PennState College of Engineering | MECHANICAL AND NUCLEAR ENGINEERING

Phase-Change Heat Transfer in Energy Systems: Outlook for Simulation Enabled Advances

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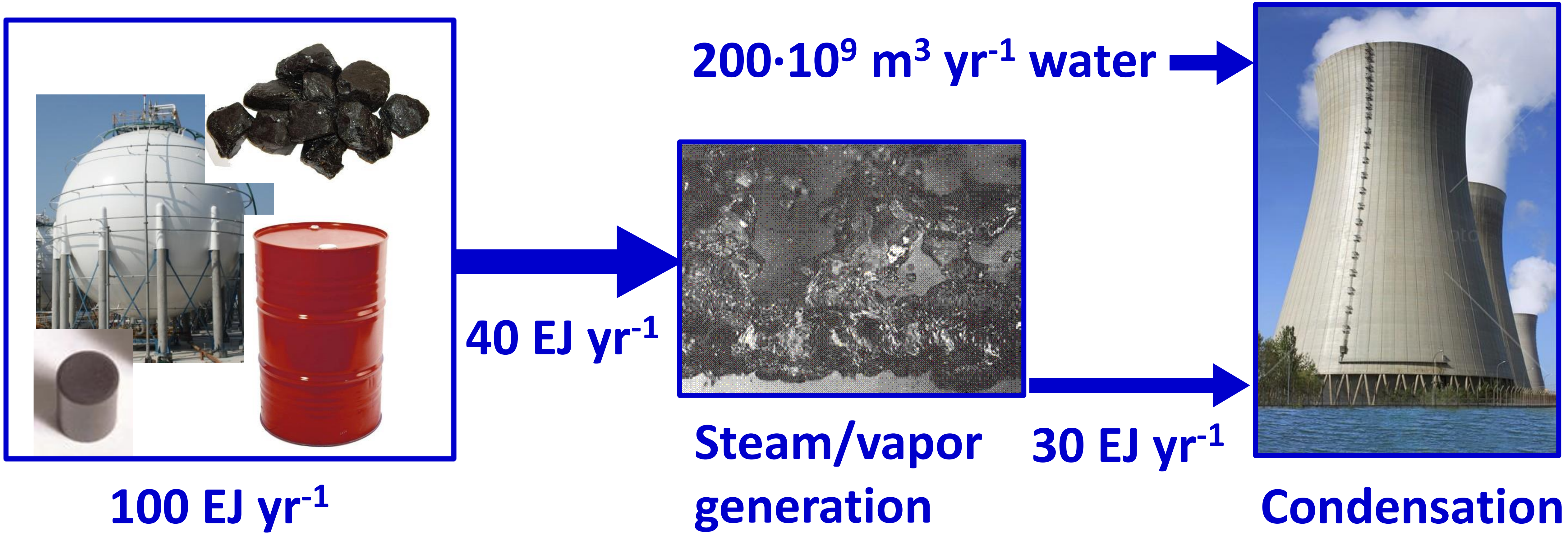
Thank You

- DOE CSGF Program
  & Krell Institute

- Prof. Srinivas Garimella
  & Sustainable Thermal Systems Laboratory
- Dr. Donna Guillen
  & Idaho National Lab

Role of Phase Change in Energy Use

- 40% of US primary energy consumed in steam and vapor generation (EIA 2012, 2013)
- 72% of which rejected through condensation (Rattner & Garimella, 2011)
  - Accounts for 41% of freshwater consumption (Kenny *et al*., 2005)



Phase Change Heat Transfer & Energy

- Phase change found in almost all energy intensive processes
- Great energy density in phase-change processes
  - 1 liter air (100 → 200°C): **96 J**
  - 1 liter water (liquid → vapor at 100°C): **2.2 MJ**

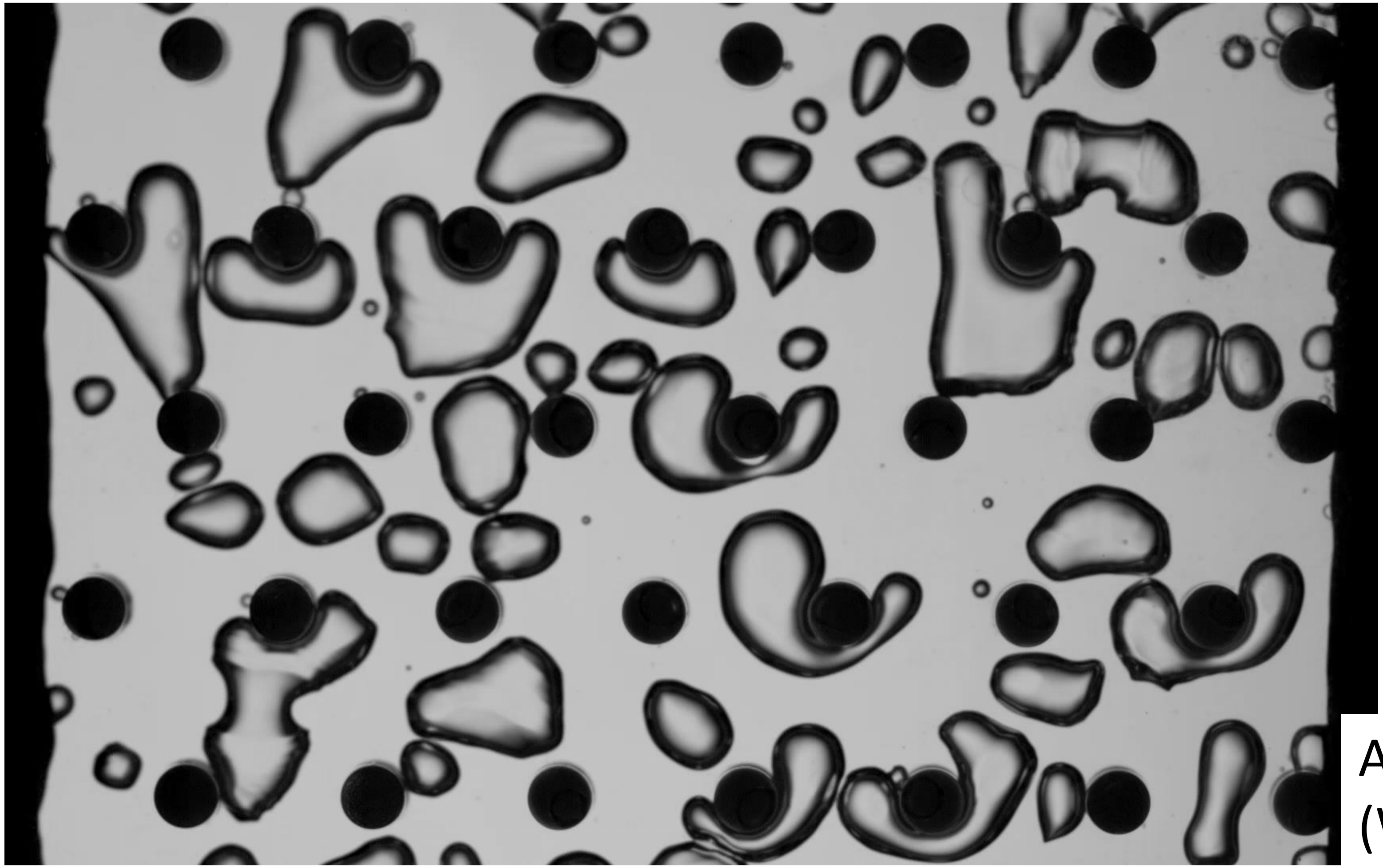
Electricity production
(Steam generation,
Steam condensation)

Air conditioning
(Evaporative cooling,
condensation heat rejection)

Distillation
(Selective evaporation,
condensation)

Challenges of Predicting Phase Change Flows

- **Multiphase flows**: distinct materials, discontinuities in domain, change of topology, orientation, interfacial forces, wide range of scales



Air-water flow
(Wood & Rattner, 2016)

Engineering Phase Change Heat Transfer Systems

- *Three pillars* applied to phase-change heat transfer

Analytic Theory

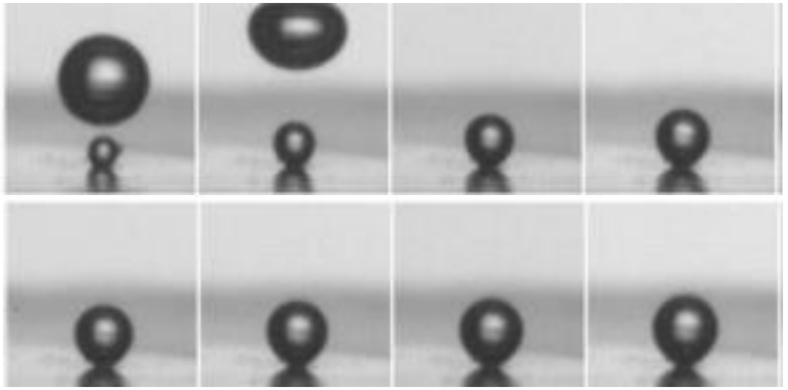
- Limited to simplest processes

Experiments

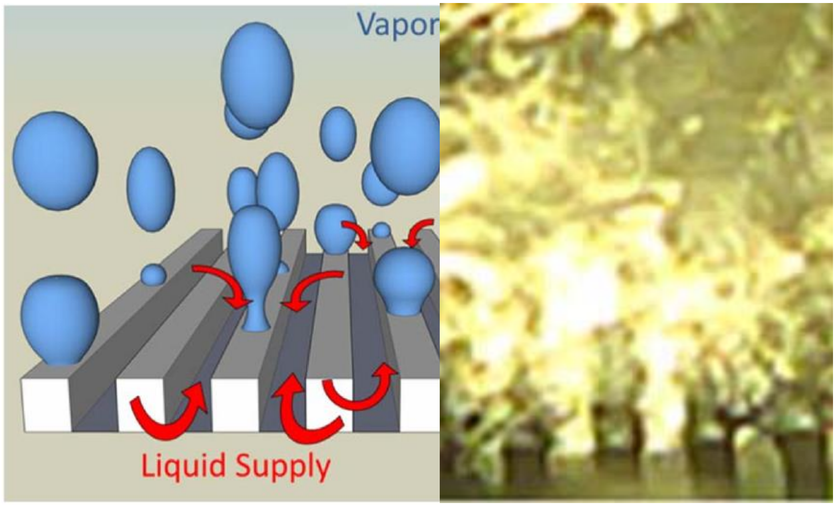
- Applicable for complex processes
- Limited generality (fluids, flow rate...)

Simulations

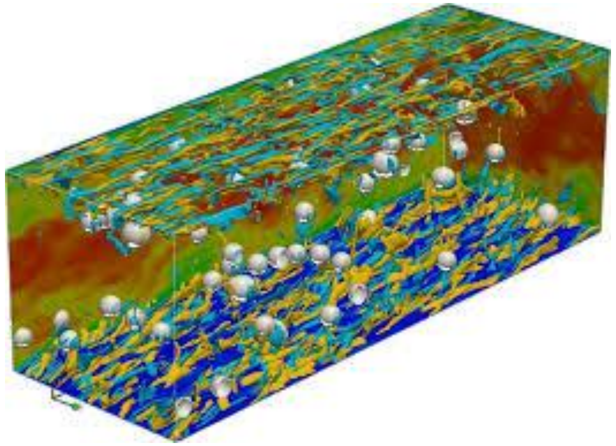
- Great potential for high fidelity results... but in infancy



(Samuel, 2012)



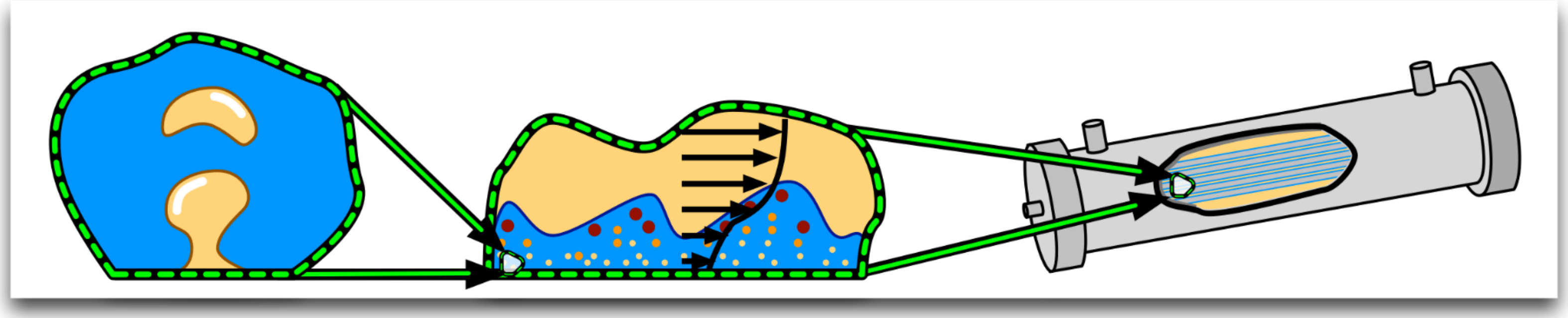
(Cooke and Kandlikar, 2011)



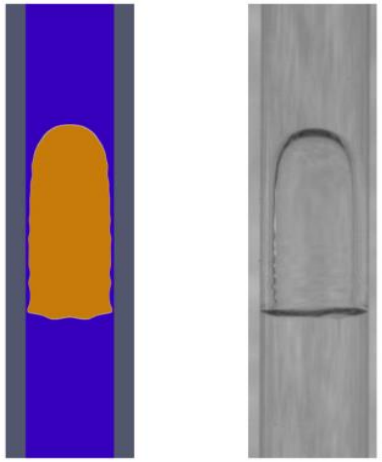
(Bolotnov, 2014)

Research Direction

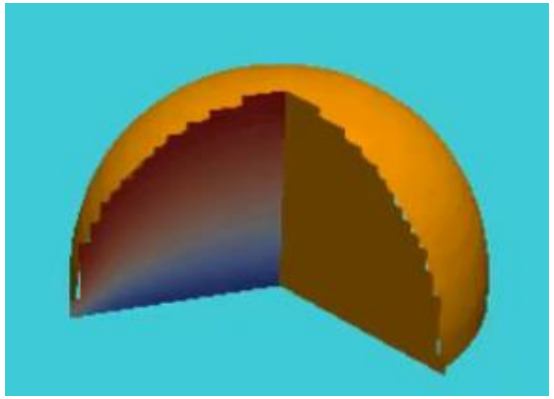
- Advance understanding of phase change heat transfer from phenomena to full system scales



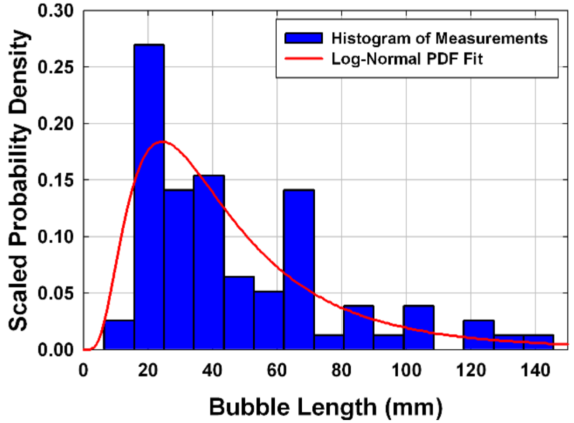
- Complementary simulation and experimental research program



Validation Studies



Simulation
(determining internal fields)



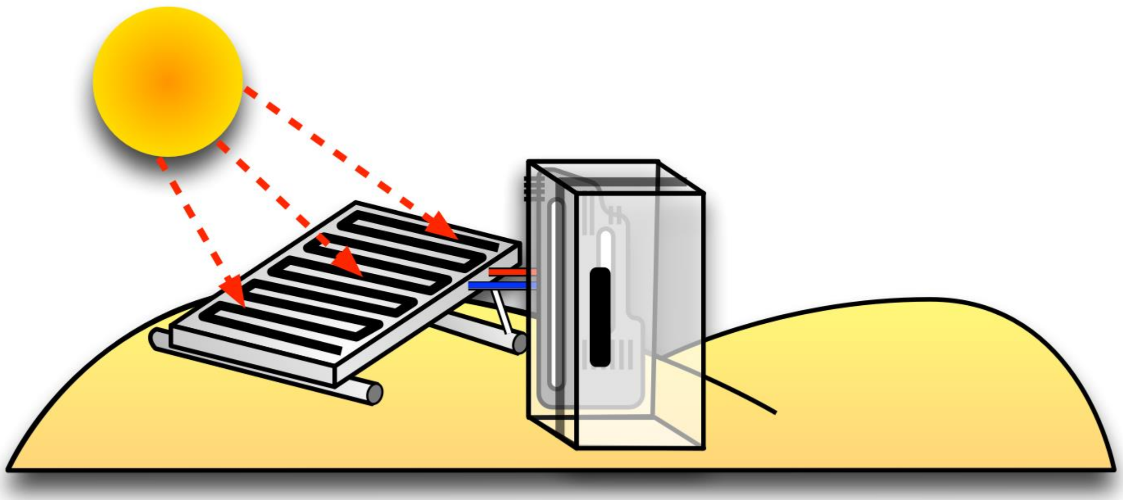
Experiments
(real-time measurements)

