol{\tau}_{\mathrm{eff}}} + \underset{\text{pressure}}{\nabla \cdot \left(\bar{p}_{\mathrm{g}} \mathbf{I}\right)} - \underset{\text{gravity}}{\varrho_{\mathrm{g}} \mathbf{g}} = 0$$

- component mass balance

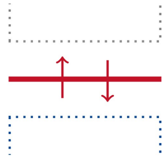
$$\underset{\text{storage}}{\frac{\partial \left(\varrho_{\mathrm{mol,g}} \bar{x}_{\mathrm{g}}^{\kappa}\right)}{\partial t}} + \underset{\text{advection}}{\nabla \cdot \left(\varrho_{\mathrm{mol,g}} \bar{x}_{\mathrm{g}}^{\kappa} \bar{\mathbf{v}}_{\mathrm{g}}\right)} + \underset{\text{effective diffusion}}{\nabla \cdot \mathbf{j}_{\mathrm{eff}}^{\kappa,\mathrm{ff}}} = 0$$

- energy balance

$$\underset{\text{storage}}{\frac{\partial \left(\varrho_{\mathrm{g}} \bar{u}_{\mathrm{g}}\right)}{\partial t}} + \underset{\text{advection}}{\nabla \cdot \left(\varrho_{\mathrm{g}} \bar{h}_{\mathrm{g}} \bar{\mathbf{v}}_{\mathrm{g}}\right)} + \underset{\text{effective diffusion}}{\sum_{\kappa \in \{\mathrm{w,a}\}} \nabla \cdot \left(\bar{h}_{\mathrm{g}}^{\kappa} \mathbf{j}_{\mathrm{mass,eff}}^{\kappa,\mathrm{ff}}\right)} + \underset{\text{effective conduction}}{\nabla \cdot \mathbf{j}_{\mathrm{cond,eff}}^{\mathrm{ff}}} = 0$$

## Model

Interface – Coupling Conditions I



- total mass

$$\left[\left(\varrho_{\mathrm{mol,g}}\mathbf{v}_{\mathrm{g}}\right)\cdot\mathbf{n}\right]^{\mathrm{ff,if}} = -\left[\left(\varrho_{\mathrm{mol,g}}\mathbf{v}_{\mathrm{g}} + \varrho_{\mathrm{mol,l}}\mathbf{v}_{\mathrm{l}}\right)\cdot\mathbf{n}\right]^{\mathrm{pm,if}}$$

- momentum (tangential)

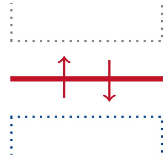
$$\left[\left(-\frac{\sqrt{K}}{\alpha_{\mathrm{BJ}}}\left(\nabla\mathbf{v}_{\mathrm{g}}\right)\mathbf{n} - \mathbf{v}_{\mathrm{g}}\right)\cdot\mathbf{t}_i\right]^{\mathrm{ff,if}} = 0$$

- momentum (normal)

$$\left[\left(\left(\varrho_{\mathrm{g}}\mathbf{v}_{\mathrm{g}}\mathbf{v}_{\mathrm{g}}^{\mathsf{T}} - \boldsymbol{\tau}_{\mathrm{eff}} + p_{\mathrm{g}}\mathbf{I}\right)\mathbf{n}\right)\cdot\mathbf{n}\right]^{\mathrm{ff,if}} = p_{\mathrm{g}}^{\mathrm{pm,if}}$$

# Model

## Interface – Coupling Conditions II



- component mass

$$\left[x_\mathrm{g}^\kappa\right]^\mathrm{ff,if} = \left[x_\mathrm{g}^\kappa\right]^\mathrm{pm,if}$$

$$\left[\left(\varrho_\mathrm{mol,g} x_\mathrm{g}^\kappa \mathbf{v}_\mathrm{g} + \mathbf{j}_\mathrm{eff}^\kappa\right) \cdot \mathbf{n}\right]^\mathrm{ff,if}$$
$$= - \left[\left(\varrho_\mathrm{mol,g} x_\mathrm{g}^\kappa \mathbf{v}_\mathrm{g} + \varrho_\mathrm{mol,l} x_\mathrm{l}^\kappa \mathbf{v}_\mathrm{l} + \mathbf{j}_\mathrm{g}^\kappa + \mathbf{j}_\mathrm{l}^\kappa\right) \cdot \mathbf{n}\right]^\mathrm{pm,if}$$

