Wetting and other interfacial phenomena during RTM

Matthew Grasinger

Air Force Research Laboratory
Materials & Manufacturing Directorate

email: matthew.grasinger.1@afrl.af.mil

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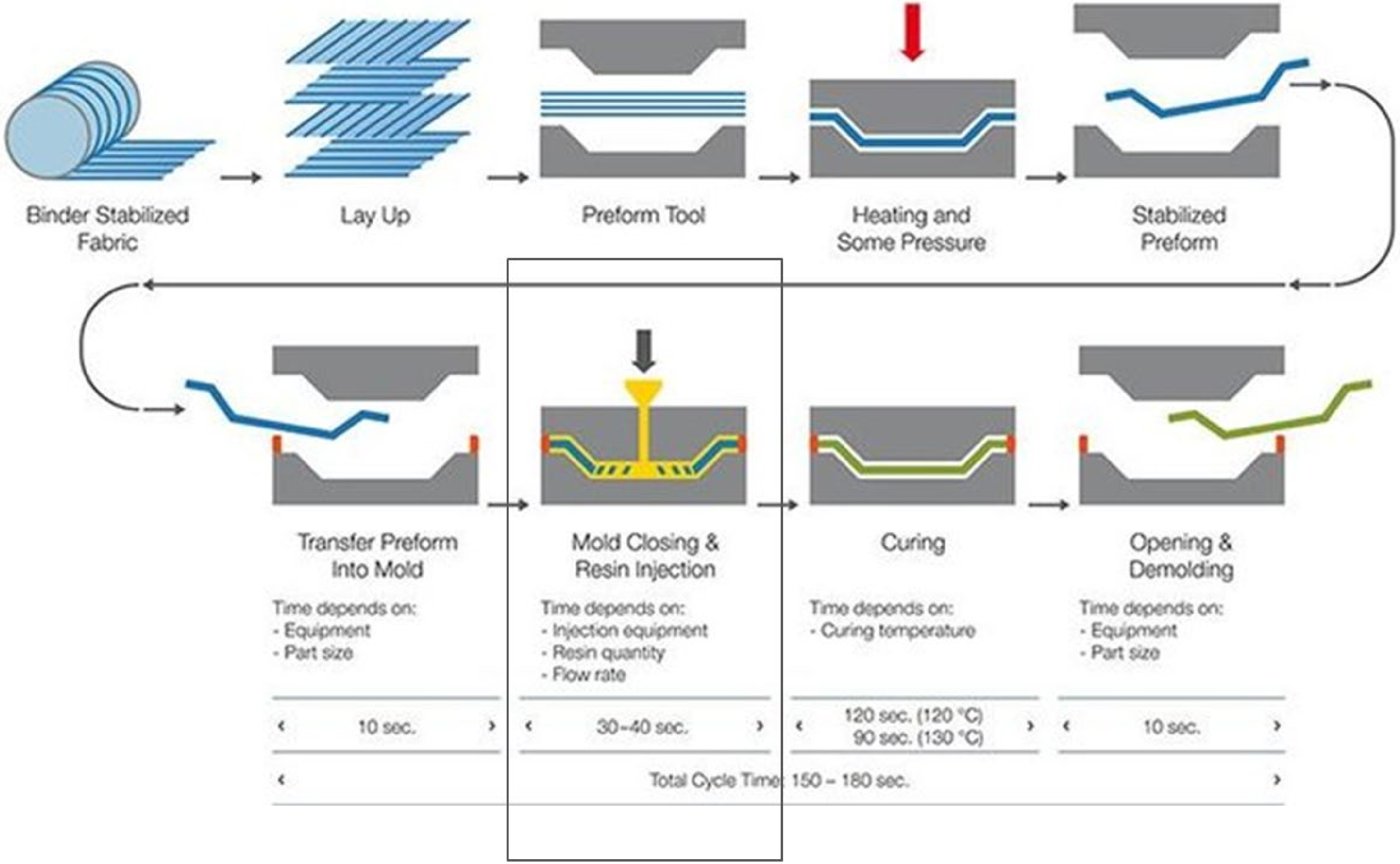
Resin transfer molding



