Leaving Equilibrium Assumptions Behind Challenges

International Research Training Group nupus

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Motivation

Modelling Non-Equilibrium

- Limits of *thermodynamic equilibrium assumption*
  → confidence in existing models
- Being able to model situation of clear non-equilibrium
  → extending range of applicability

Current Work

Thermal Non-Equilibrium

$$\frac{\partial\left(\phi\varrho_w S_w u_w\right)}{\partial t}+\nabla\cdot\left(\varrho_w\mathbf{v}_w h_w+\sum_\kappa \mathbf{j}_w^\kappa h_w^\kappa\right)-\nabla\cdot\left(\phi S_w\lambda_w\nabla T_w\right)=$$
$$+\mathrm{Nu}(\mathrm{Re},\,\mathrm{Pr})a_{wn}\frac{\overline{\lambda}_{wn}}{L}\left(T_n-T_w\right)+\mathrm{Nu}(\mathrm{Re},\,\mathrm{Pr})a_{ws}\frac{\overline{\lambda}_{ws}}{L}\left(T_s-T_w\right)$$
$$+\sum_\kappa q_{\kappa\rightsquigarrow w}h^\kappa_{\mathrm{origin}}+q_w^{\mathrm{energy}}$$

$$\frac{\partial\left(\phi\varrho_n S_n u_n\right)}{\partial t}+\nabla\cdot\left(\varrho_n\mathbf{v}_n h_n+\sum_\kappa \mathbf{j}_n^\kappa h_n^\kappa\right)-\nabla\cdot\left(\phi S_n\lambda_n\nabla T_n\right)=$$
$$-\mathrm{Nu}(\mathrm{Re},\,\mathrm{Pr})a_{wn}\frac{\overline{\lambda}_{wn}}{L}\left(T_n-T_w\right)+\mathrm{Nu}(\mathrm{Re},\,\mathrm{Pr})a_{ns}\frac{\overline{\lambda}_{ns}}{L}\left(T_s-T_n\right)$$
$$+\sum_\kappa q_{\kappa\rightsquigarrow w}h^\kappa_{\mathrm{origin}}+q_n^{\mathrm{energy}}$$

$$\frac{\partial\left((1-\phi)\varrho_s c T_s\right)}{\partial t}-\nabla\cdot\left((1-\phi)\lambda_s\nabla T_s\right)=$$
$$-\mathrm{Nu}(\mathrm{Re},\,\mathrm{Pr})a_{ws}\frac{\overline{\lambda}_{ws}}{L}\left(T_s-T_w\right)-\mathrm{Nu}(\mathrm{Re},\,\mathrm{Pr})a_{ns}\frac{\overline{\lambda}_{ns}}{L}\left(T_s-T_n\right)+q_s^{\mathrm{energy}}$$