- energy

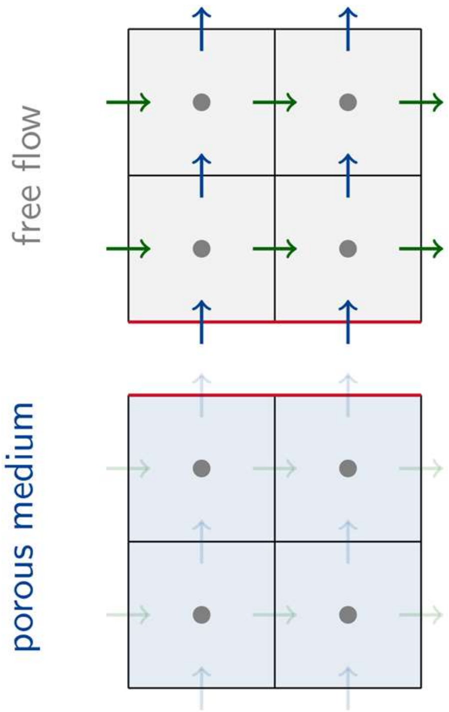
$$[T]^\mathrm{ff,if} = [T]^\mathrm{pm,if}$$

$$\left[\left(\varrho_\mathrm{g} h_\mathrm{g} \mathbf{v}_\mathrm{g} + h_\mathrm{g}^\mathrm{a} \mathbf{j}_\mathrm{mass,eff}^\mathrm{a} + h_\mathrm{g}^\mathrm{w} \mathbf{j}_\mathrm{mass,eff}^\mathrm{w} - (\lambda_\mathrm{g} + \lambda_\mathrm{t}) \nabla T\right) \cdot \mathbf{n}\right]^\mathrm{ff,if}$$
$$= - [(\varrho_\mathrm{g} h_\mathrm{g} \mathbf{v}_\mathrm{g} + \varrho_\mathrm{l} h_\mathrm{l} \mathbf{v}_\mathrm{l} - \lambda \nabla T) \cdot \mathbf{n}]^\mathrm{pm,if}$$

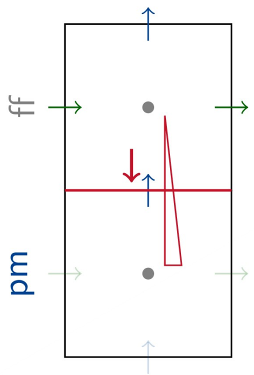
# Implementation

## Coupling

staggered grid / CCFV




- $\varphi \in \{p_g, S_l / x_g^w, T\}$
- $\rightarrow$ $v_x$
- $\uparrow$ $v_y$
- — interface