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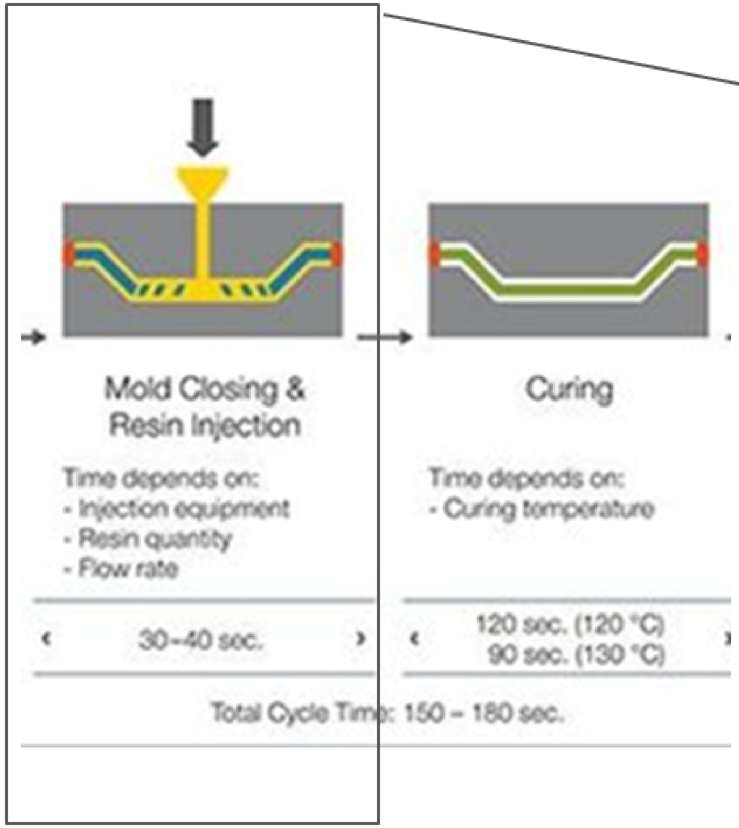