Outline

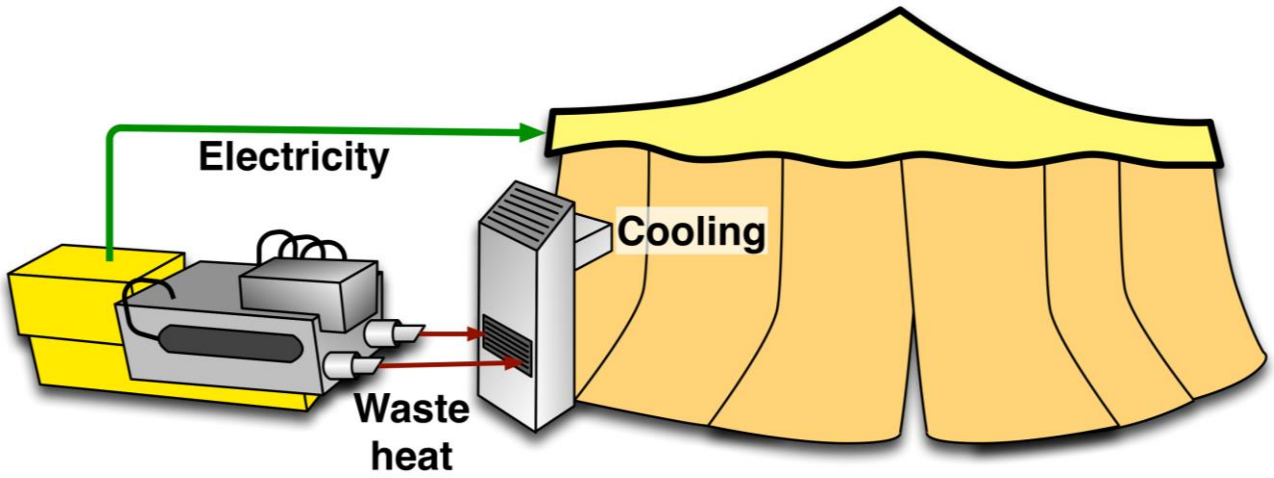
- Introduction and Background
- **Application: Flow evaporation and bubble pumps for off-grid refrigeration needs**
- Application: Dropwise condensation for desalination
- Open research challenges in phase-change simulations and potential directions
- Summary and conclusions

Diffusion Absorption Refrigeration Cycle

- Conventional refrigeration systems require electrical input (compressor & pumps)
  - Limits applications to settings with electrical infrastructure
- Single-pressure (DAR cycle) absorption requires **only** thermal input



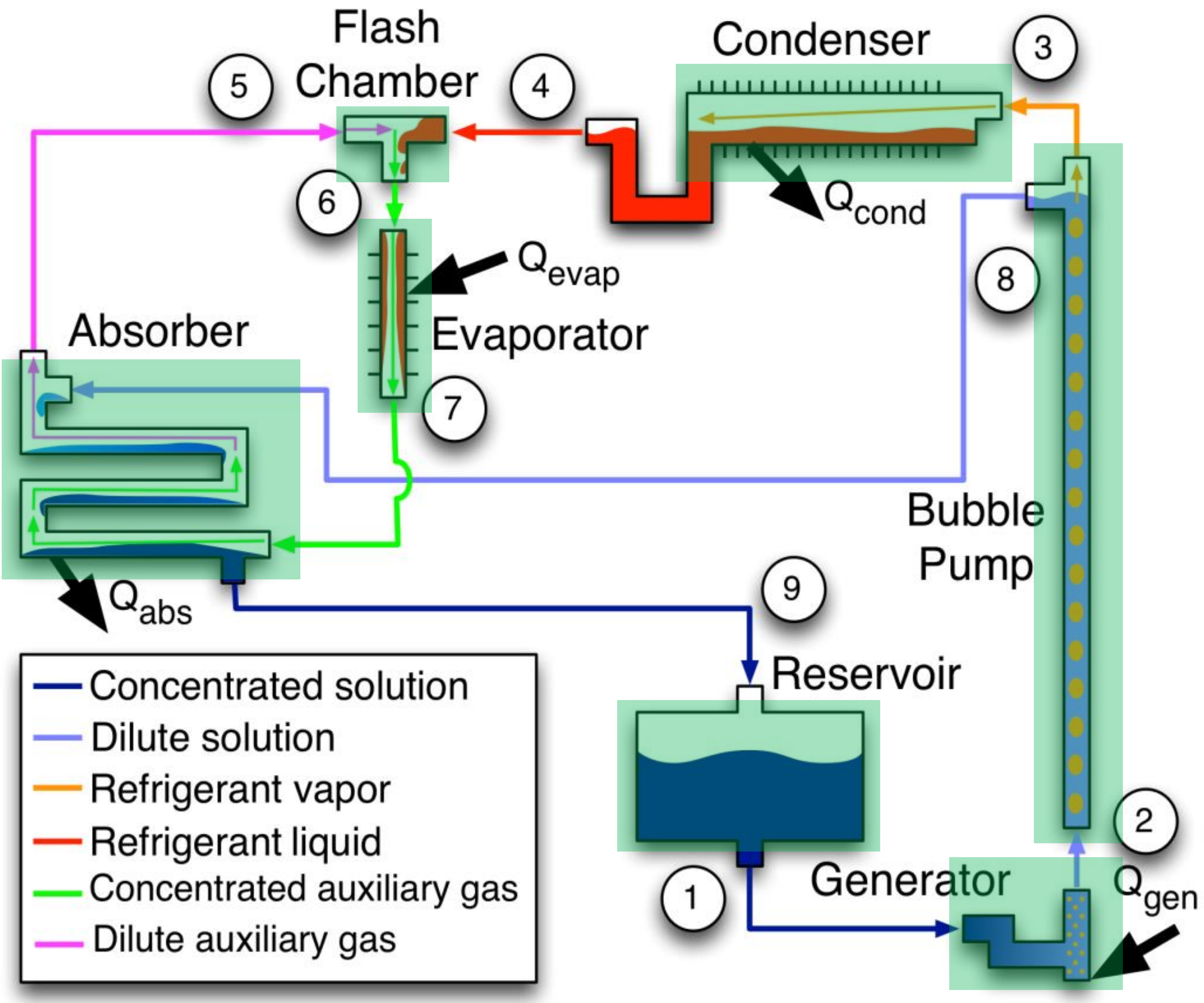
Solar-thermal refrigeration for vaccines and medicine in developing countries



Fully thermally activated air-conditioning in remote locations

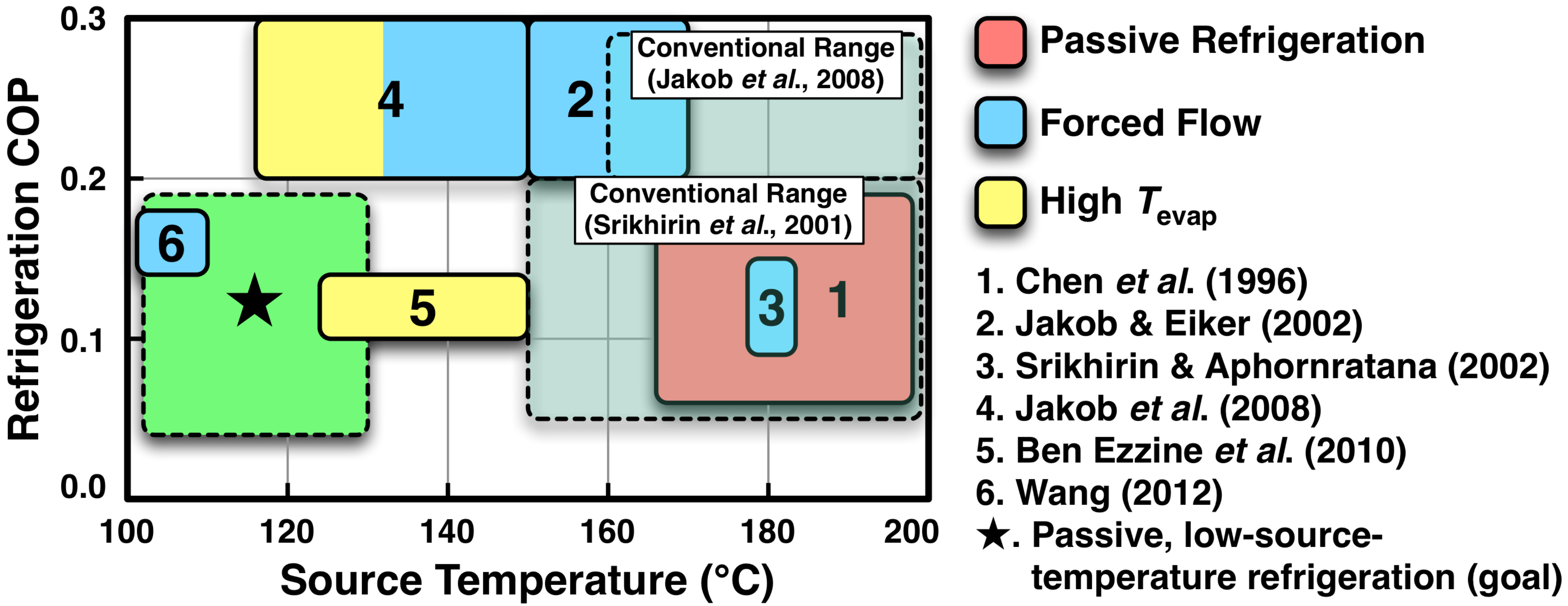
DAR Thermodynamic Cycle

- Only thermal input
- Single-pressure operation
- Three working fluids (**refrigerant**, **absorbent**, **auxiliary gas**)
- Buoyancy driven internal flows (bubble pump, gas loop)



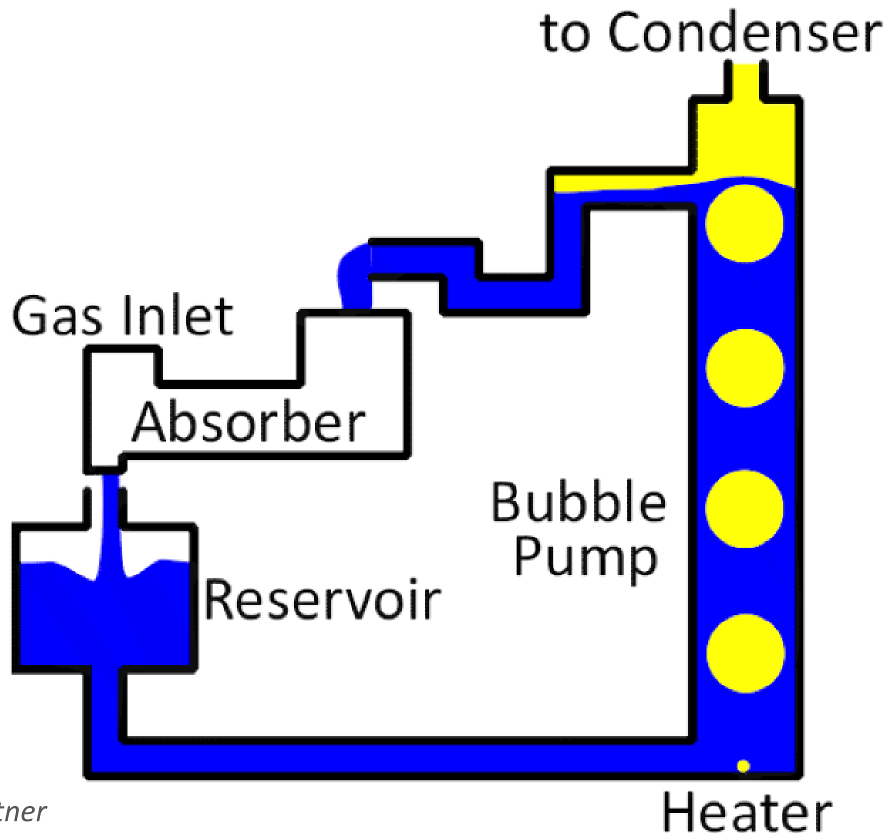
Research Objectives

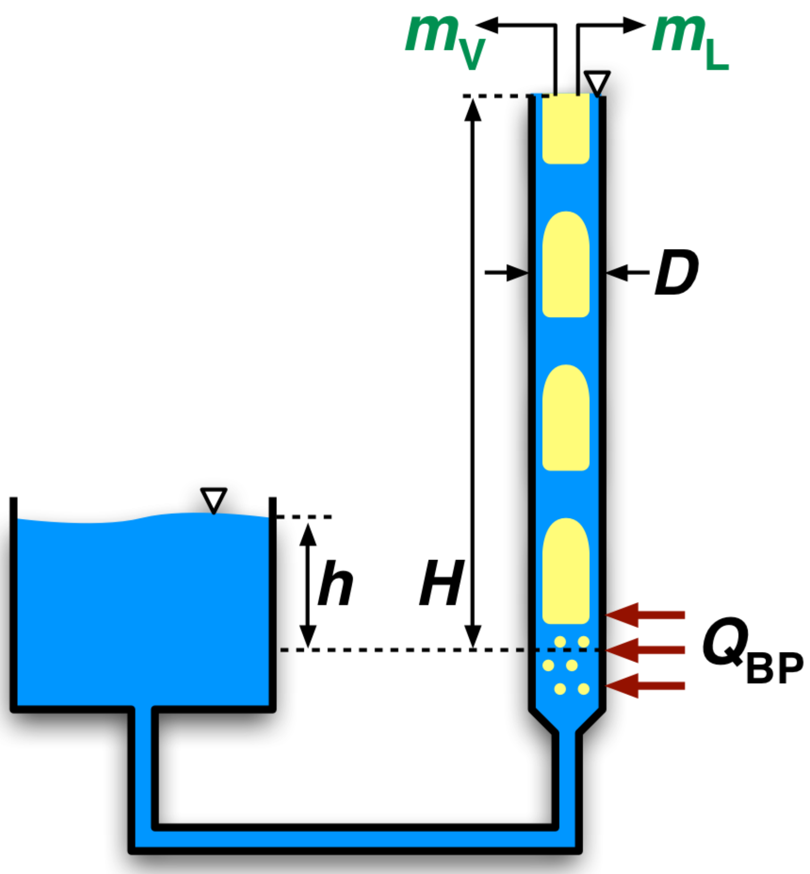
- Existing DAR systems require high T_{source}, high T_{evap}, or forced liquid cooling
- **Goal**: fully passive, low T_{source} (110 – 130°C), low T_{evap} (~5°C) operation



Bubble-Pump Generator

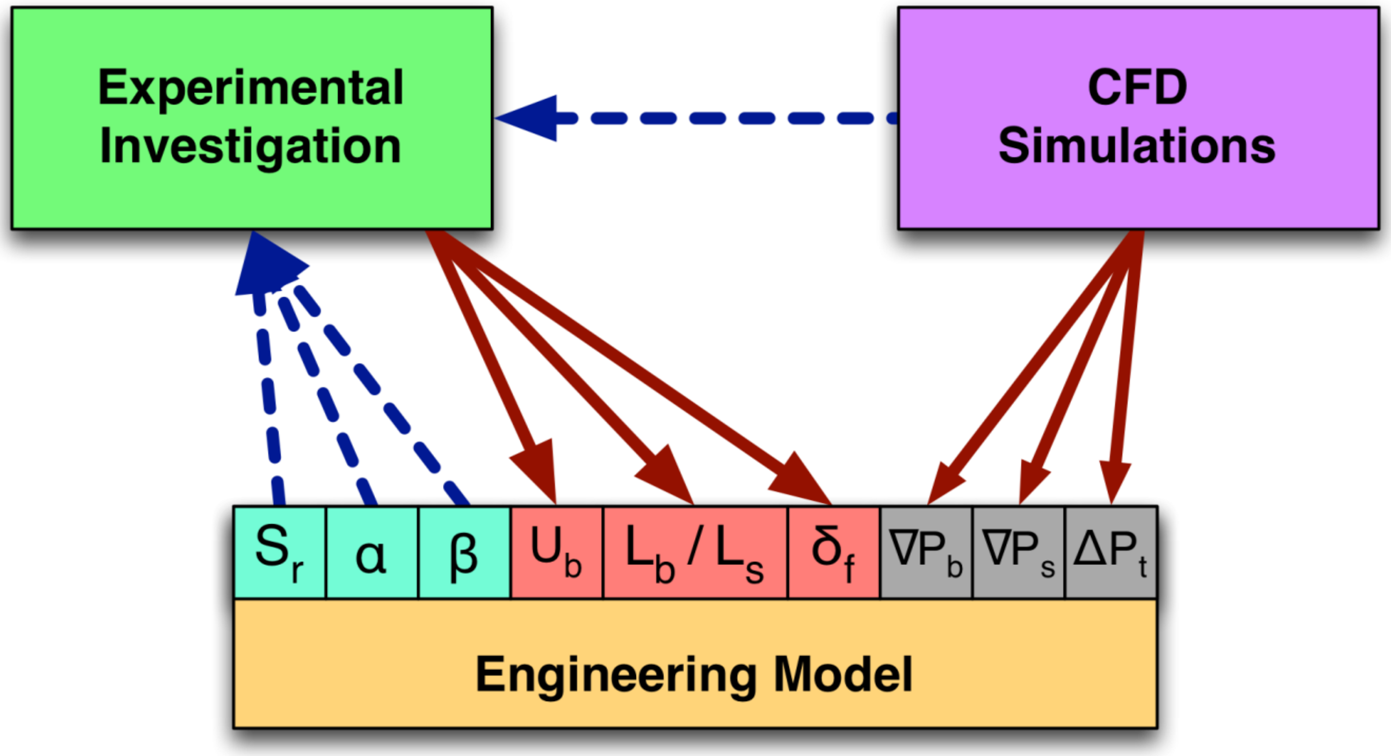
- BPG establishes flow rates and performance in full system
- **Challenge**: Predict $\boldsymbol{m}_L$ & $\boldsymbol{m}_V$ given: $\boldsymbol{D}$, $\boldsymbol{S}_r = h/H$, $\boldsymbol{Q}_{BP}$, fluid properties
- Incomplete understanding of Taylor flow at intermediate-diameter scale