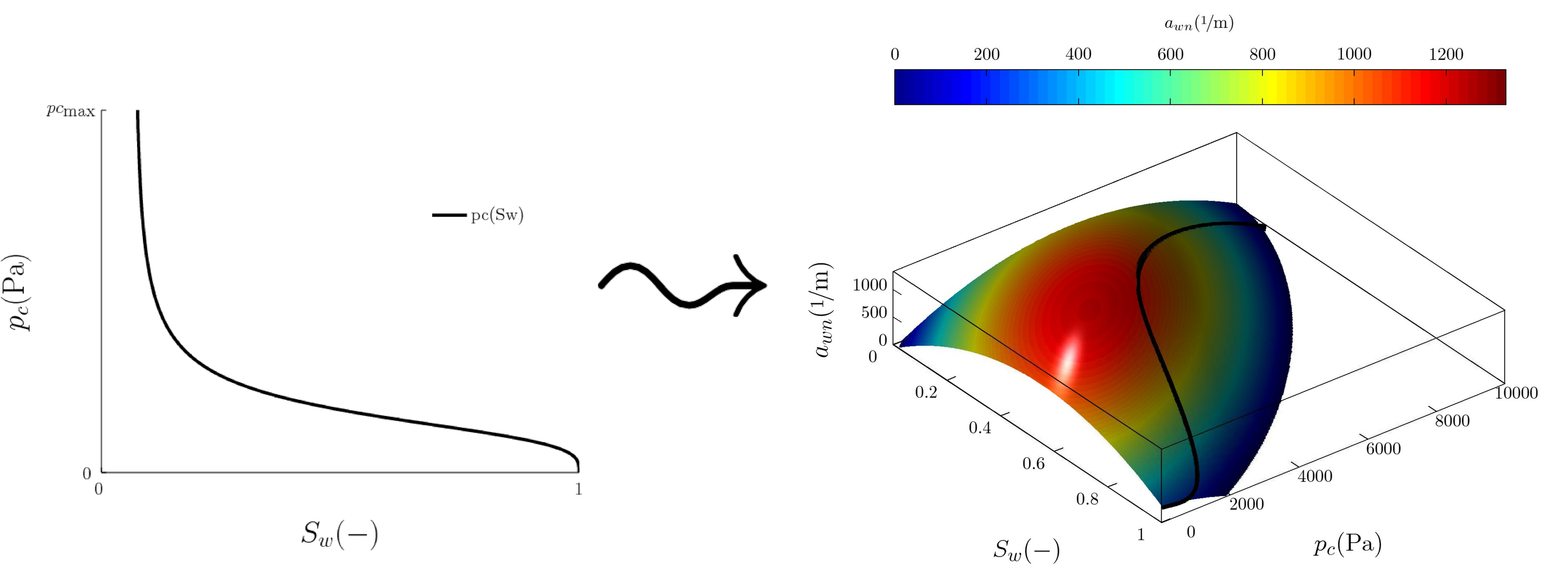

*Figure 1: Capillary pressure - saturation relationship (**left**), capillary pressure - saturation - interfacial area relationship (**right**)*

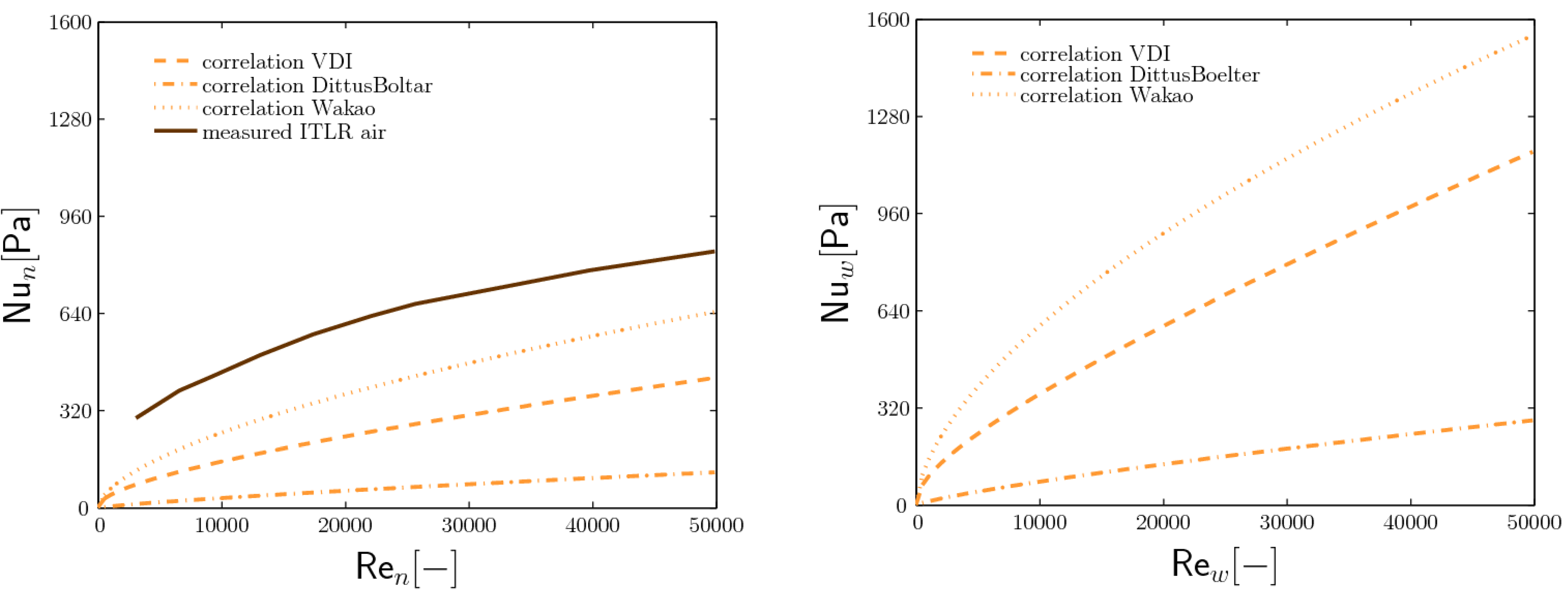

*Figure 2: Nusselt Correlations water (**left**), Nusselt Correlations air (**right**)*

Standard Energy Equation

$$\frac{\partial\left((1-\phi)\varrho_s c T\right)}{\partial t}+\sum_\alpha\frac{\partial\left(\phi\varrho_\alpha S_\alpha u_\alpha\right)}{\partial t}-\nabla\cdot\left(\overline{\lambda}_{\mathrm{pm}}\nabla T\right)$$
$$+\sum_\alpha\nabla\cdot\left(\varrho_\alpha\mathbf{v}_\alpha h_\alpha+\sum_\kappa\mathbf{j}_\alpha^\kappa h_\alpha^\kappa\right)=0$$