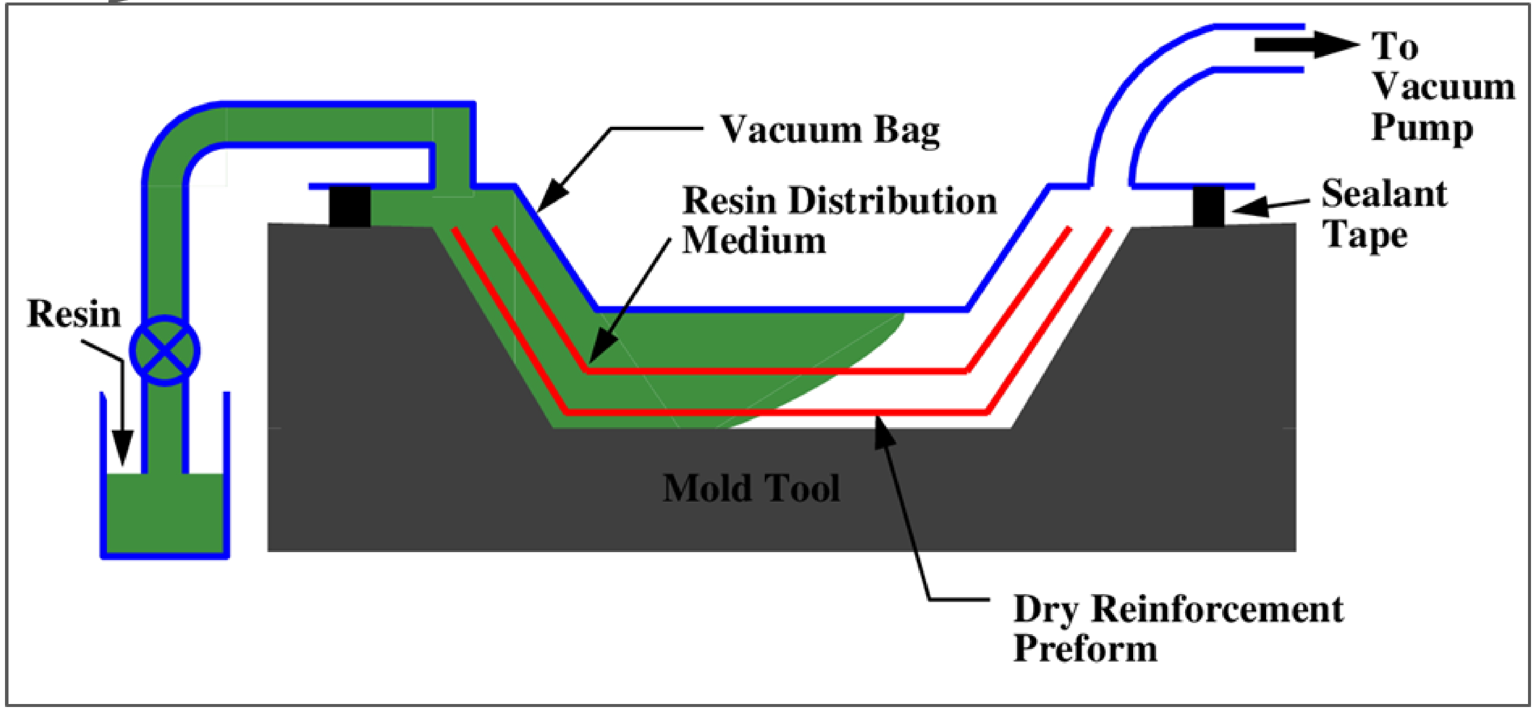
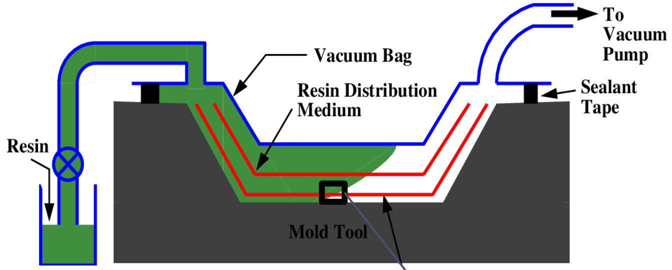
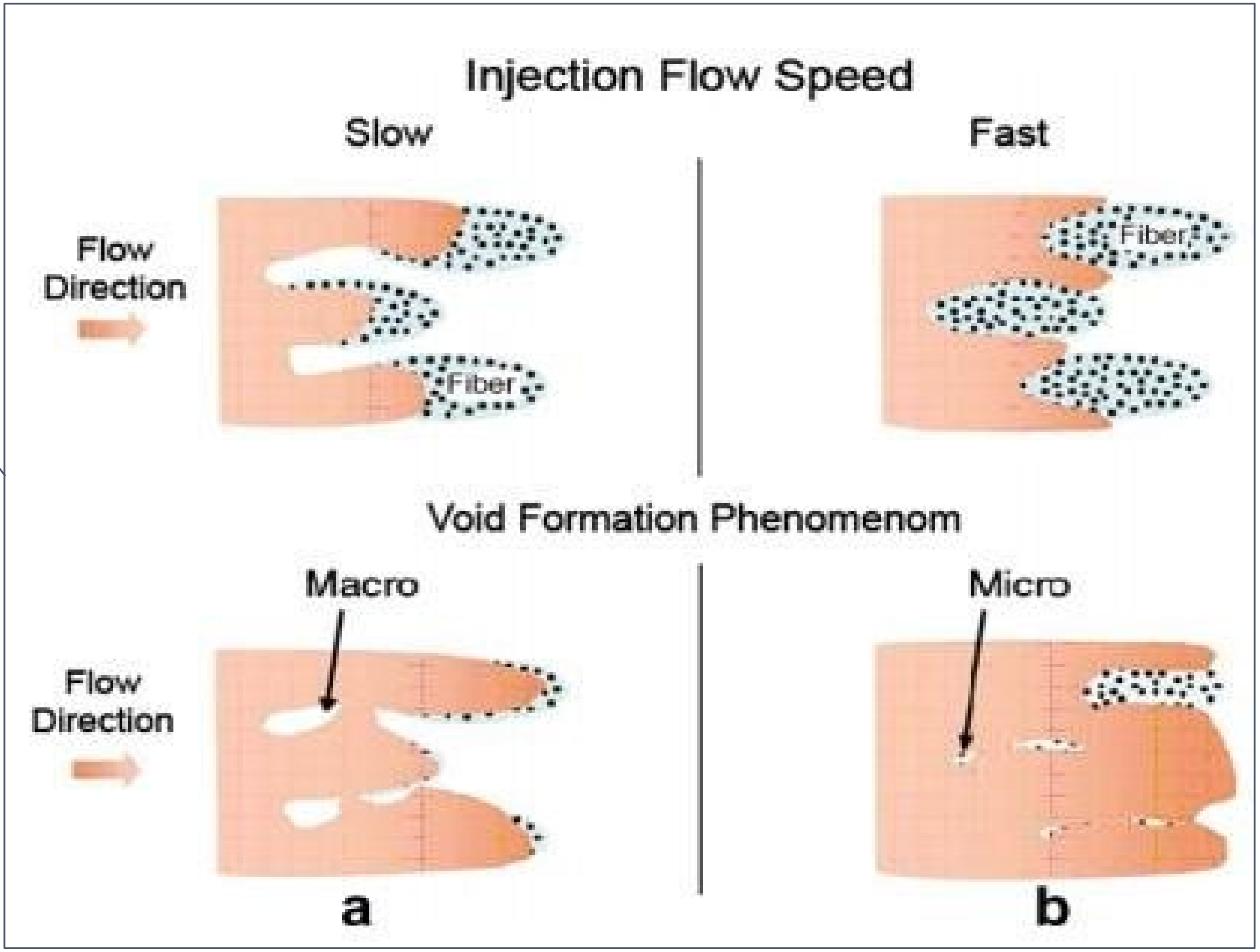