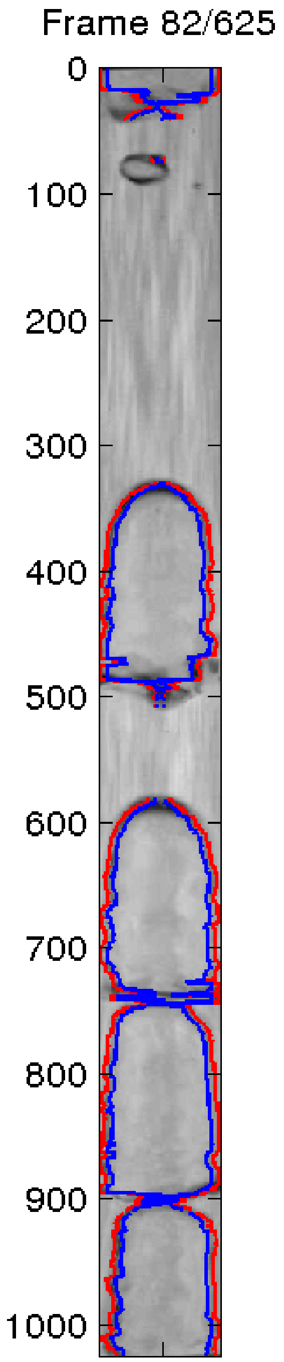


Experimental Investigations of Taylor Flow

- High speed video to measure: U_b, α, δ_f, L_b, L_s
  → Universal Taylor flow rise velocity model
- Integrate with simulation for dynamic closure

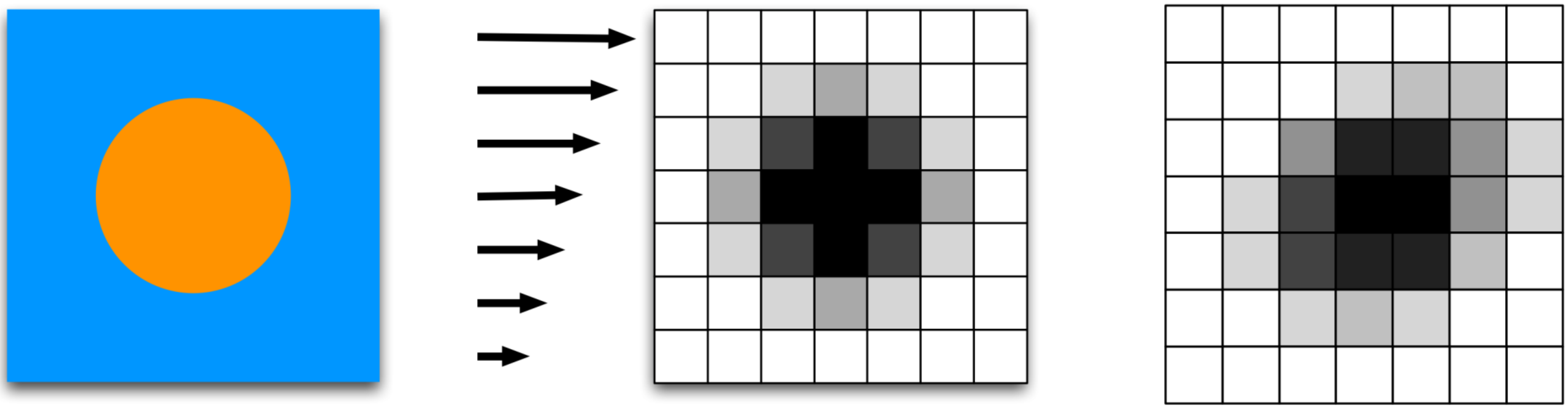


Experimental Rise Velocity (m s^{-1})



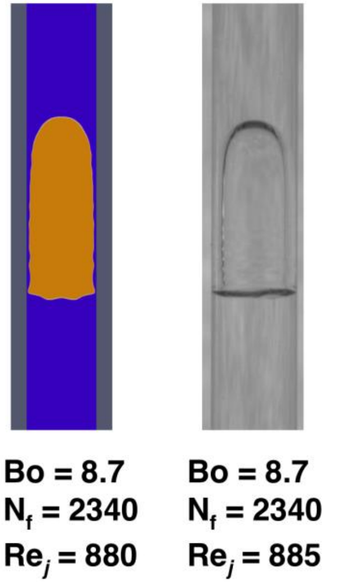
VOF Simulation Approach

- Represent phase fraction in each cell with: $\alpha \in [0,1]$
- Solve advection equation for α: $\frac{\partial \alpha}{\partial t} + \frac{\partial}{\partial x_{\mathrm{i}}}(u_{\mathrm{i}}\alpha) = 0$
- Weight fluid properties with α: $\theta = \alpha\theta_{\mathrm{L}} + (1-\alpha)\theta_{\mathrm{G}}$
- Volumetric surface tension force in interface cells

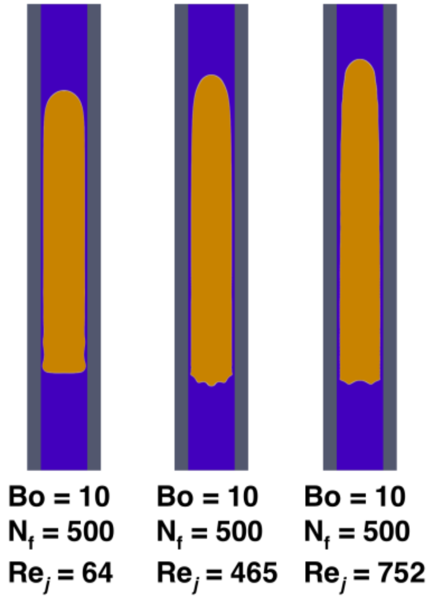


Two-Phase Flow Morphologies

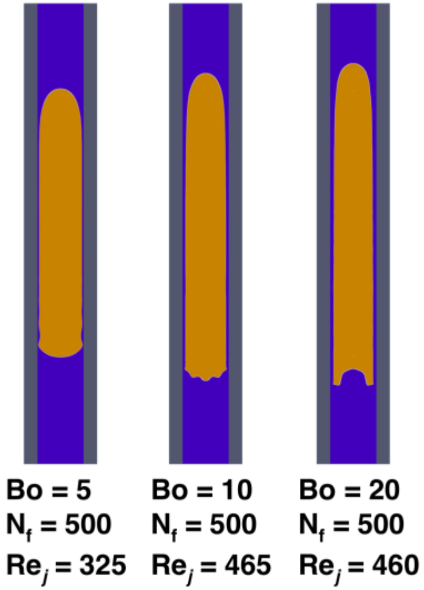
Comparison with experiment



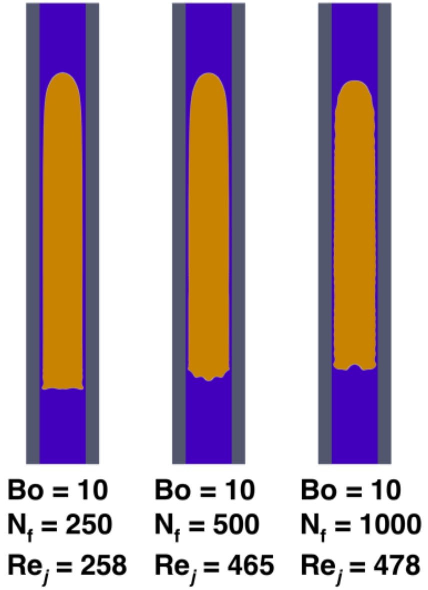
Increasing Flow rate (Re_j)



Reducing relative surface tension (Bo)

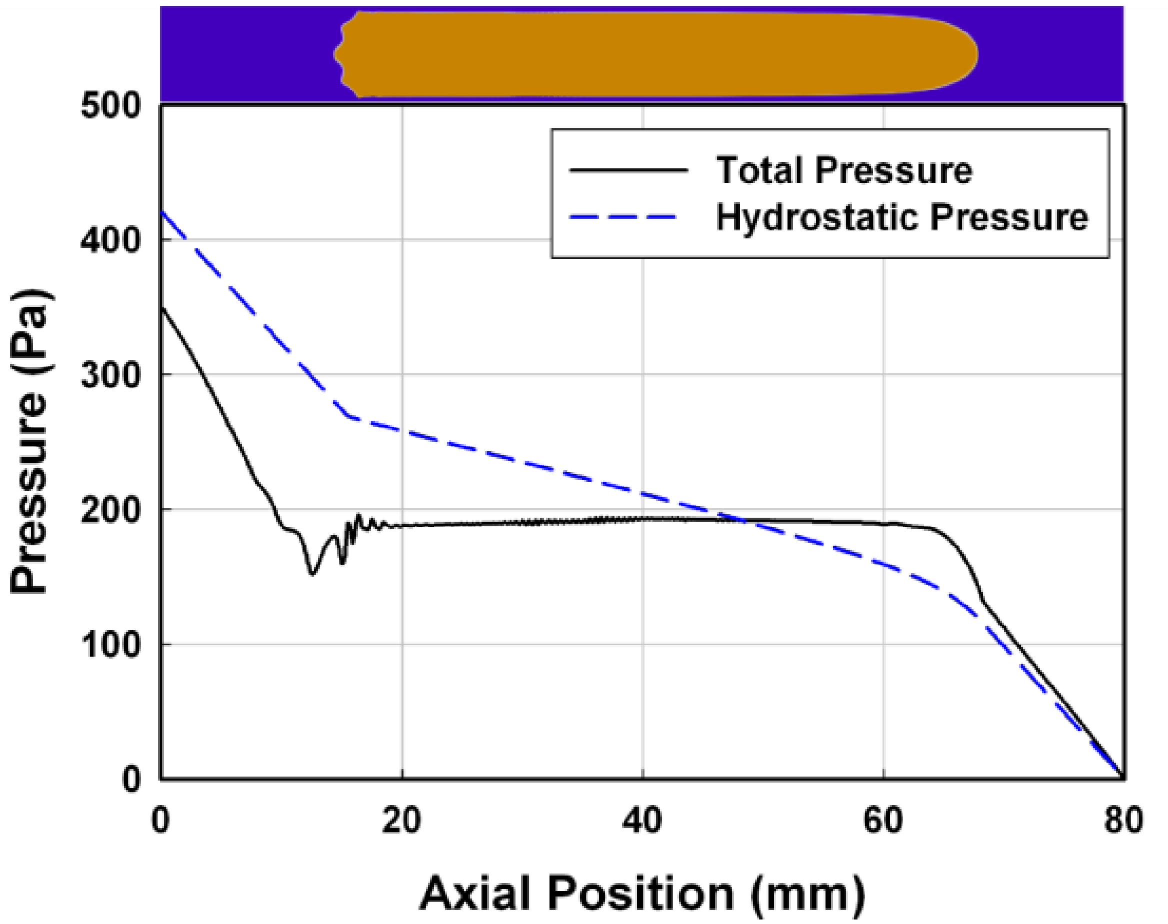


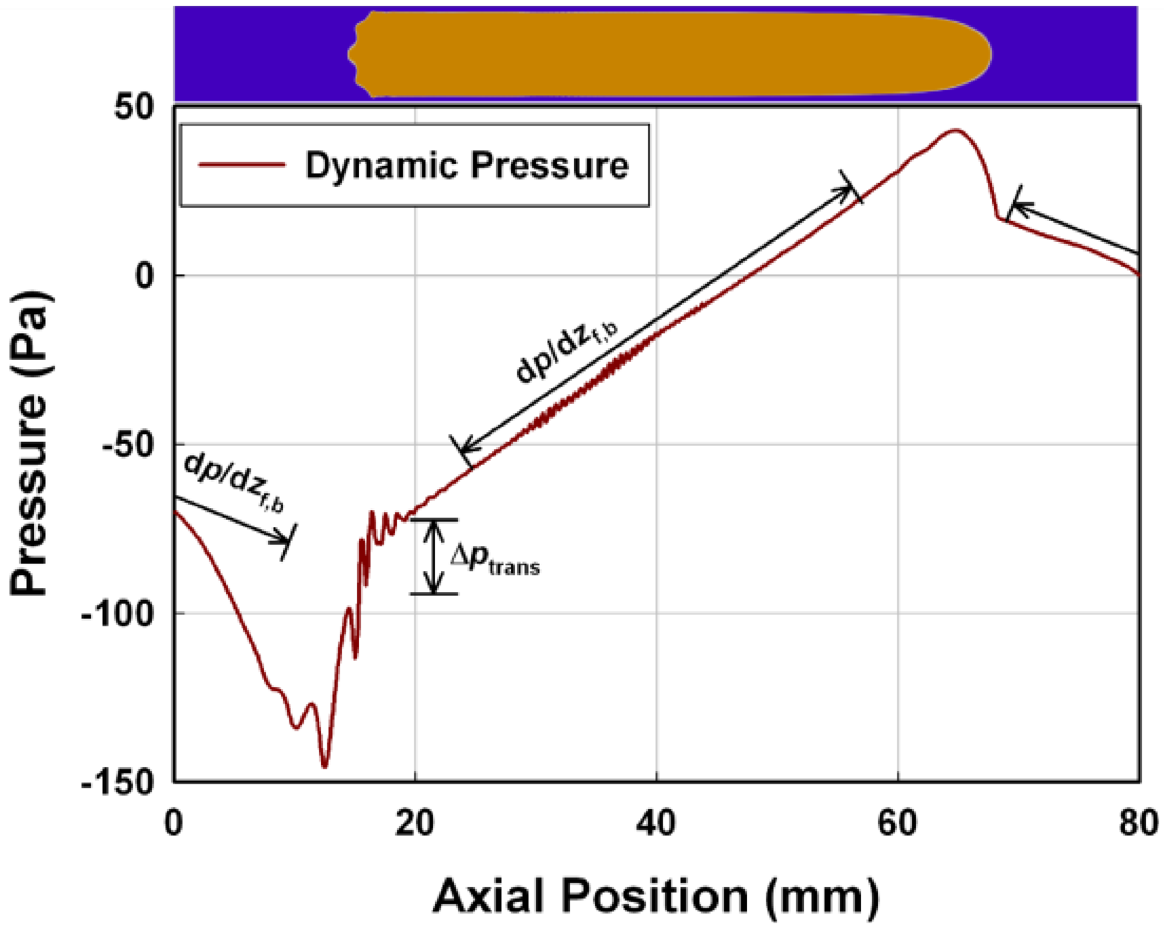
Reducing relative viscosity (N_f)



Decomposing Hydrodynamics

- Simulation decomposed to identify hydrodynamic contributions



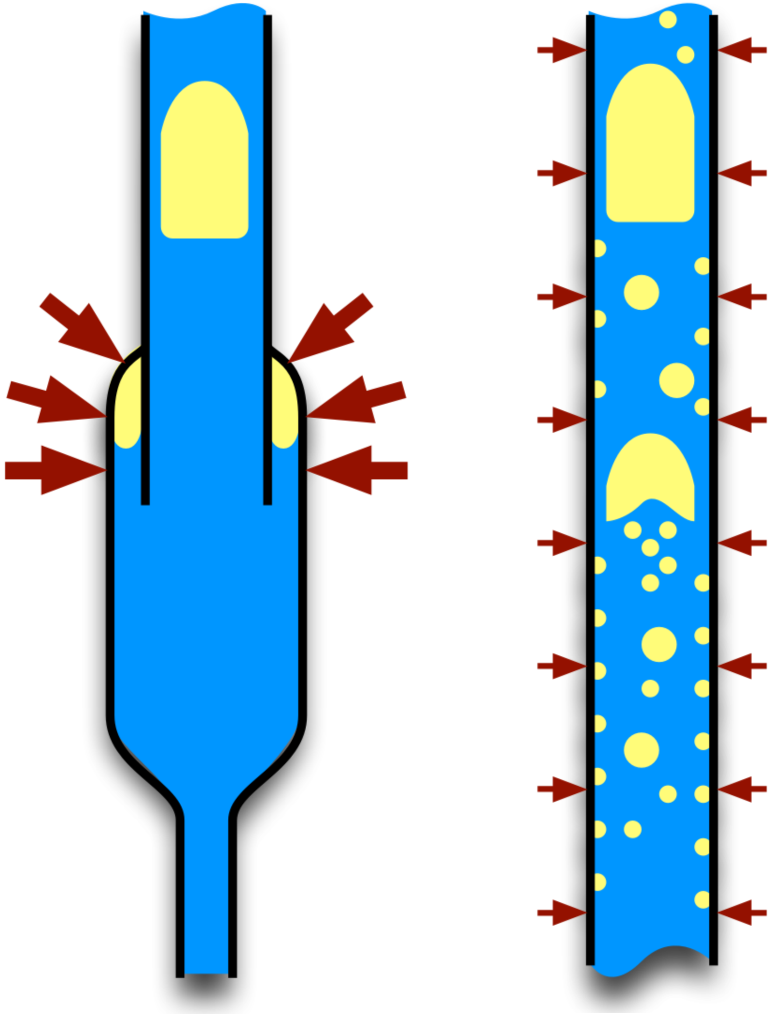


Need for Enhanced Bubble Pump Design

- Conventional configurations are **spot-heated**
  - Needs high source temperatures (T_{gen} > 180°C)
- Limits applications to settings with high grade thermal sources