Challenges

Volume changing work

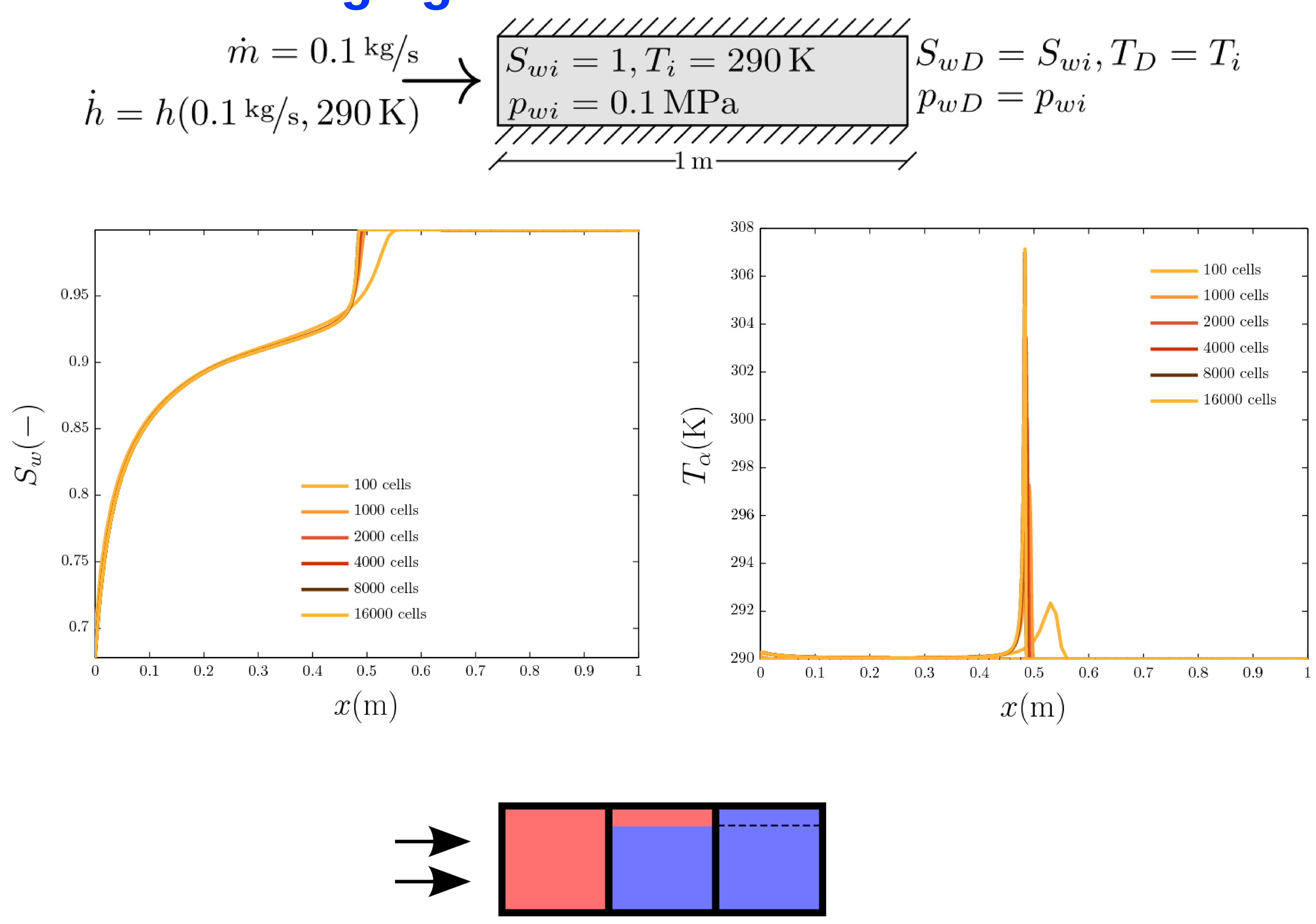

*Figure 2: Schematic of the simulation setup (**top**), convergence study (**middle**), helper cartoon (**bottom**)*

$$\sum_\alpha\frac{\partial\left(\phi\varrho_\alpha S_\alpha u_\alpha\right)}{\partial t}+\sum_\alpha\left(\mathbf{v}_\alpha\varrho_\alpha h_\alpha\right)=0$$

$$\frac{\partial\left(\phi\varrho_w S_w u_w\right)}{\partial t}+\left(\mathbf{v}_w\varrho_w h_w\right)=Q_{n\rightsquigarrow w}$$
$$\frac{\partial\left(\phi\varrho_n S_n u_n\right)}{\partial t}+\left(\mathbf{v}_n\varrho_n h_n\right)=Q_{w\rightsquigarrow n}$$

Enthalpy of solvation

- When mass changes from one phase to another, there is an energy change associated with it.
- Where do I find the data?

Visualization of Temperature in Micro model

- There are existing Micro models.
- How to measure temperature distribution?

Sensitivity Analysis

- Many new parameters are in the model
- How to find out which one needs most attention?

Scenarios

- Up to now rather academic examples have been simulated.
- Ideas for more realistic setting welcomed!

Indicators

- It would be nice to know when a model is leaving it's range of validity
- As little limitations / assumptions should go into the development of theses indicators

Outlook

Identify Need for Complex Model

- Under which circumstances is thermodynamic equilibrium a good assumption?
- Sensitivity Analysis: Which Parameters / choices have most influence?

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