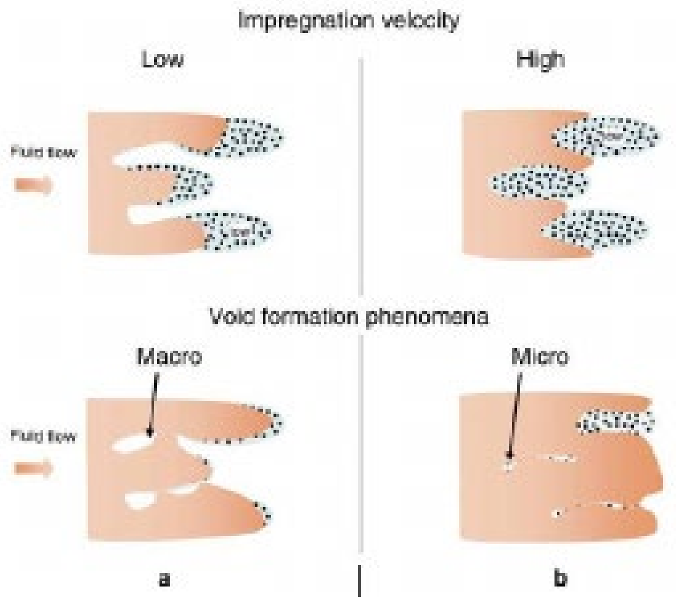
Void formation during resin infusion



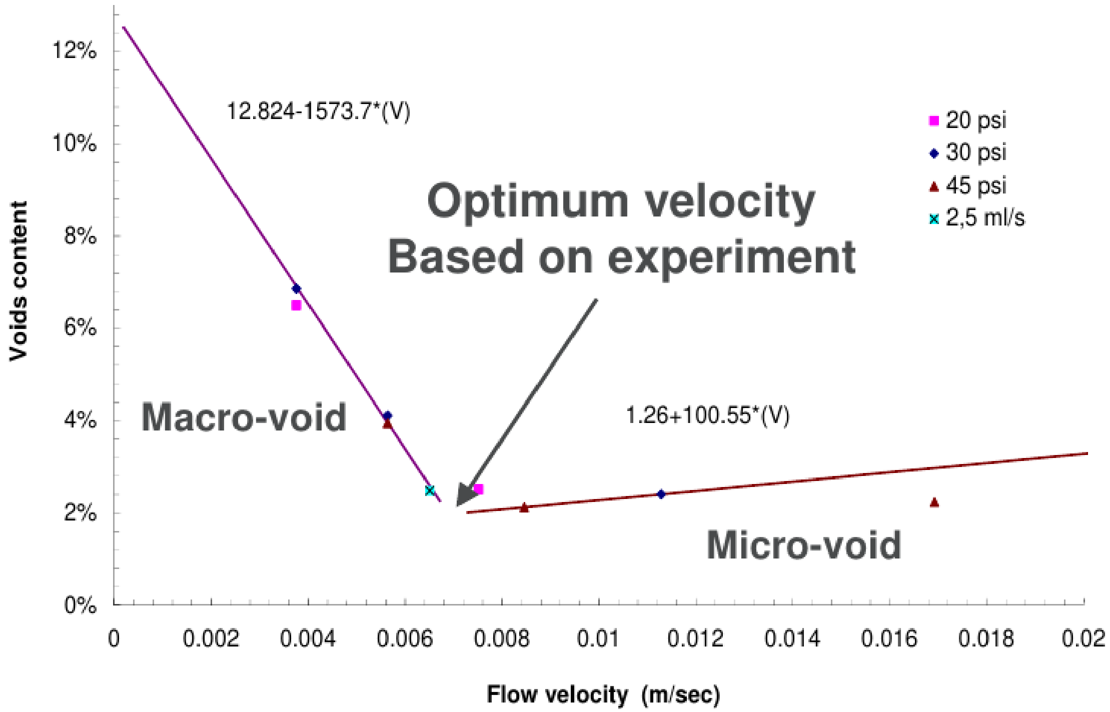


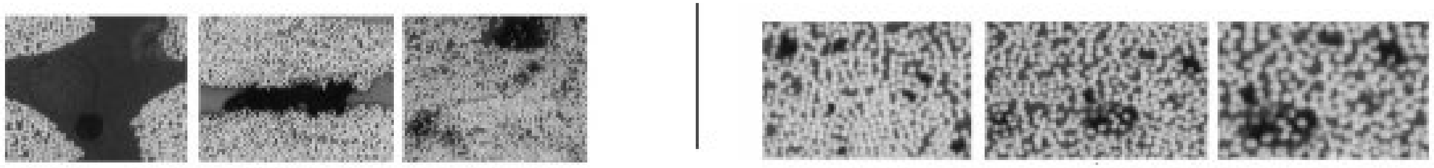
Void formation during resin infusion

$$\max\left\|\vec{v}_{front}\right\| \le \left\|\vec{v}_{crit}\right\|$$



“Optimum”





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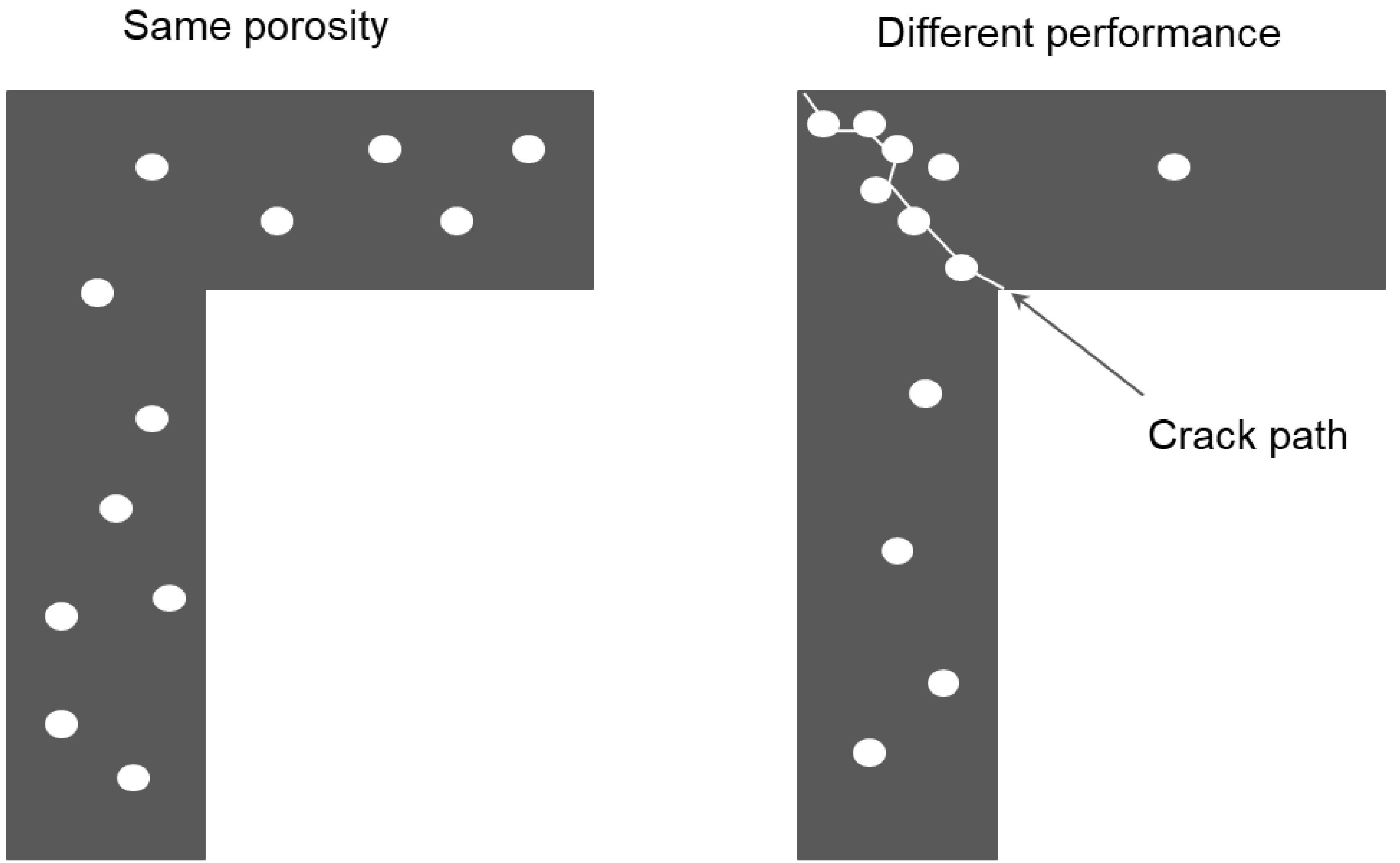