Research Needs

- Continuously heated BPG
- Flow develops along full component length
  - Need phase-change simulation approach to study this process



$Q = U A \mathbf{\Delta T}$ $Q = U \mathbf{A} \Delta T$

Phase Change Formulation

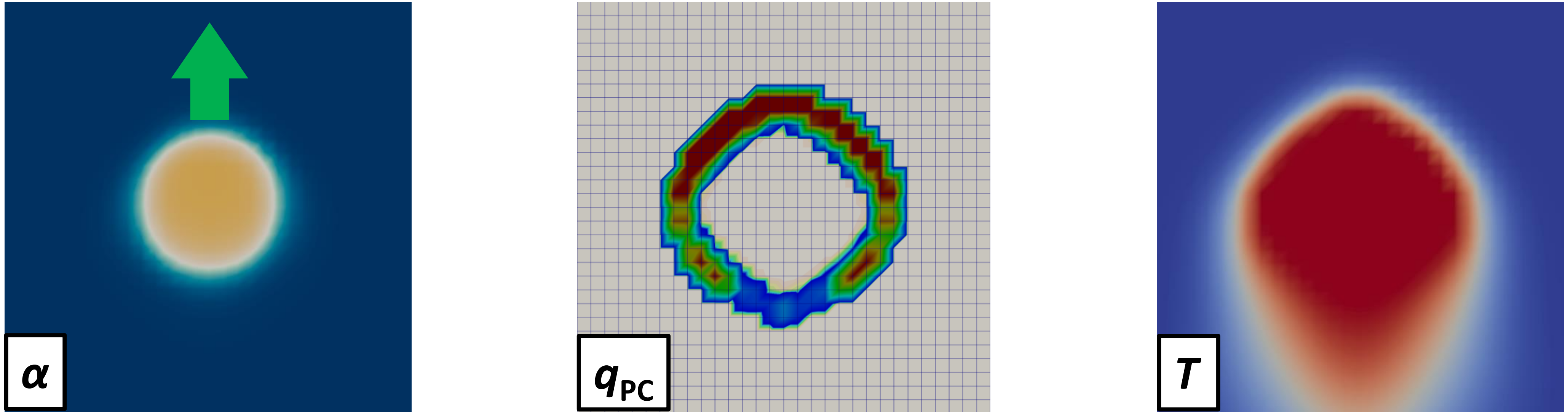
- Phase-change rate from **simulation** time scale: $\dot{q}'''_{\mathrm{PC}} = \left(\rho c_{\mathrm{p}}\right)(T - T_{\mathrm{sat}})/\Delta t$
- Phase ($\dot{\alpha}_{\mathrm{PC}}$) and volume ($\dot{v}_{\mathrm{PC}}$) source terms from $\dot{q}'''_{\mathrm{PC}}$

Continuity $$\frac{\partial u_{\mathrm{i}}}{\partial x_{\mathrm{i}}} = \dot{v}_{\mathrm{PC}}$$

Momentum $$\rho \frac{\partial u_{\mathrm{i}}}{\partial t} + \rho u_{\mathrm{j}} \frac{\partial u_{\mathrm{i}}}{\partial x_{\mathrm{j}}} = -\frac{\partial p}{\partial x_{\mathrm{i}}} + \mu_{\mathrm{eff}} \frac{\partial^2 u_{\mathrm{i}}}{\partial x_{\mathrm{i}} \partial x_{\mathrm{j}}} + f_{\mathrm{i}}$$

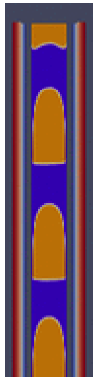
Phase $$\frac{\partial \alpha}{\partial t} + \frac{\partial}{\partial x_{\mathrm{i}}}\left(u_{\mathrm{i}} \alpha\right) = \dot{\alpha}_{\mathrm{PC}}$$

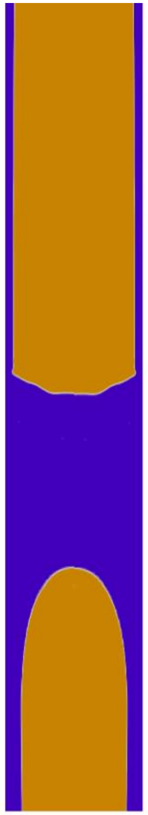
Energy $$\frac{\partial\left(\rho h\right)}{\partial t} + \frac{\partial}{\partial x_{\mathrm{i}}}\left(\rho u_{\mathrm{i}} h\right) = \frac{\partial}{\partial x_{\mathrm{i}}}\left[k_{\mathrm{eff}} \frac{\partial T}{\partial x_{\mathrm{i}}}\right] - \dot{q}'''_{\mathrm{PC}}$$

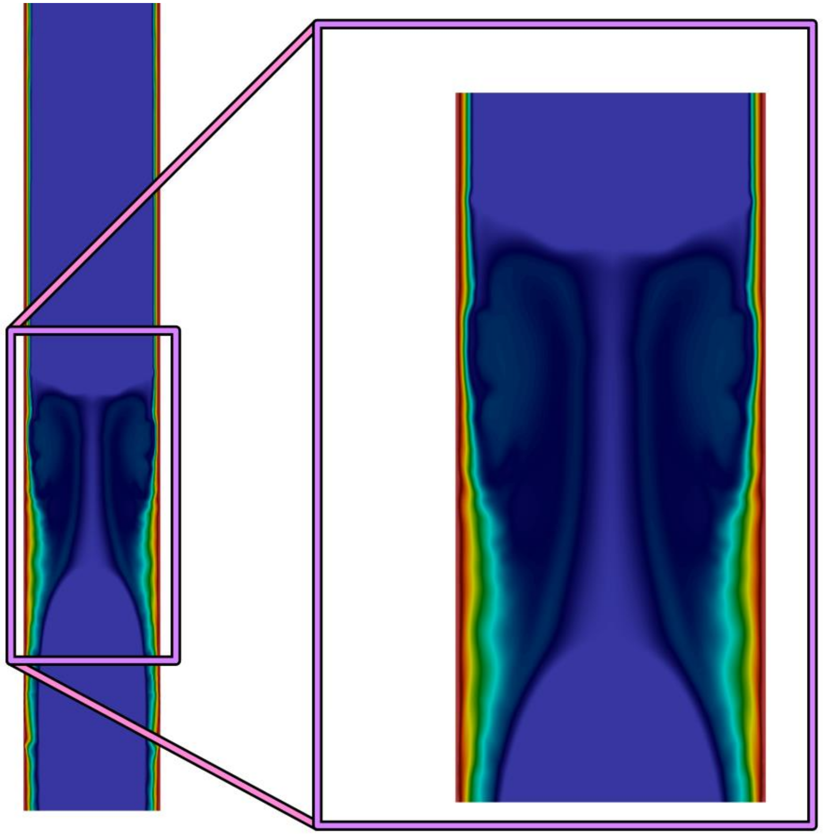


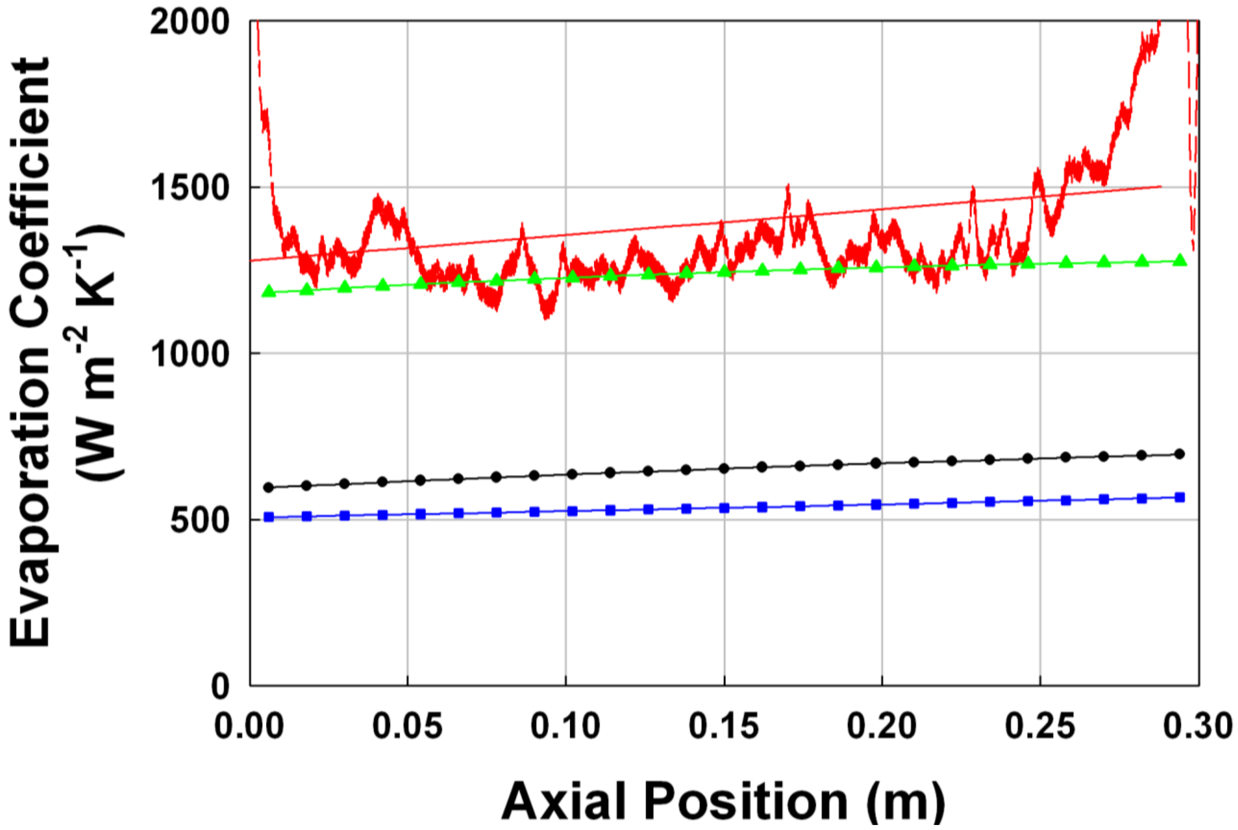
Applications: Taylor Flow Evaporation

- Simulation of coupling-fluid-heated evaporating Taylor flow
- Informed new wake-region heat transfer model