$q_n^{ff} = -q_n^{pm}$

$v_{g,n}^{ff}$

$\nabla\varphi_n^{ff} = \nabla\varphi_n^{pm}$

$D_{avg}^{ff} = ?$, $\lambda_{avg}^{ff} = ?$

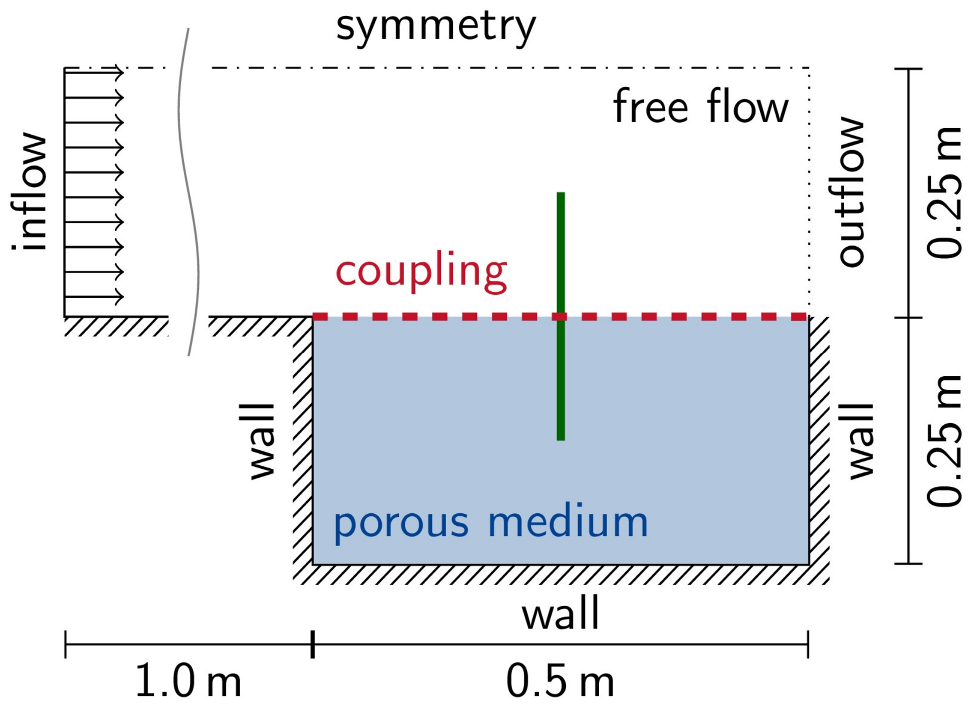
Introduction
Model
Implementation

# Examples

# Examples

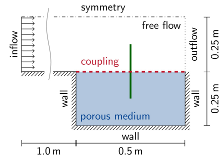
## Basic Simulation Setup

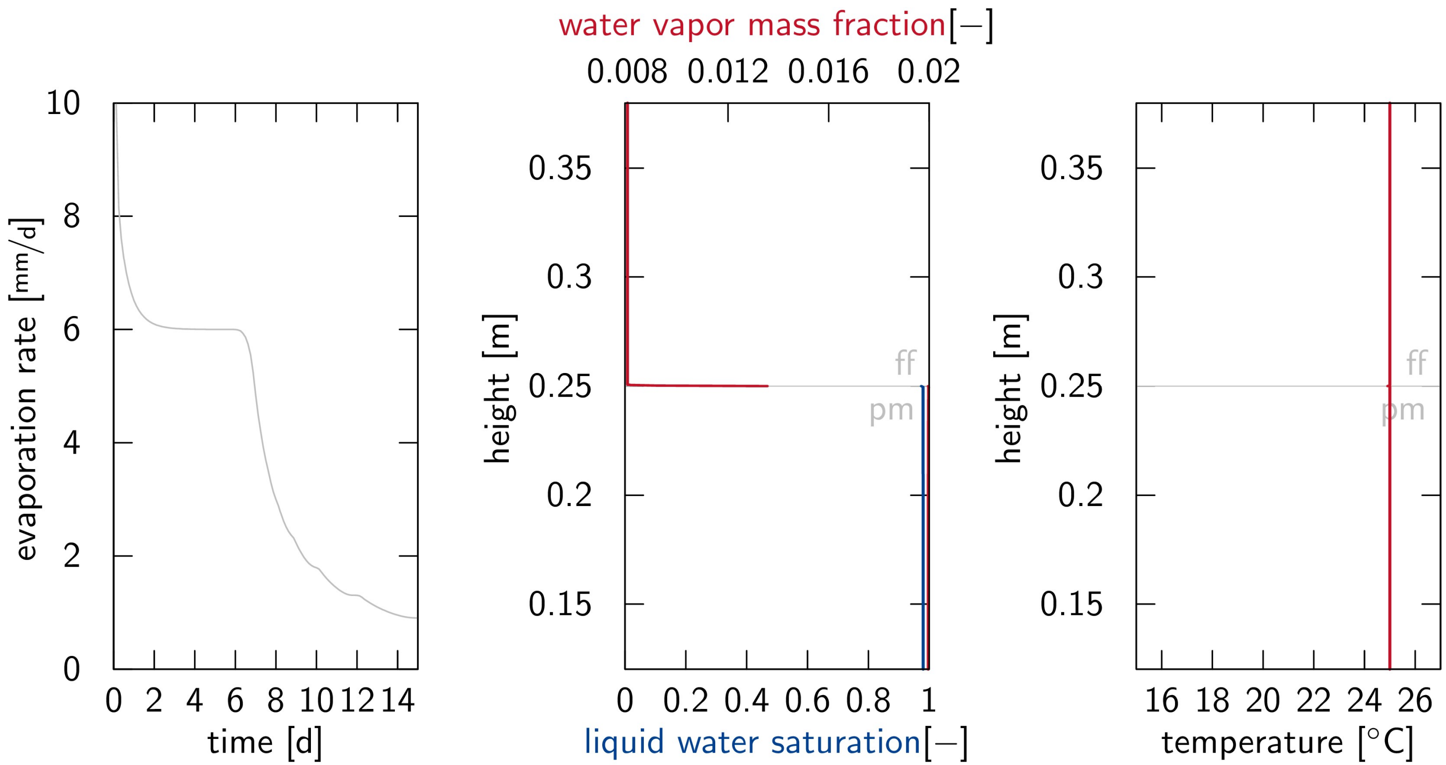
| parameter | value |
|---|---|
| $\mathbf{v}_{\mathrm{g}}^{\mathrm{ff}}$ [m/s] | $(3.5, 0)^{\mathrm{T}}$ |
| $p_{\mathrm{g}}^{\mathrm{ff}}$ [Pa] | 1E5 |
| $X_{\mathrm{g}}^{\mathrm{w,ff}}$ [–] | 0.008 |
| $T^{\mathrm{ff}}$ [K] | 298.15 |
| $p_{\mathrm{g}}^{\mathrm{pm}}$ [Pa] | 1E5 |
| $S_{\mathrm{l}}^{\mathrm{pm}}$ [–] | 0.98 |
| $T^{\mathrm{pm}}$ [K] | 298.15 |