Tow permeability, void formation, and void transport

… as a function of

- Processing conditions and “flow schedule”
  - Inlet pressure/flow rate, temperatures, etc.
- Tow geometry and fiber packing
- Resin rheology
  - Viscosity (as a function of time and temperature), shear thinning/thickening, etc.
- Degree of saturation
- Resin surface tension
- Fiber wetting and surface chemistry
  - What role does sizing play?
  - … electrowetting? Electrowetting schedule?

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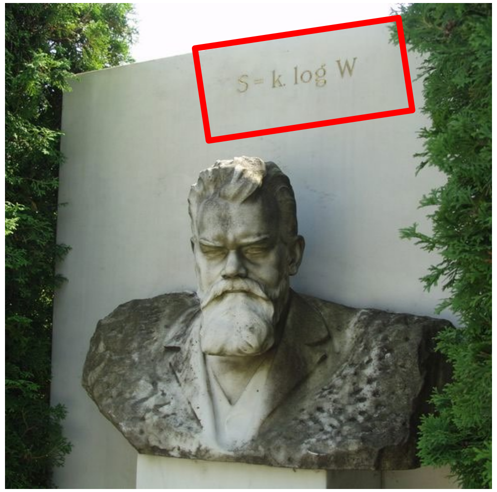
Lattice Boltzmann method

$$f\left(x, v, t\right) \equiv$$ Probability density of particle at ‘x’, with velocity ‘v’, at time ‘t’



Continuous Boltzmann equation

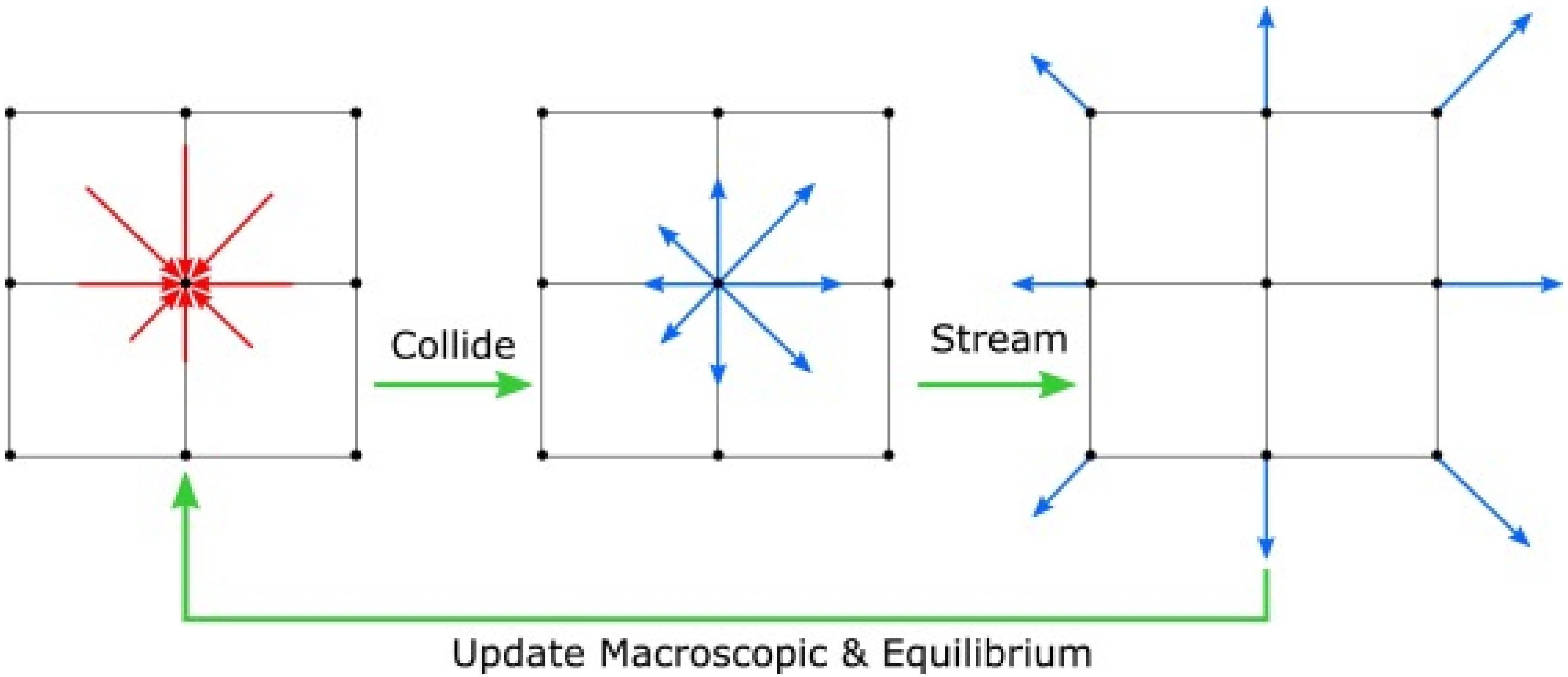
$$\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + \frac{F}{m} \cdot \frac{\partial f}{\partial v} = \Omega\left(f\right)$$