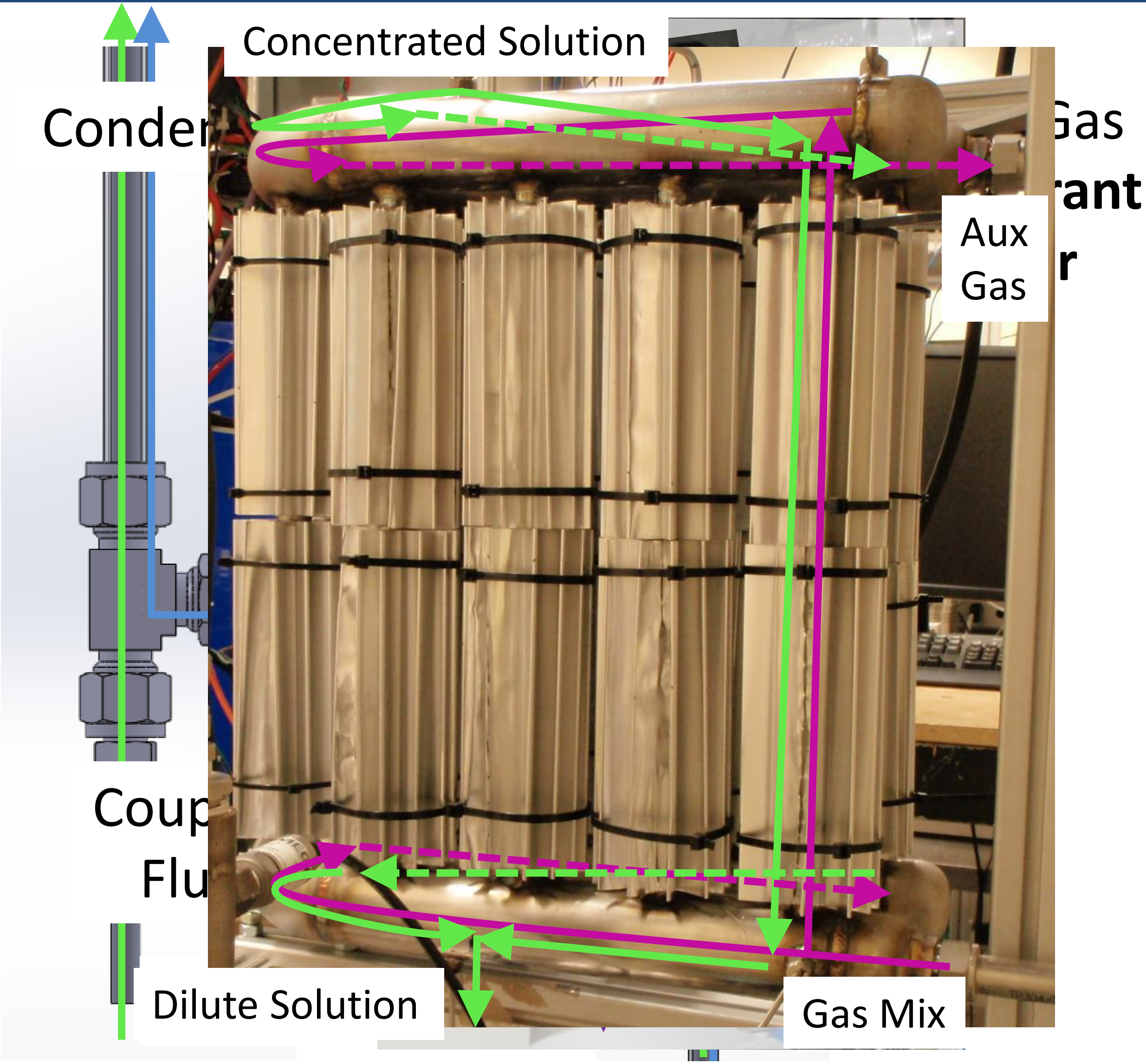


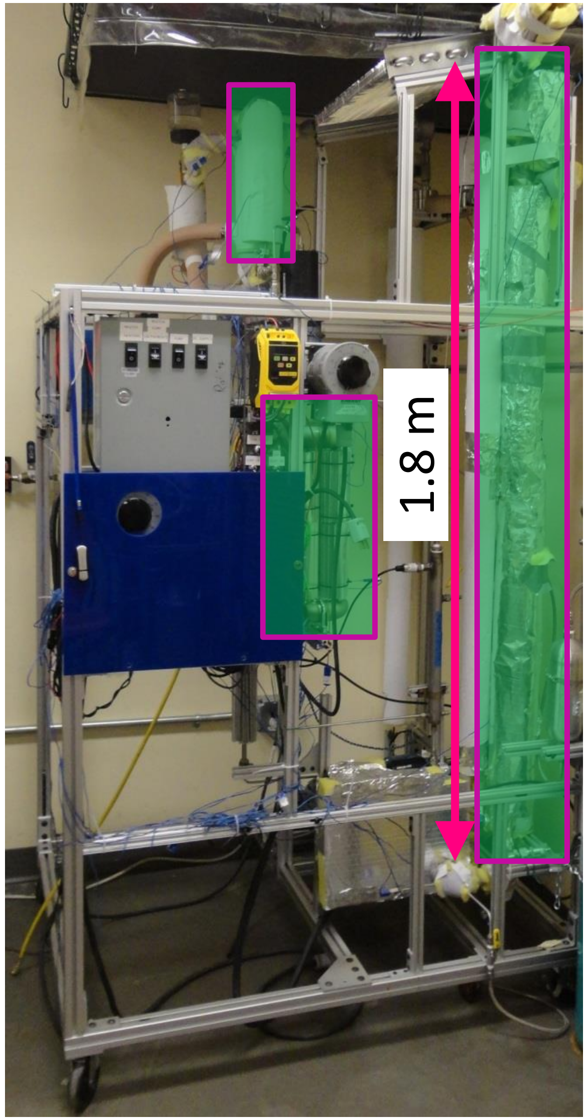






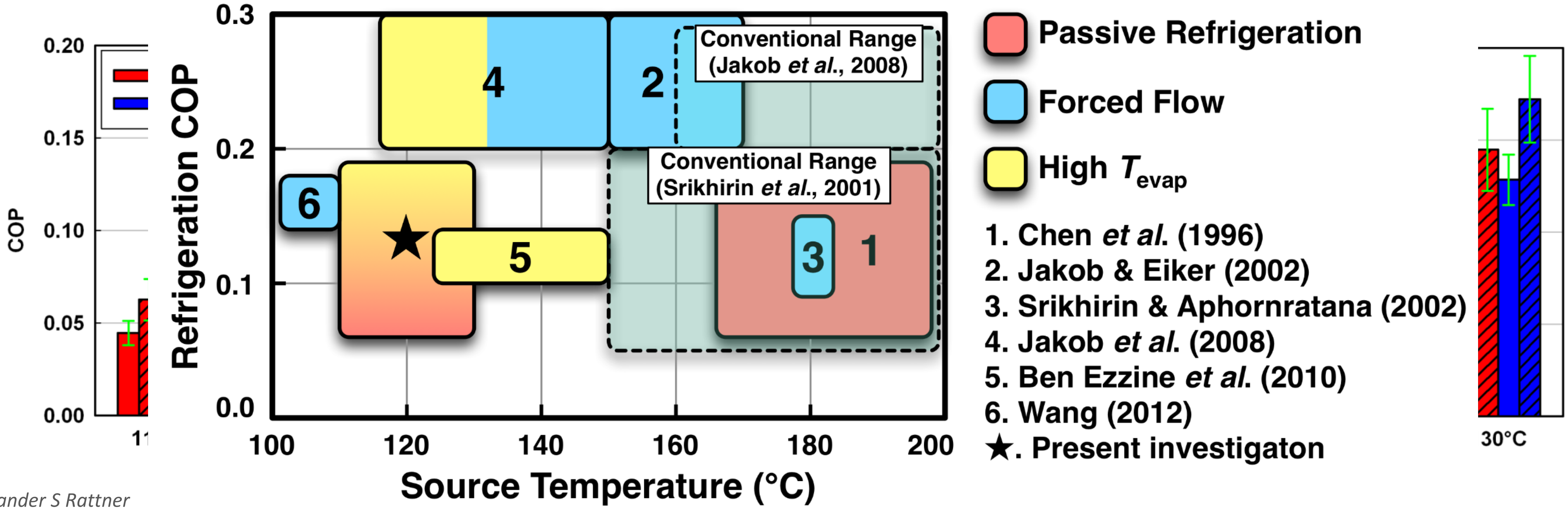
Absorber





Experimental System Evaluation

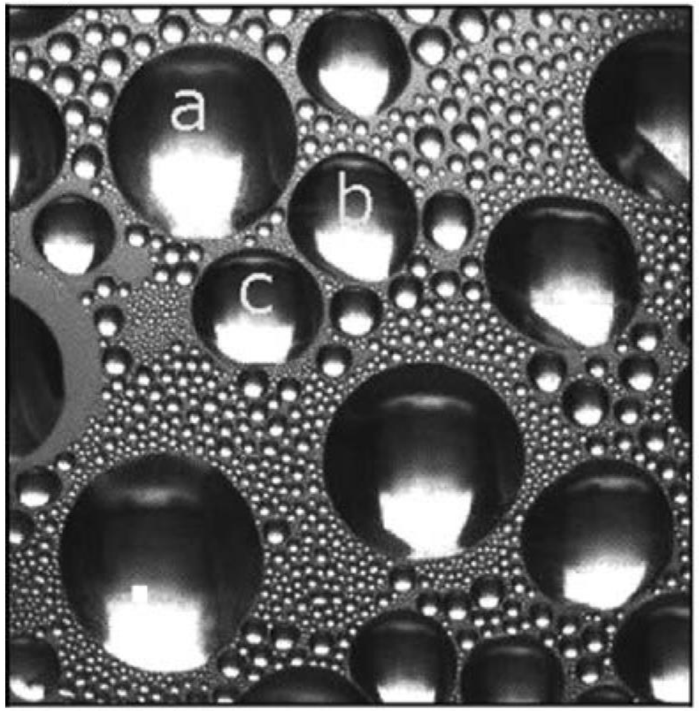
- Passive air-cooled operation at T_{source} = **110 – 130°C**
- Refrigeration (T_{evap}: 6 → 3°C) with *internal* COP: **0.06**
- Chiller *internal* COP: **0.14** (T_{evap}: 12 → 8°C)
- Minimum T_{evap} = **-2°C**



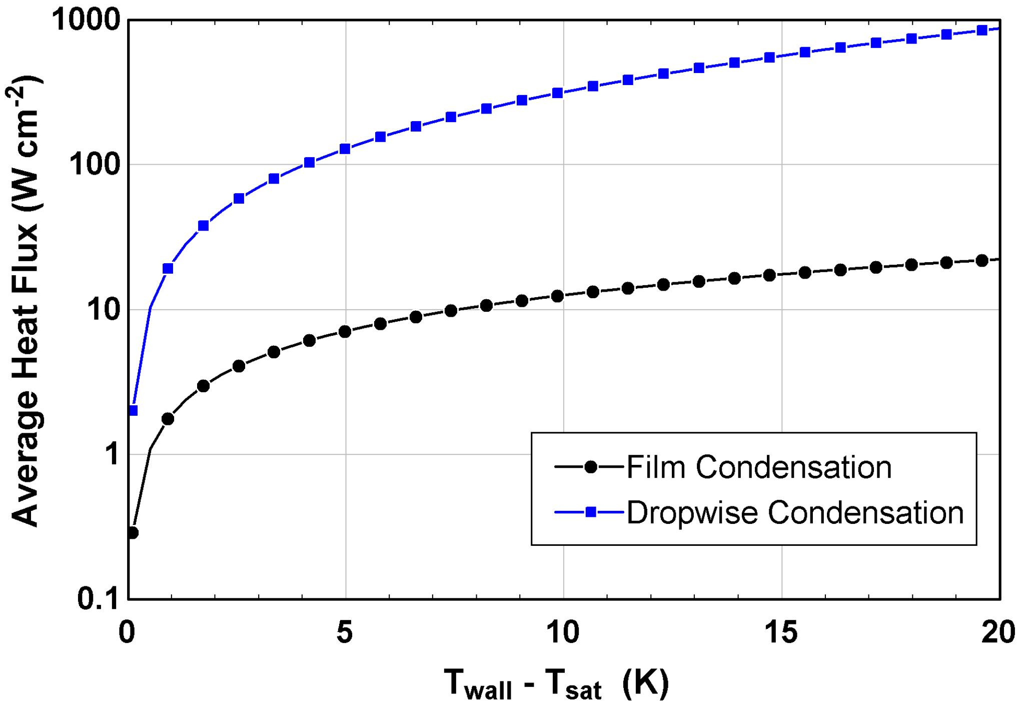
Dropwise Condensation Simulation Toward Water Desalination Applications

Overview of Dropwise Condensation

- Condensation can occur in film or dropwise modes
- High dropwise contact-line density enables ~10× heat transfer
- Challenge: delaying/avoiding dropwise-to-film transition



Sikarwar *et al.* (2010)

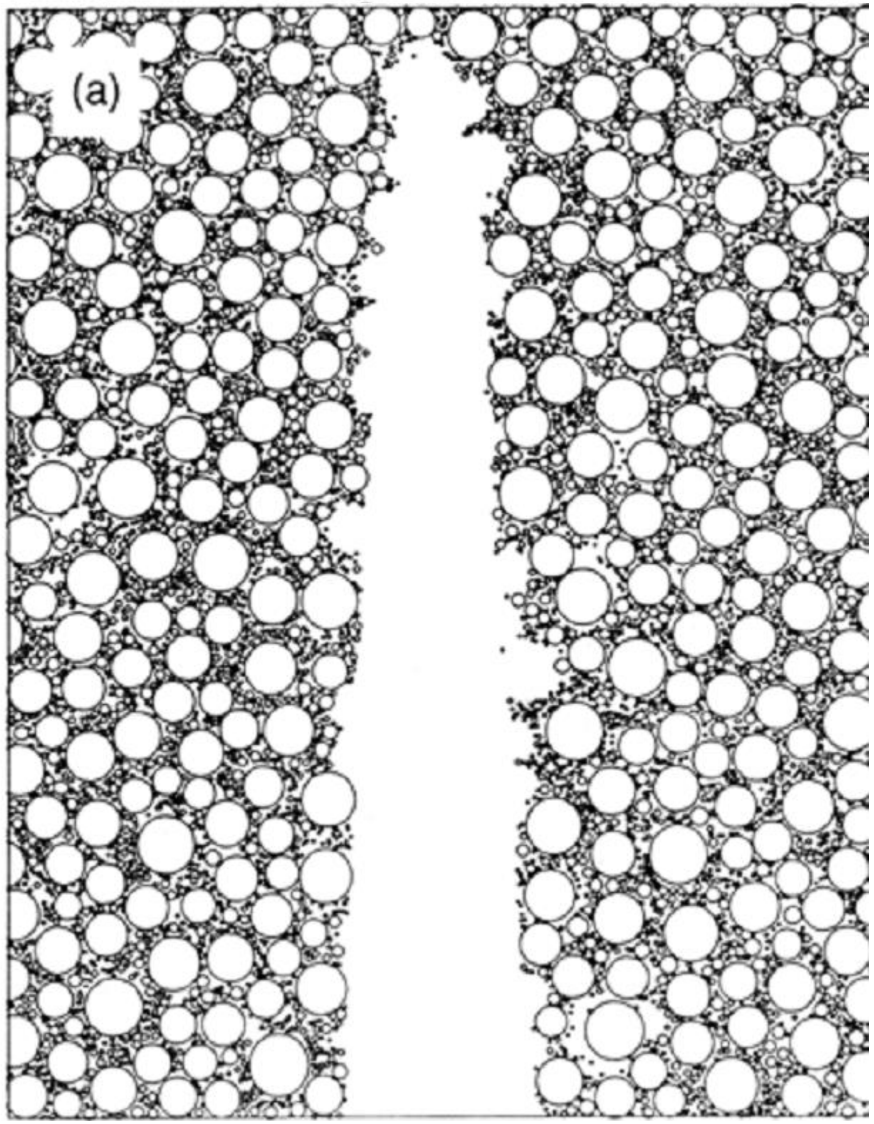


Steam (P = 1 atm, 10 cm square)

Dropwise Condensation Mechanism

- Droplets form at discrete nucleation sites on surface (10^7 – 10^9 mm^{-2})
- Drops grow and merge until removed by body forces (refreshes surface)

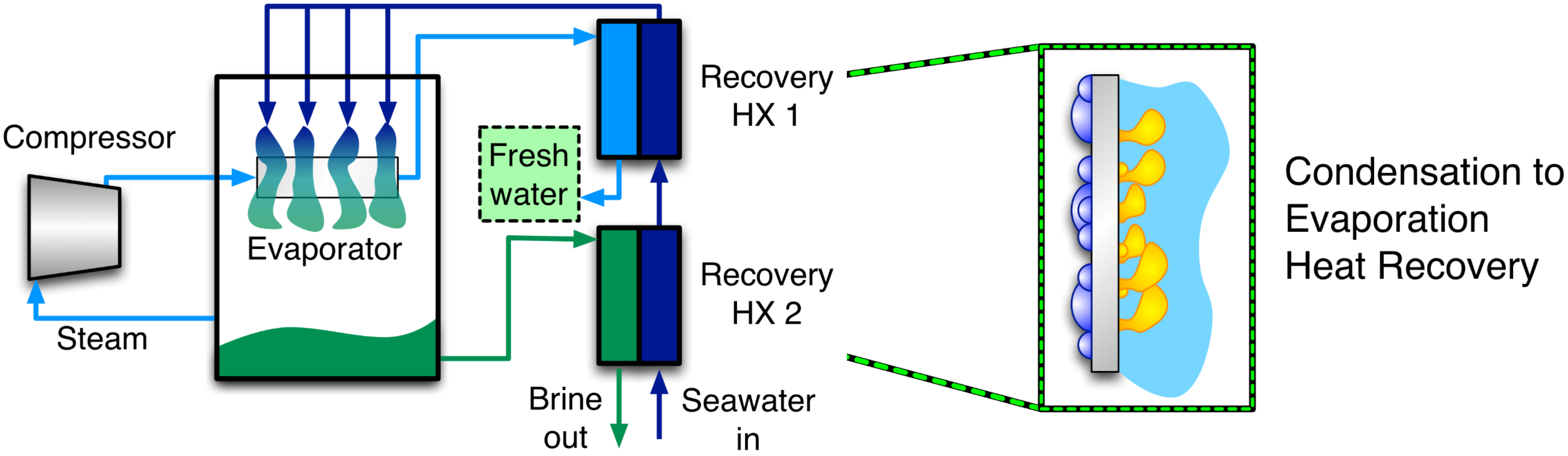
- Most heat transfer from rigid microscale drops
- Renewal driven by hydrodynamics (coalescence and sliding)



Meakin (1992)

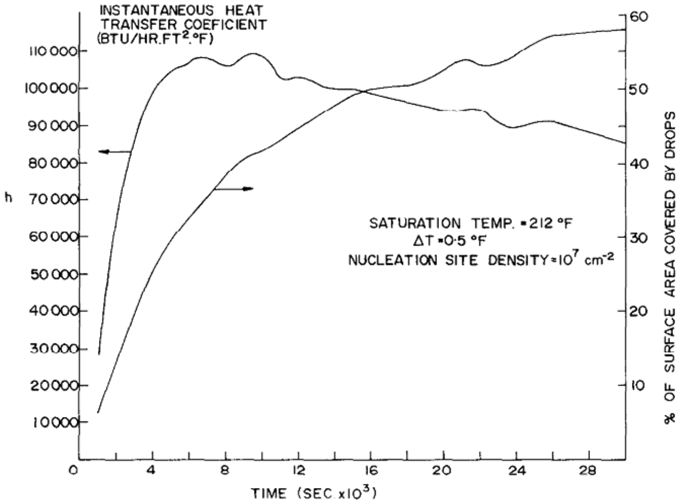
Vapor Compression Desalination

- Recuperative distillation process
  - Dropwise condensation-to-evaporation recovery: potential 35% capital cost reduction (Lukic *et al.*, 2010)
- Need simulation approaches to predict and prevent dropwise-to-filmwise flooding transition

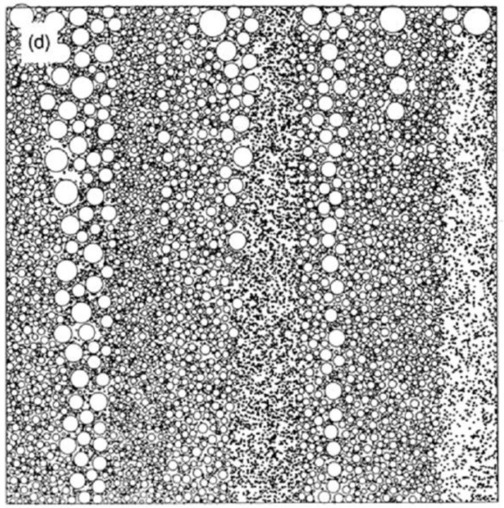


Open Research Challenges for Dropwise Condensation

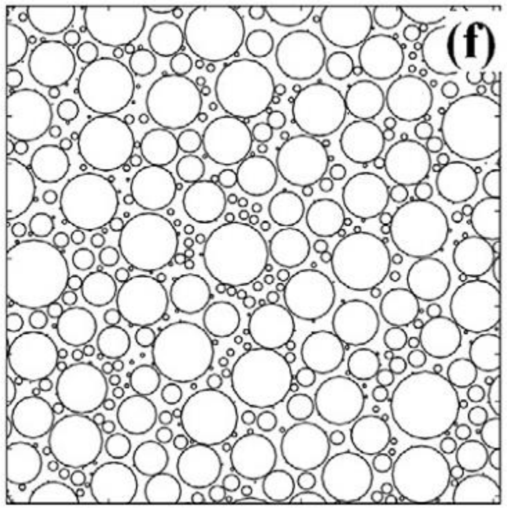
- How to predict heat transfer rate from first principles?
- Flow behavior and contributions of large droplets?
- Engineering film removal paths
- Prior models: track all droplets as rigid bodies
  - Can only capture part of active scales (10^9 droplets / mm^2)
  - Cannot account for *hydrodynamics*



Glicksman & Hunt (1972)