# Examples

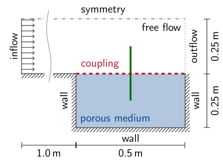
## Typical Stages of Evaporation

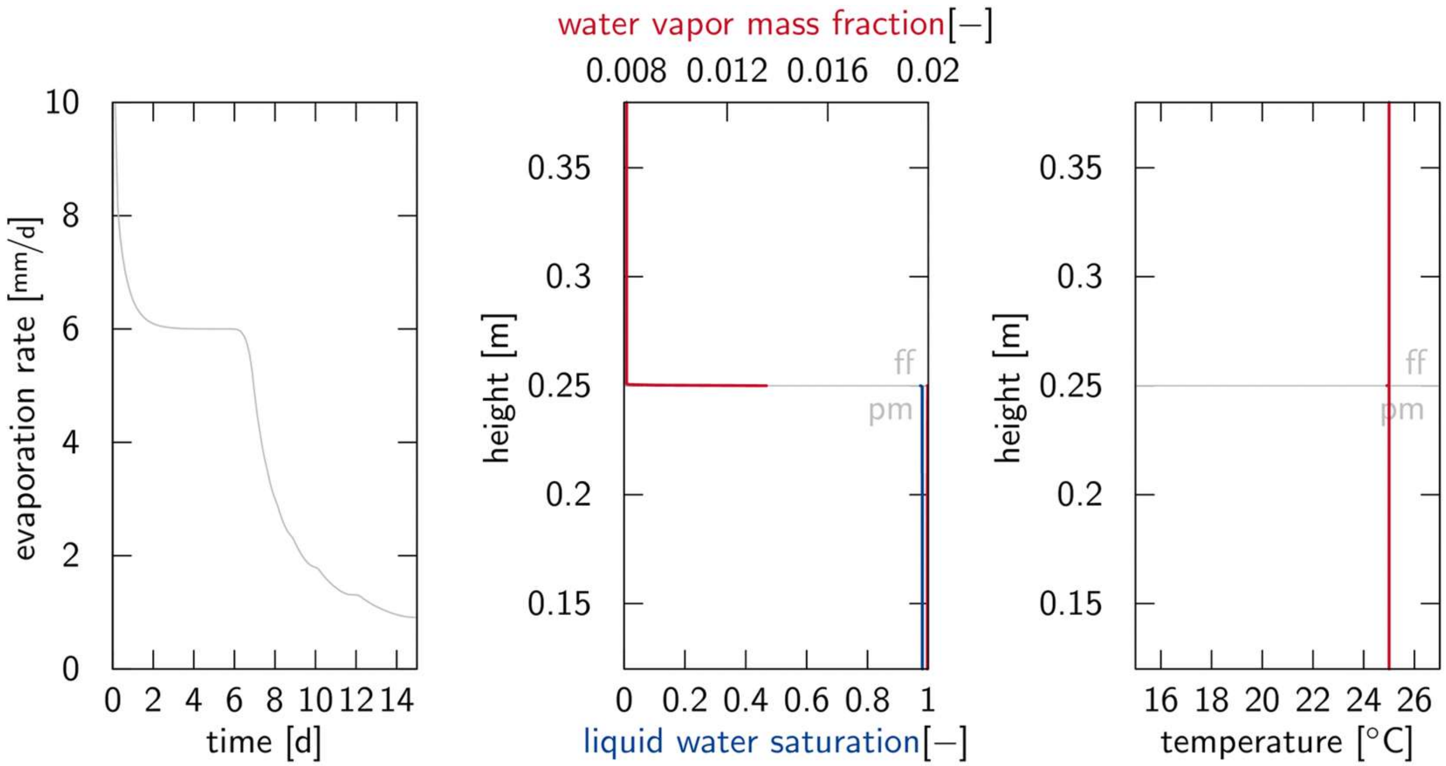


# Examples

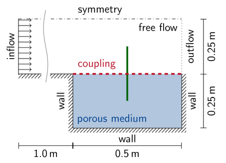