Lattice Boltzmann equation

$$f_k\left(x + \xi_k \Delta t, t + \Delta t\right) - f_k(x, t) + \tilde{F}_k = \Omega_k\left(f\right)$$

Lattice Boltzmann method

$$f_k\left(x+\xi_k \Delta t, t+\Delta t\right)-f_k(x, t)+\tilde{F}_k=\Omega_k\left(f\right)$$

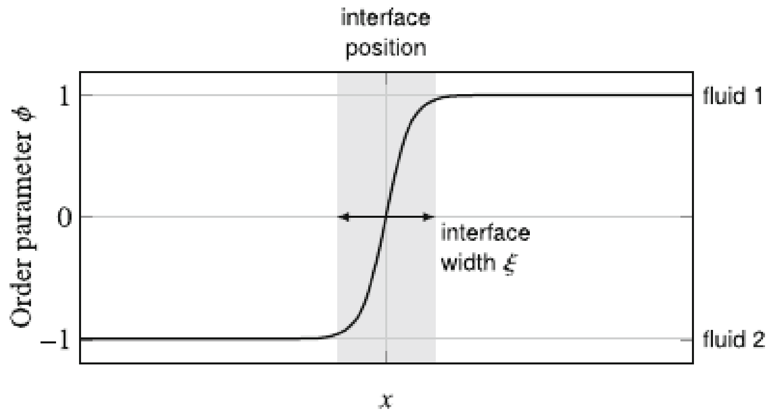


$$\rho\left(x, t\right)=\sum_k f_k\left(x, t\right), \quad \rho u\left(x, t\right)=\sum_k \xi_k f_k\left(x, t\right)$$

Multicomponent flow

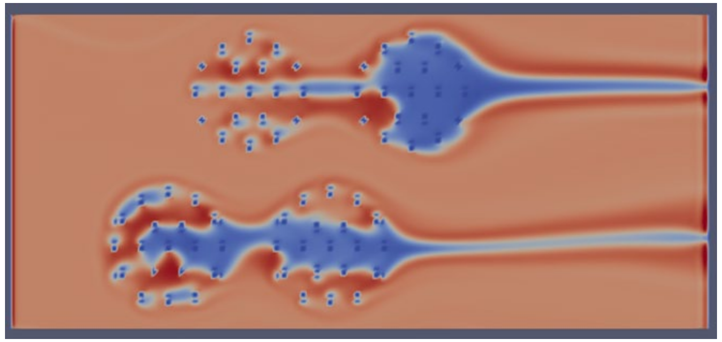
- Simulate both fluids on separate lattices
- Calculate order parameter

$$\phi = \frac{\rho^{(1)} - \rho^{(2)}}{\rho^{(1)} + \rho^{(2)}}$$



- Define a free energy functional based on the order parameter
  - Immiscible fluids: energy penalize gradients in the order parameter
- Momentum is transferred to each fluid via gradients in free energy

Blue: $\phi = -1$
Red: $\phi = 1$



Free energy and thermodynamics

Bulk fluid thermodynamics

$$\Psi = \int_V [\psi_b + \psi_g] \, dV = \int_V \left[c_s^2 \rho \ln \rho + \frac{A}{4}\left(\phi^2 - 1\right)^2 + \frac{\kappa}{2}(\nabla \phi)^2 \right] dV$$

Recall:

$$\phi = \frac{\rho^{(1)} - \rho^{(2)}}{\rho^{(1)} + \rho^{(2)}}$$

Penalizes mixing of fluids

Penalizes change in order parameter; Controls the equilibrium *interface width*

$$\xi = \sqrt{\kappa / A}$$

Free energy and thermodynamics

Bulk fluid thermodynamics

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Interface thermodynamics

$$\gamma_{12} = \int_{-\infty}^{\infty} \left[\frac{A}{4}\left(\phi^2 - 1\right)^2 + \frac{\kappa}{2}(\nabla\phi)^2 \right] dx = \sqrt{\frac{8\kappa A}{9}}.$$

Equilibrium surface energy between two fluids

(Assuming flat interface between fluids at x = 0)

Free energy and thermodynamics

Surface thermodynamics

$$\gamma_{12} = \int_{-\infty}^{\infty} \left[\frac{A}{4}\left(\phi^2 - 1\right)^2 + \frac{\kappa}{2}(\nabla\phi)^2 \right] \mathrm{d}x = \sqrt{\frac{8\kappa A}{9}}.$$

Equilibrium surface energy between two fluids

(Assuming flat interface between fluids at x = 0)