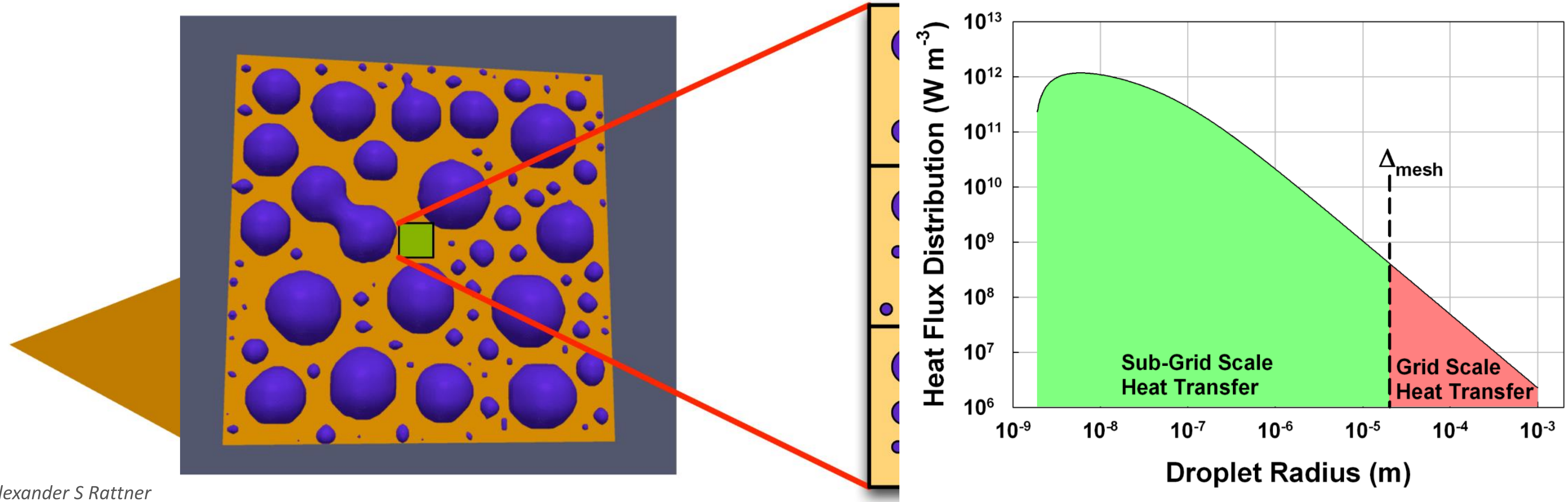
Meakin (1992)



Mei *et al.* (2011)

Approach and Objectives

- Multiscale simulation approach
  - Large scale flows: Direct *volume-of-fluid* (VOF) simulation (expensive)
  - Microscale transport: Eulerian averaged formulation

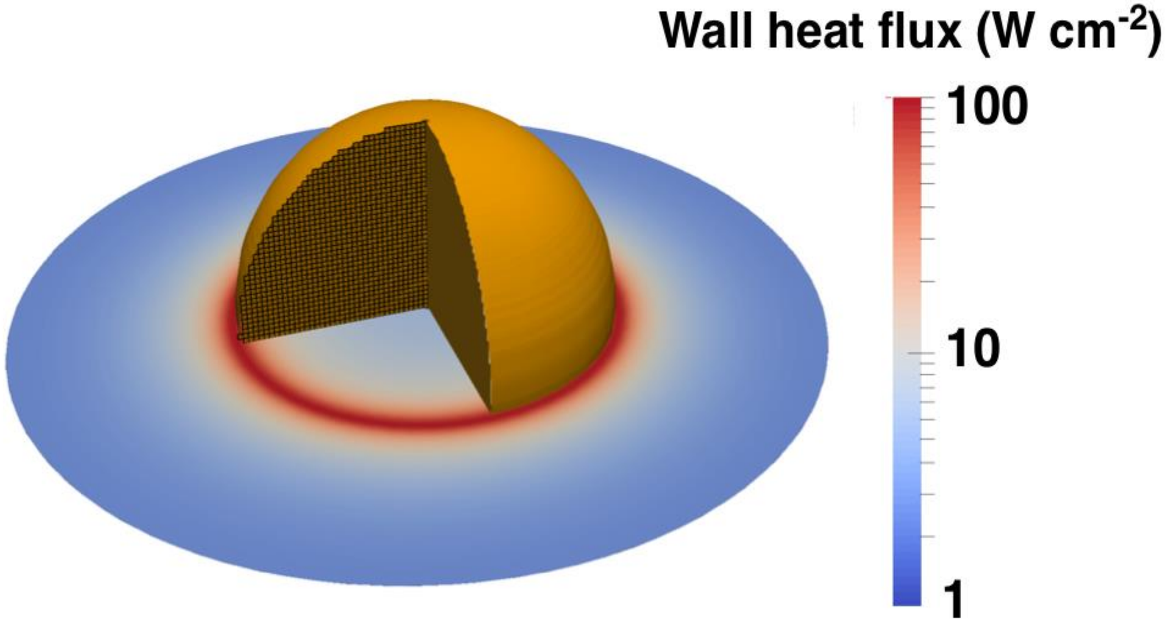


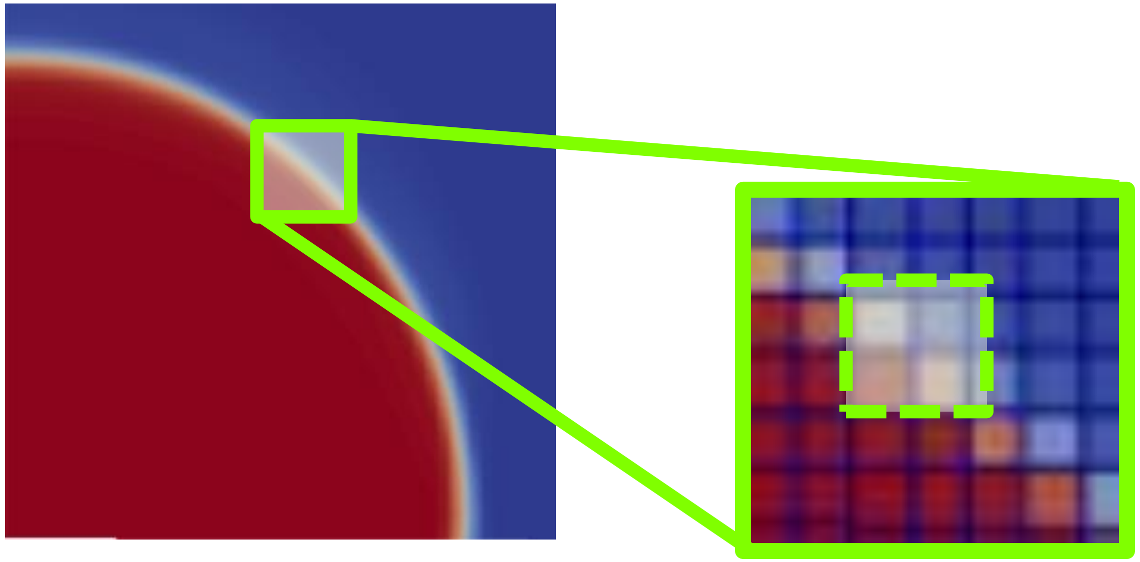
Alexander S Rattner

Phase Change Model with Interfacial Resistance

- In dropwise condensation, most heat transfer near contact-line
  - Here interfacial thermal resistance dominant (sub-continuum)
- Model with closure model centered on interface

$$\dot{q}'''_{\mathrm{pc}} \equiv \frac{T \;\; - T_{sat}}{R''_{\mathrm{int}}}\left(A\delta(\vec{x} - \vec{x}_{int})\right)$$

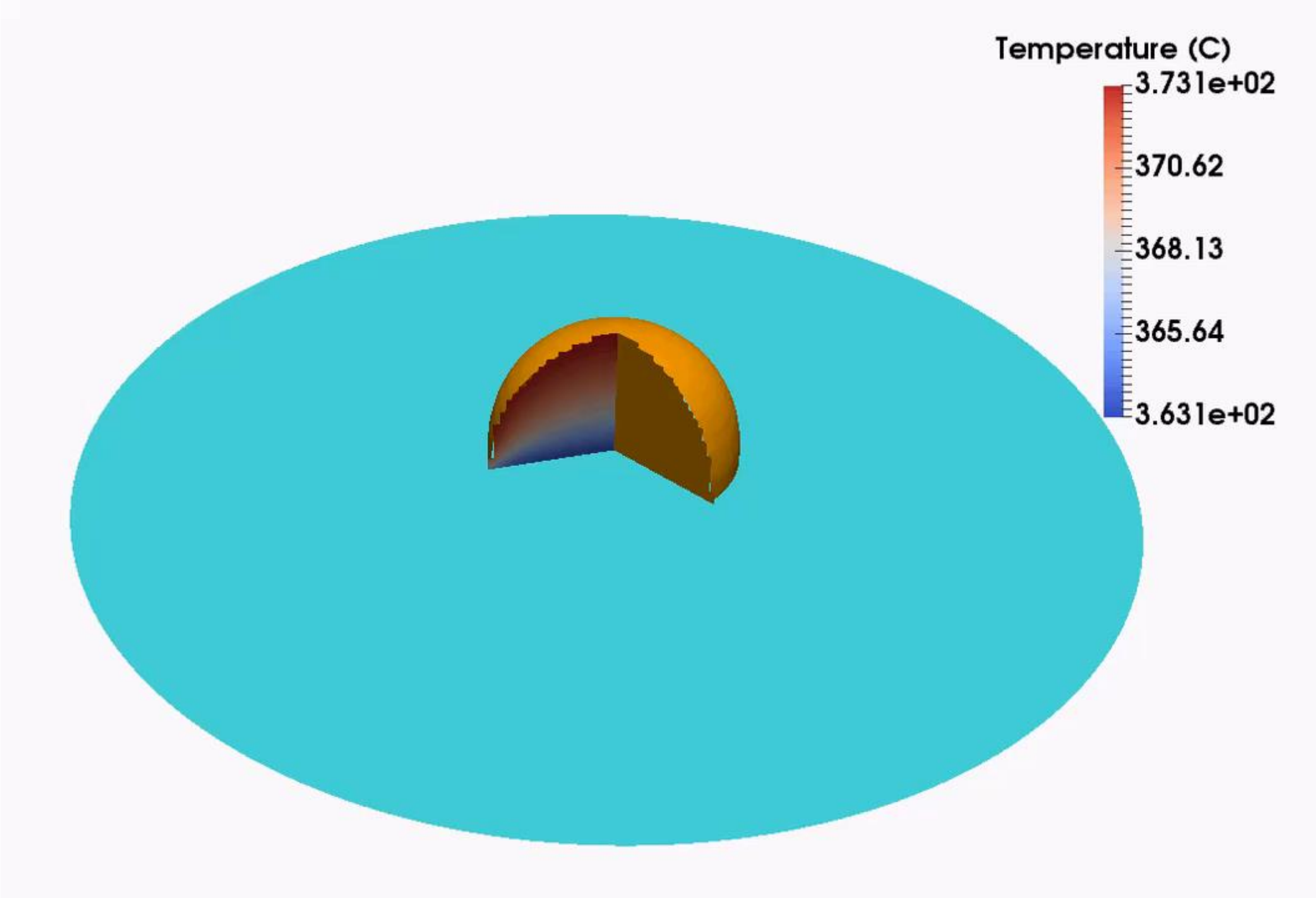


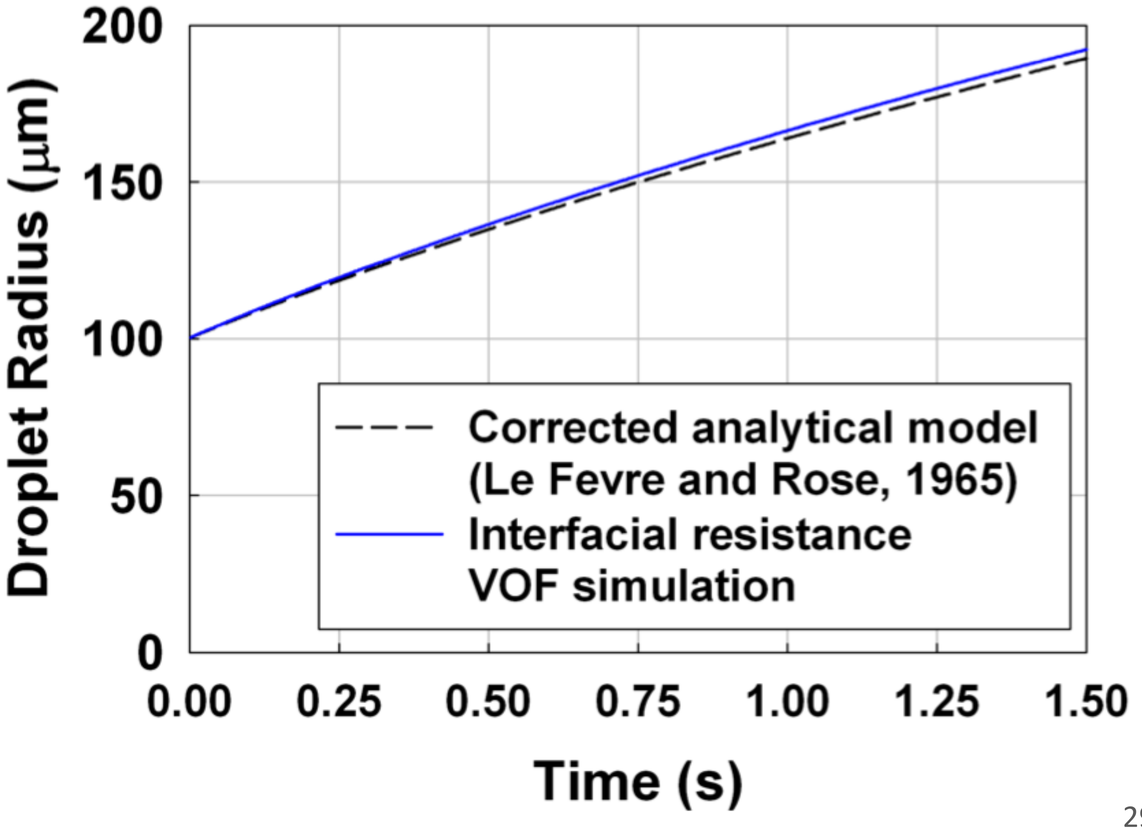


$$A\delta(\vec{x} - \vec{x}_{int}) = |\nabla\alpha_1| V_{\mathrm{cell}}$$

Validation for Droplet Growth

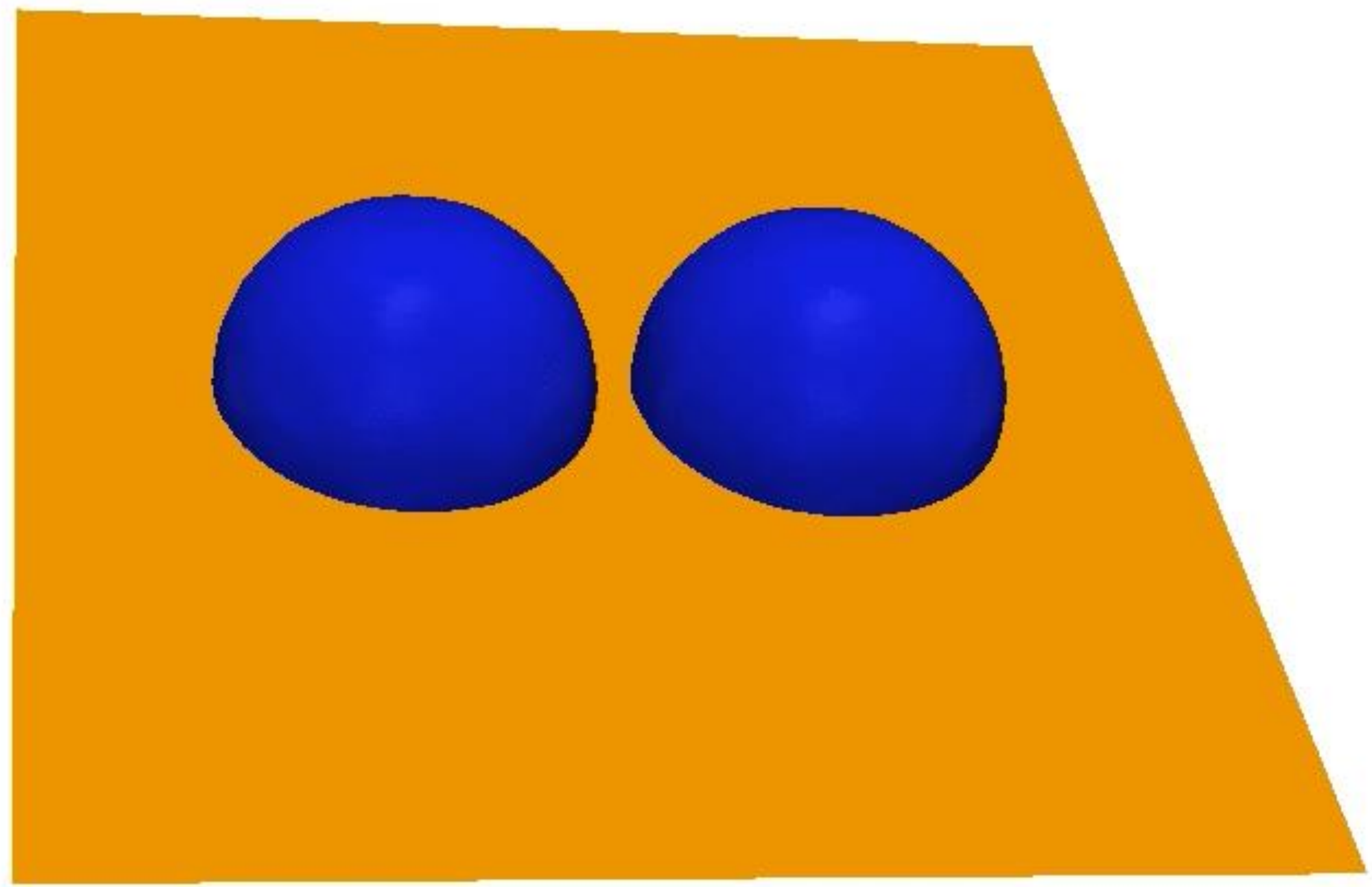
- Validation study for condensing water, P_{atm}, $T_{wall} = T_{sat} - 10$ K
- Comparison with growth rate model of Le Fevre and Rose (1965)