## Typical Stages of Evaporation – Stage-I (Constant Rate)

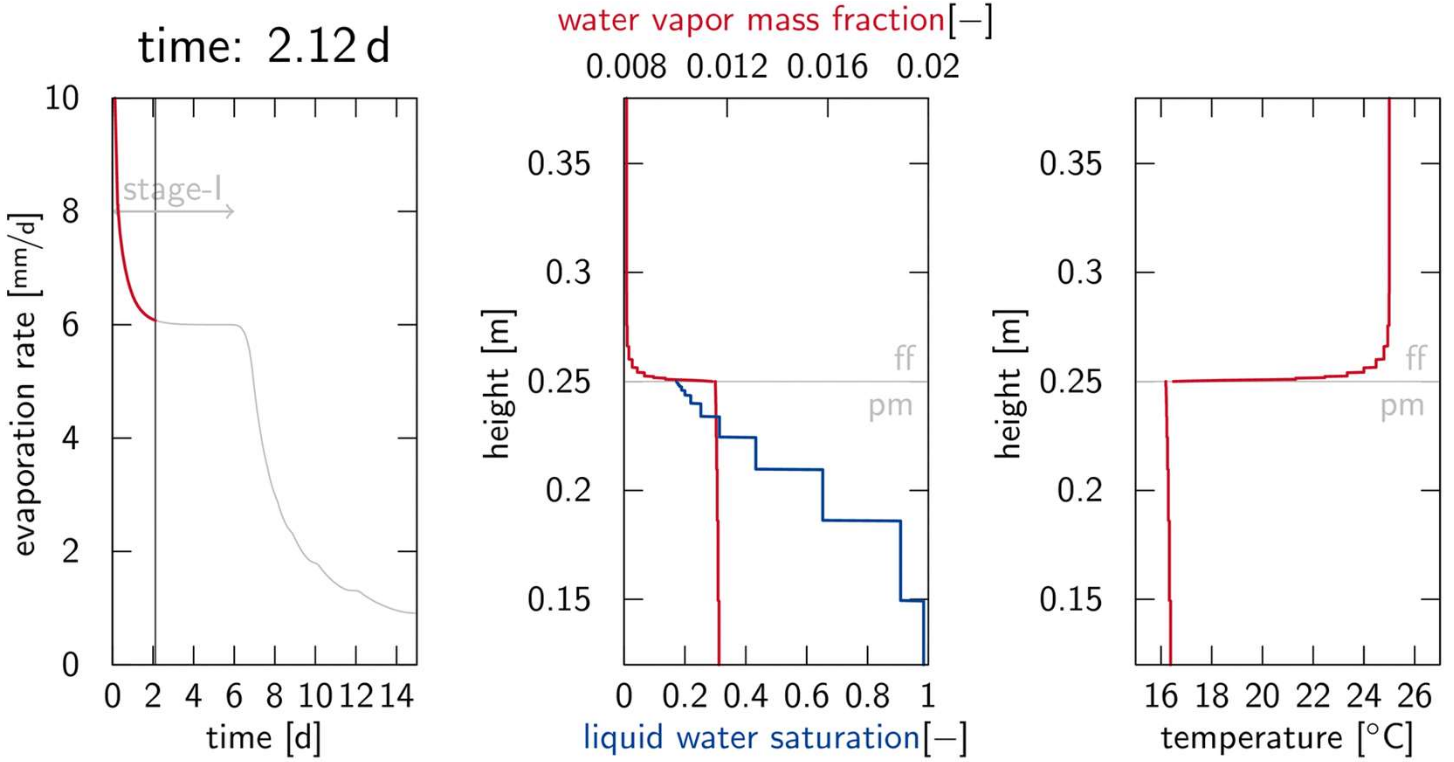


## Examples

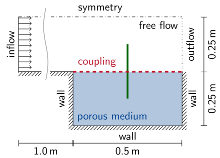
Typical Stages of Evaporation – Stage-I (Constant Rate)