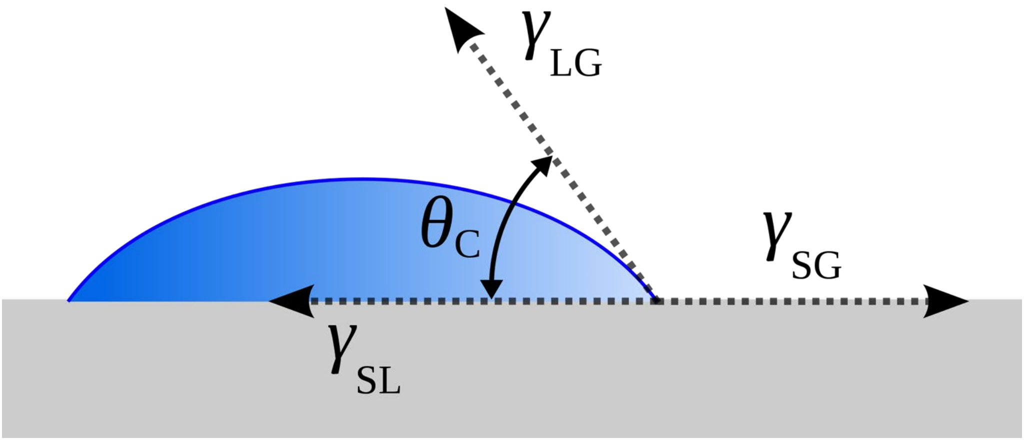
$$\Psi_s = \int_A \psi_s \, \mathrm{d}A = -\int_A h\phi_s \, \mathrm{d}A$$

Free energy at solid boundary
(h > 0, fluid 1 is preferred
h < 0, fluid 2 is preferred)

$$\gamma_{s1} = \frac{\gamma_{12}}{2}\left[1 - (1 + \Omega)^{3/2}\right]$$

$$\gamma_{s2} = \frac{\gamma_{12}}{2}\left[1 - (1 - \Omega)^{3/2}\right]$$

$$\Omega = h\sqrt{2/(\kappa A)}$$



Free energy and thermodynamics

Surface thermodynamics

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Surface tension parameter

Equilibrium surface energy between two fluids

(Assuming flat interface between fluids at x = 0)

$$\Psi_s = \int_A \psi_s \, \mathrm{d}A = - \int_A h \phi_s \, \mathrm{d}A$$

Free energy at solid boundary
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Surface affinity

$$\gamma_{s1} = \frac{\gamma_{12}}{2} \left[1 - (1 + \Omega)^{3/2} \right]$$

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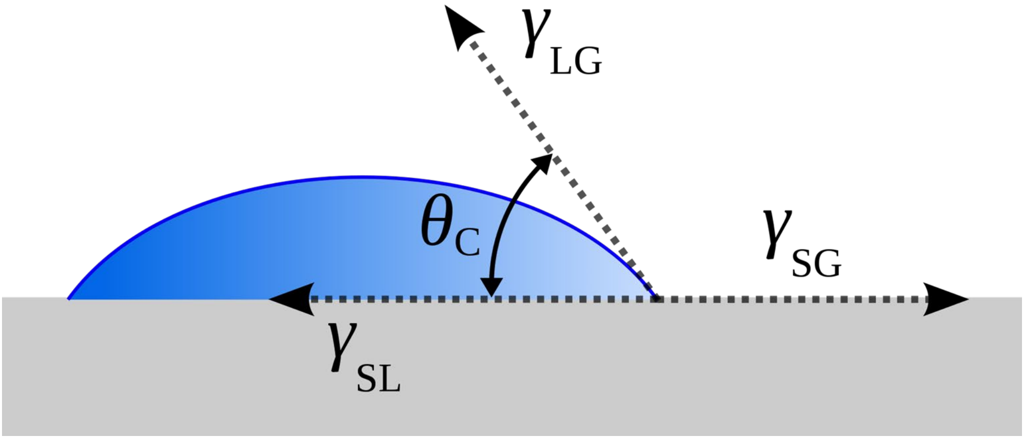
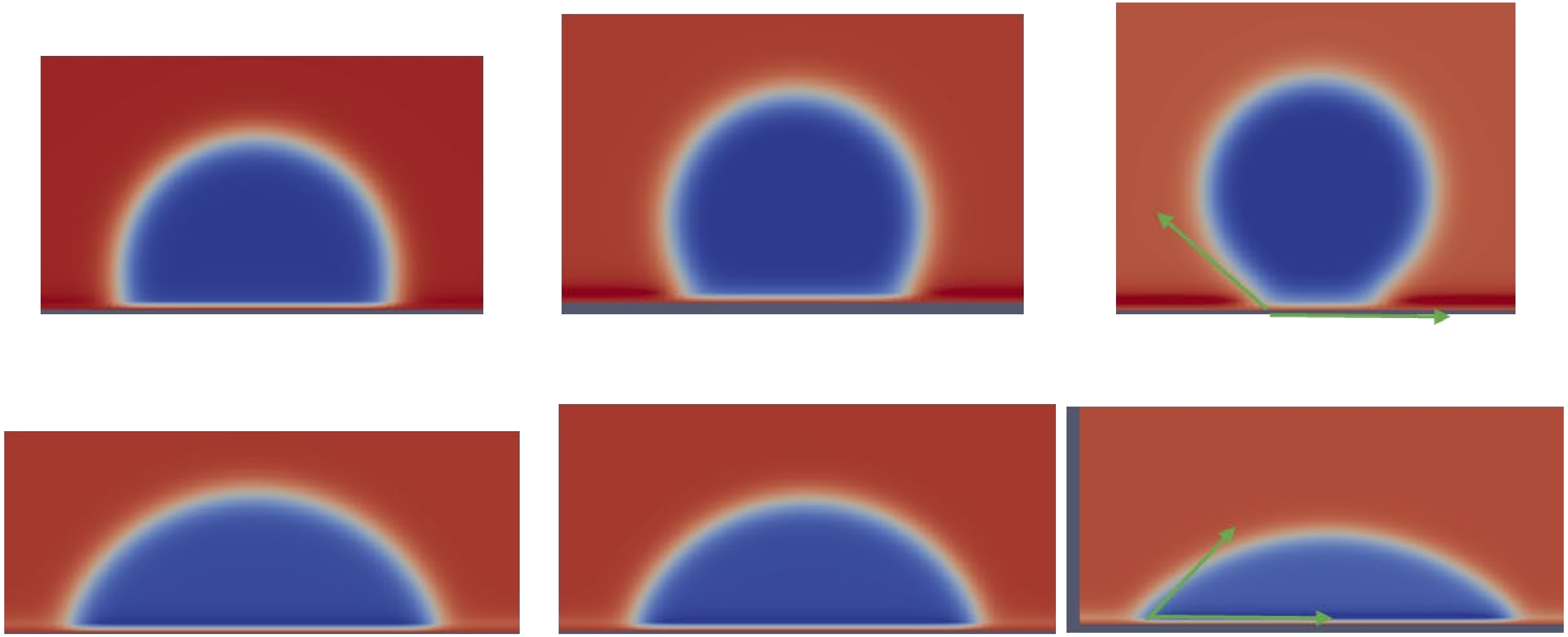