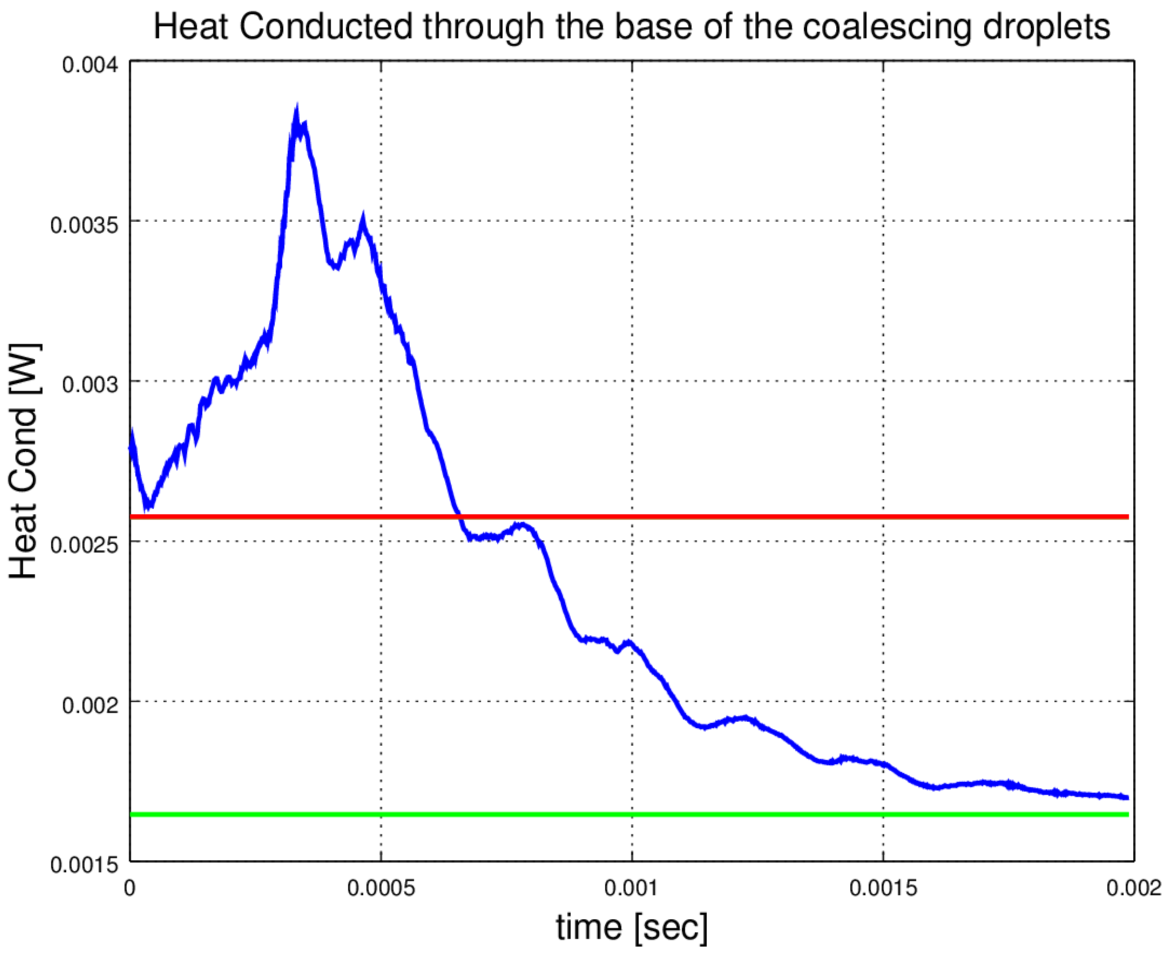
Application to Large-Scale Dynamics

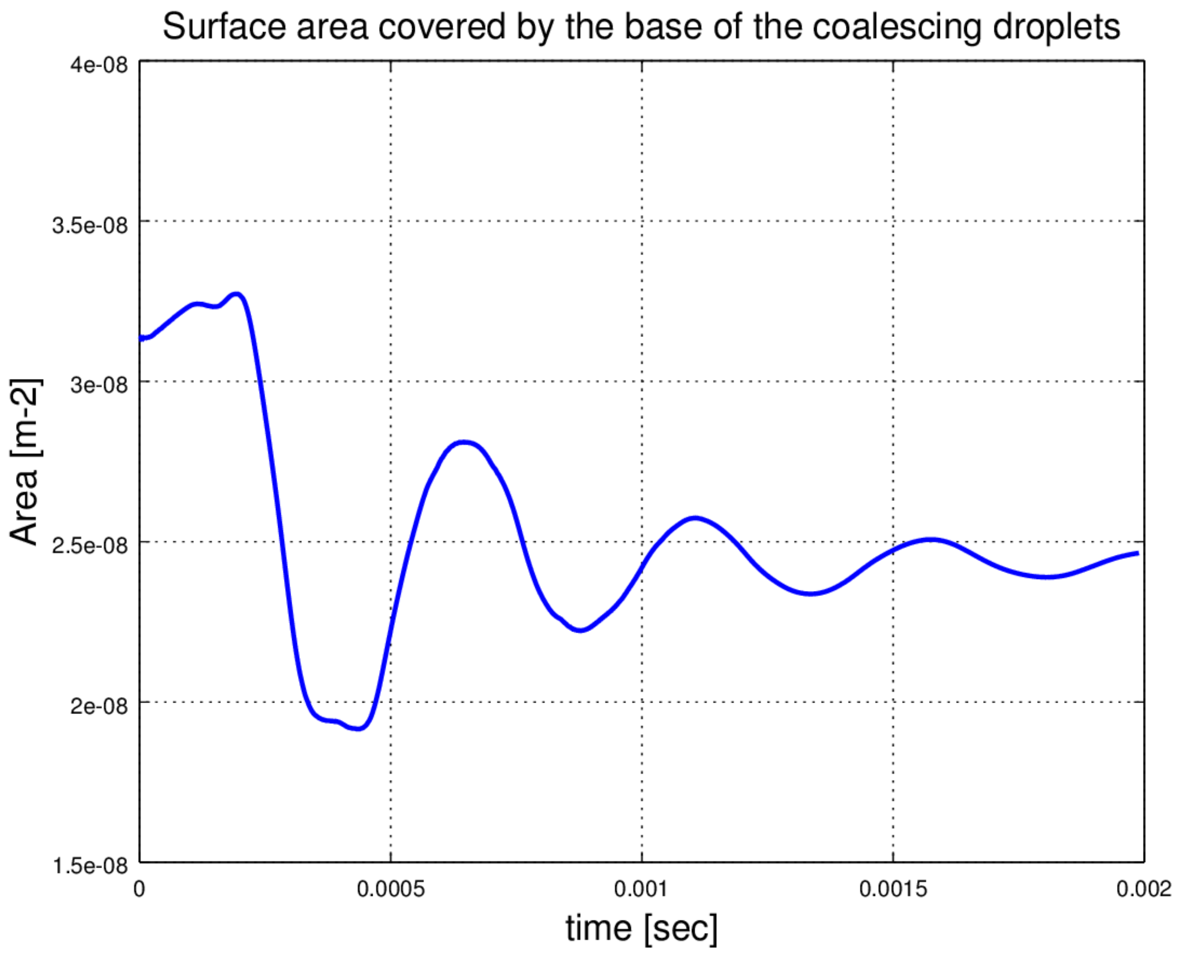
- VOF method applied to large-droplet dynamics
- Here: coalescence of two D = 100 μm droplets



Coalescence Results and Assessment

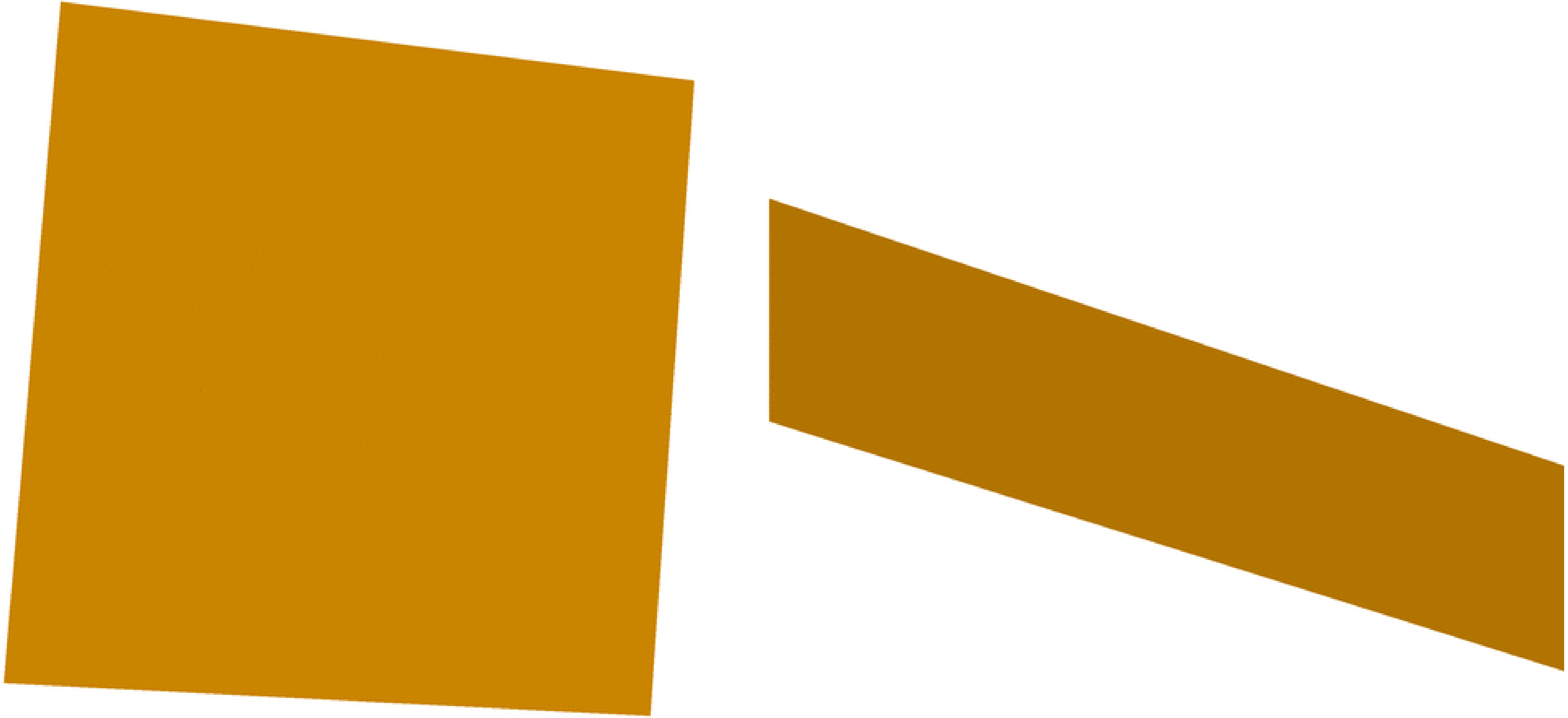
- Heat transfer enhancement due to droplet mixing
- Finite coalescence time





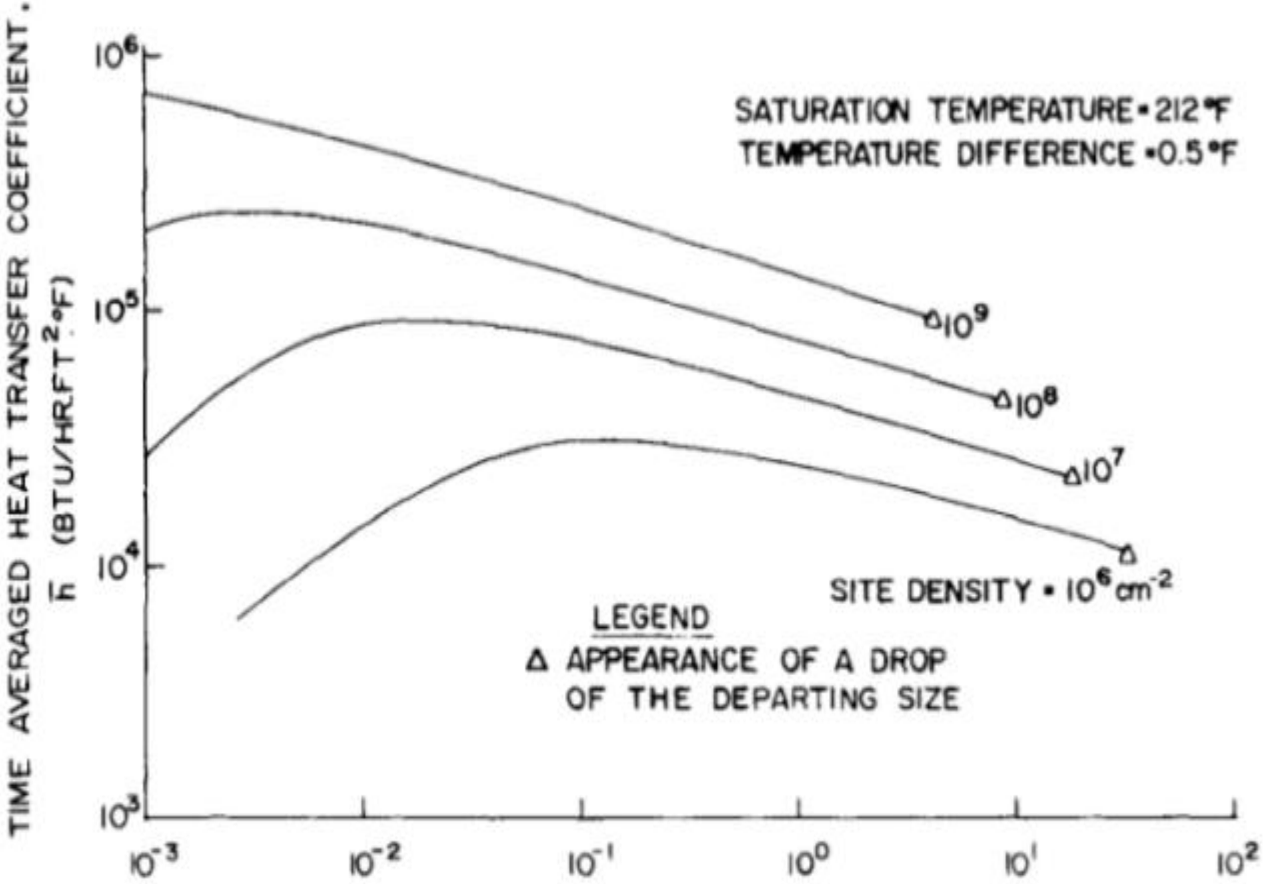
Grid-Scale Condensation Simulation

- Preliminary simulations of grid-scale condensation
- (Water 127°C, reduced σ, ΔT = 10 K, 2 × 2 mm plate, t ~ 0.05 s)