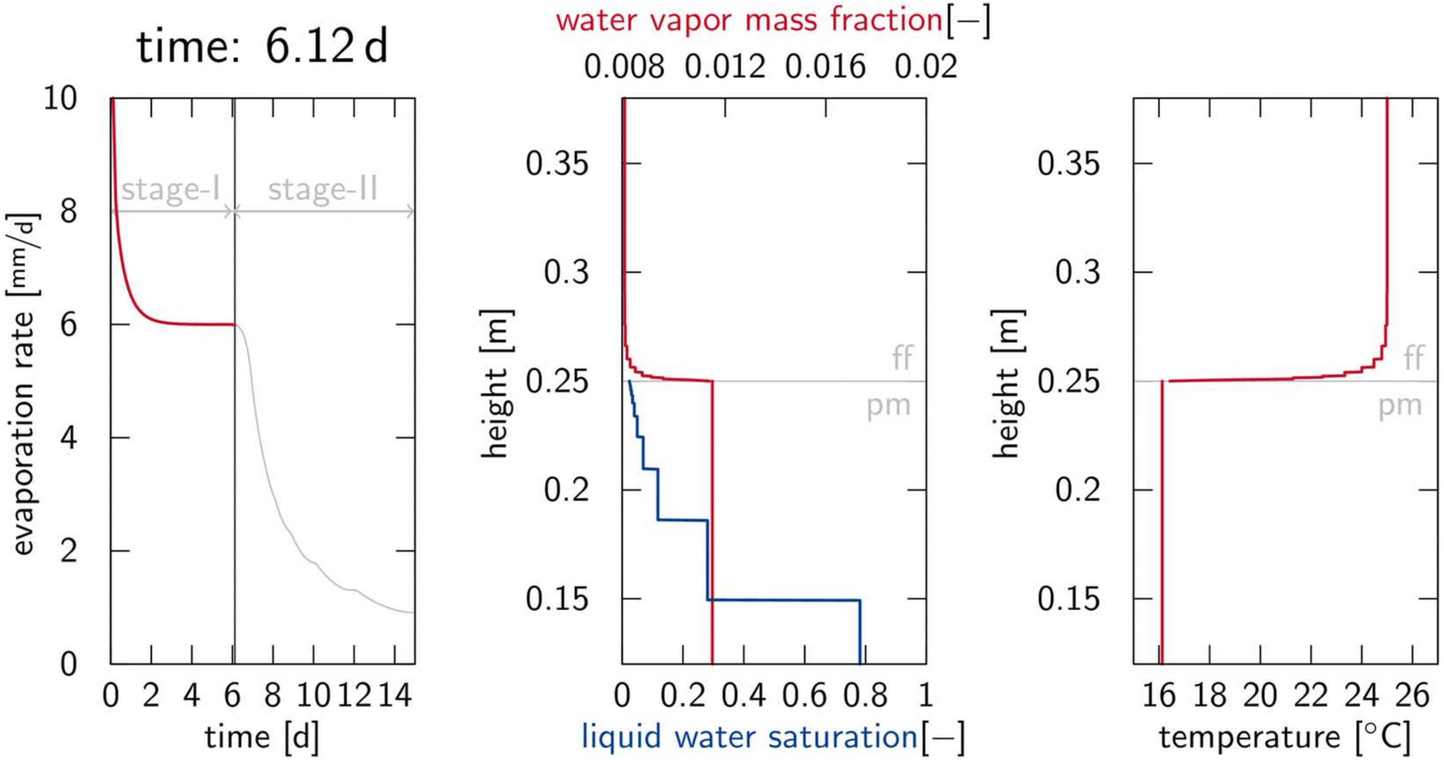


## Examples

Typical Stages of Evaporation – Stage-II (Falling Rate)



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# Vielen Dank!

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