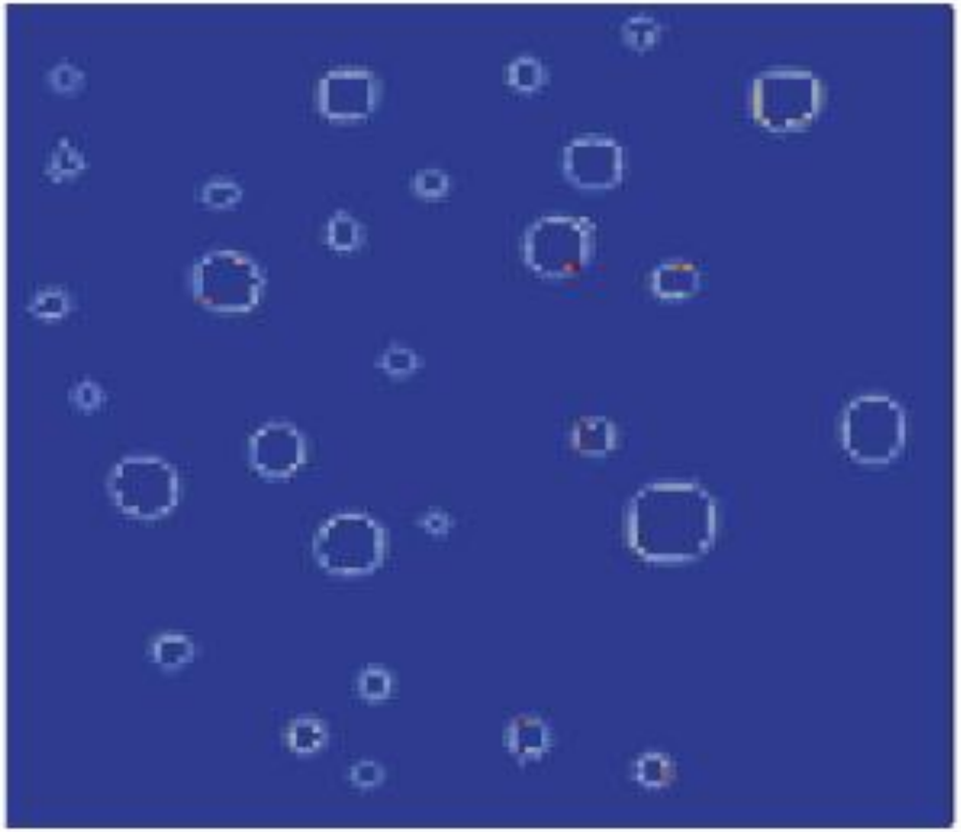
Grid-Scale Condensation Simulation

- Integrate resolved grid-scale with SGS heat transfer model
- Based on *age* since last dry or wiped clear between large droplets
  - $q''_{\mathrm{SGS}}(\tau)$ from Glicksman and Hunt (1972)

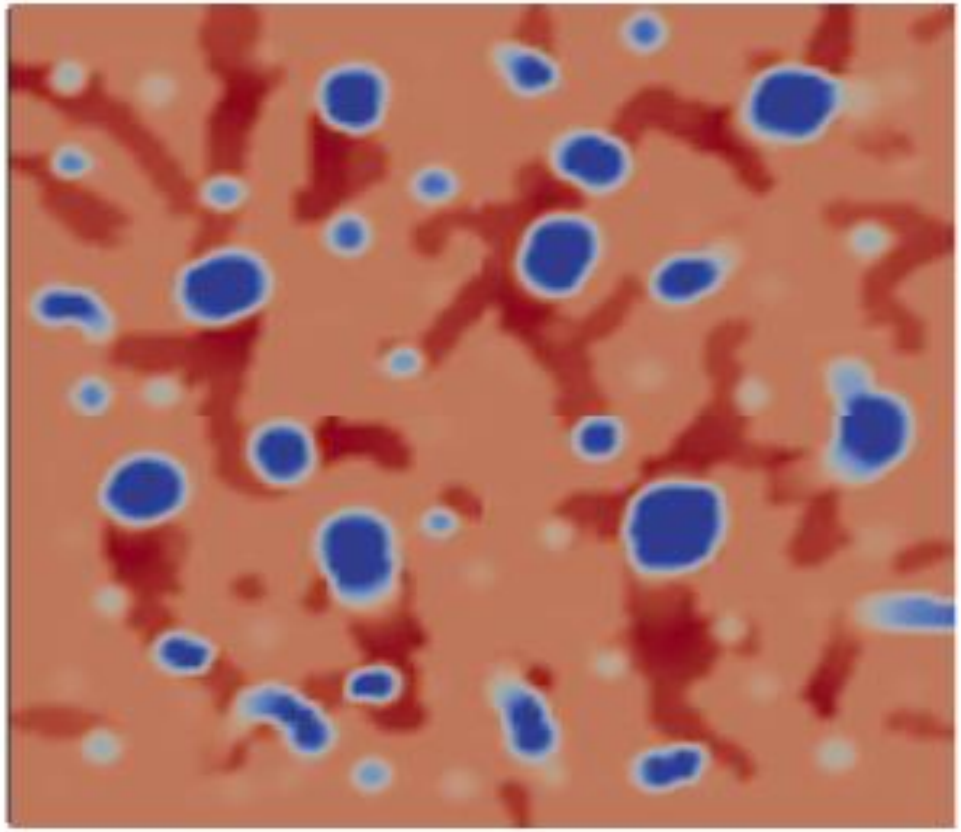


Grid-Scale Condensation Simulation

- Preliminary results, wall heat flux
- Coalescence & sliding events reset droplet growth cycle



Grid Scale

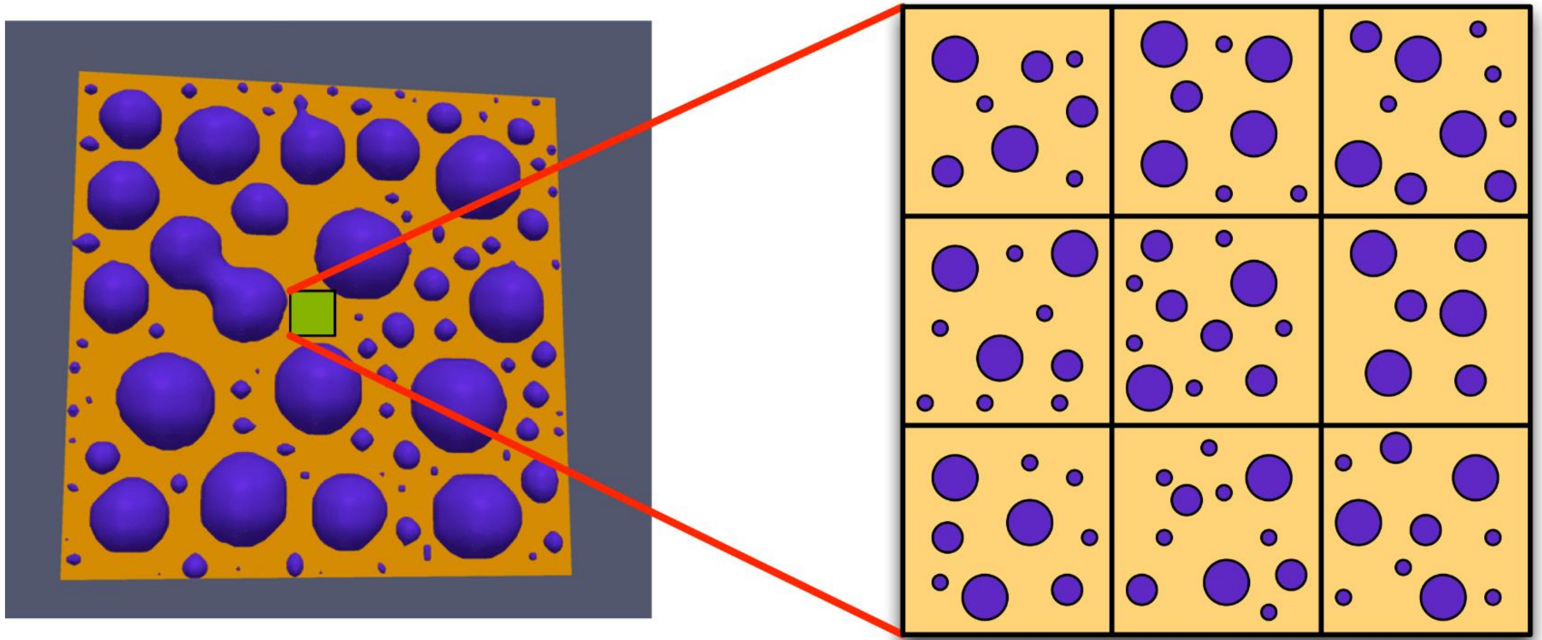


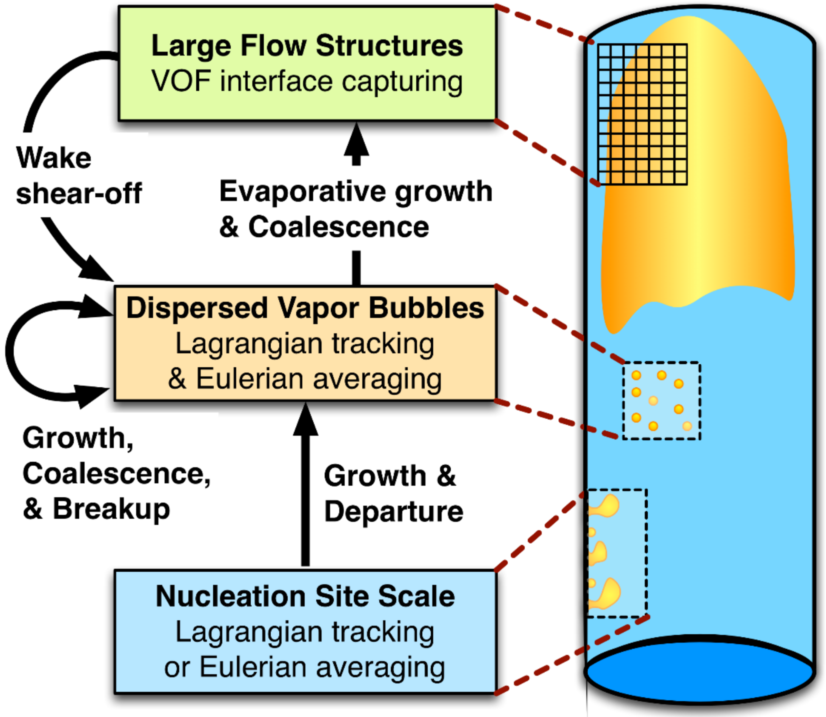
Sub Grid Scale

Some Open Challenges in Phase-Change CFD & Potential Research Directions

Extreme Ranges of Scales in Boiling and Condensation

- Dropwise condensation: up to 10^9 active sites / mm^2
  - 5 cm square, storing x, y, and r (FP doubles): 55 TB memory!
- Boiling: μm-scale nucleation sites up to cm-scales vapor slugs
- Potential for multiscale approaches with low-cost microscale models





Interface Breakup and Coalescence

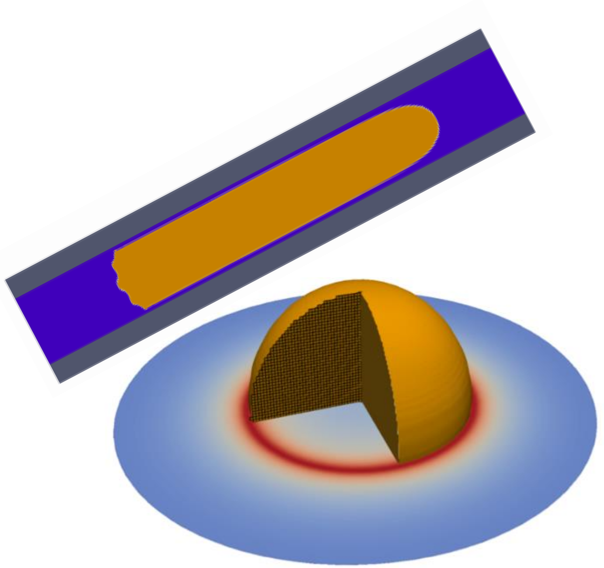
- Most solvers predict coalescence/breakup when meniscus $\lesssim \Delta_{\text{mesh}}$
  - – Fail to predict real interface dynamics (bubble bouncing)
- Need hybrid continuum-MD methods (Bardia *et al.*, 2016)

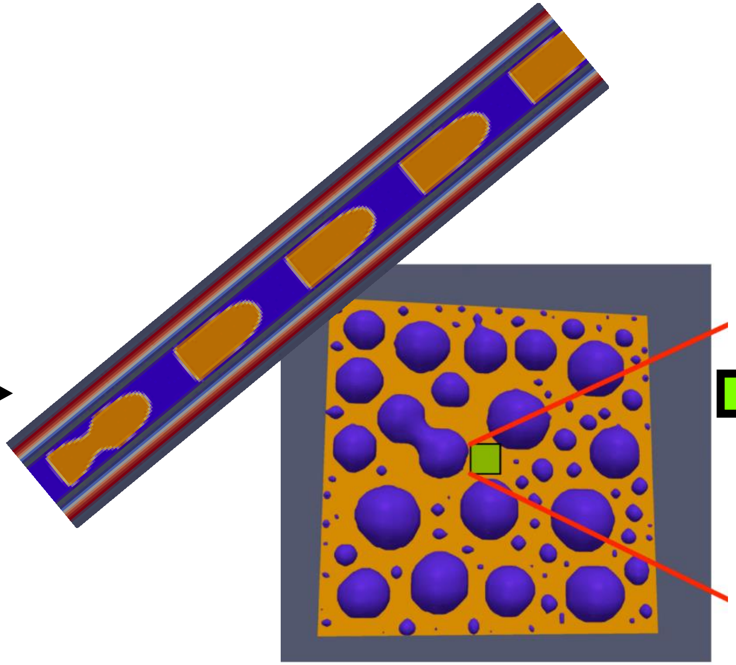
Air-water flow (Alnajdi & Rattner, 2016)

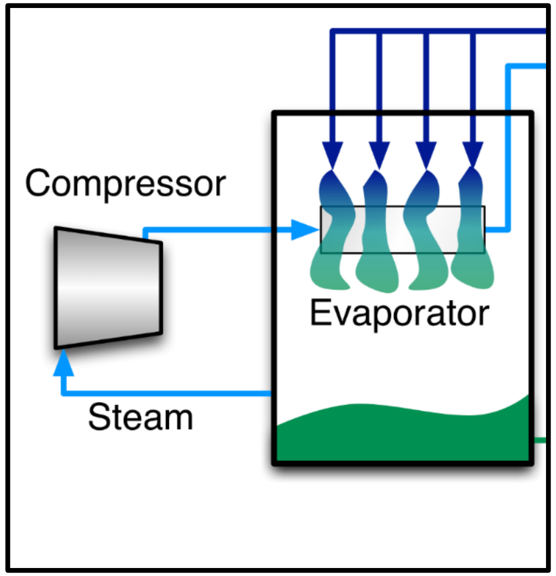
Summary and Outlook

Summary and Outlook

- Apply phase change simulations at **phenomena** and **process** scales to advance **energy systems**







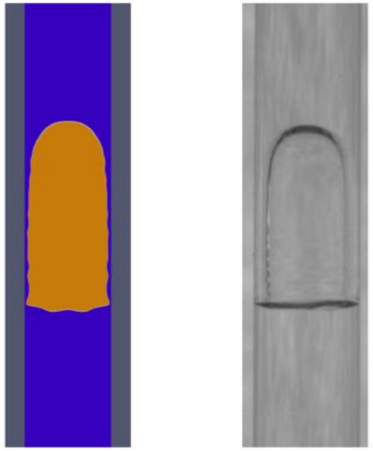
Transport Phenomena

Phase Change Processes

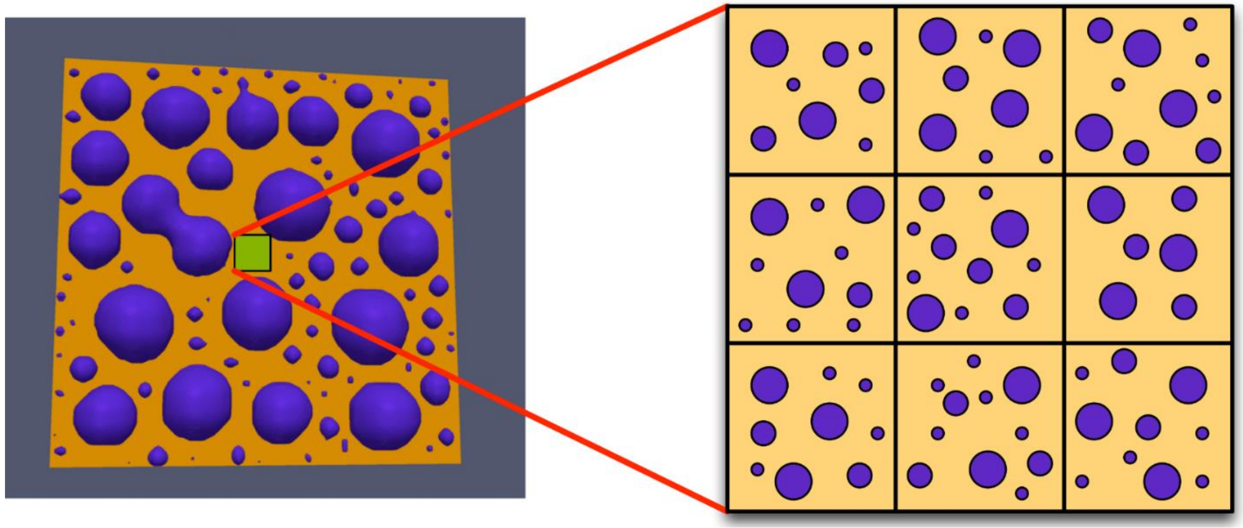
Thermal Energy Systems

Summary and Outlook

- Potential for complementary simulations and experiments (beyond validation)



- **Open research challenges:** highly multiscale processes, approaching continuum limits



Thank You

- Dr. Srinivas Garimella, STSL at Georgia Tech
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