Contact angle simulations

Can relate model parameters to surface tension and contact angle

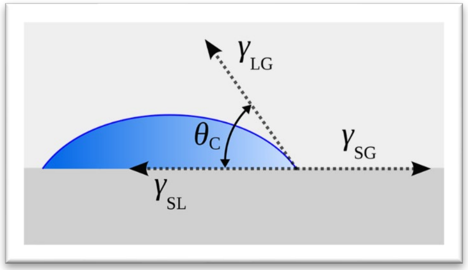
Degrees of incompatibility

Degrees of wetting

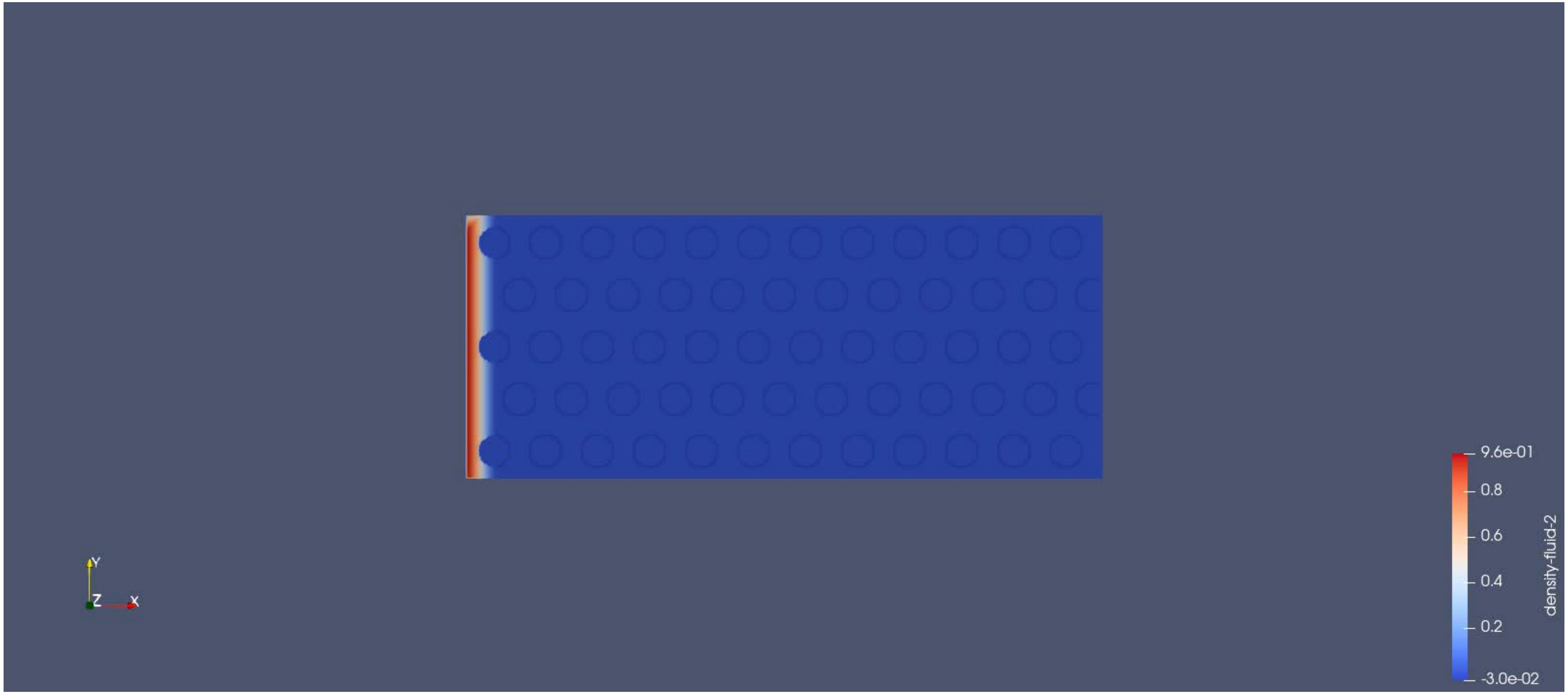


Surface effects on voids and flow front

< 90, “wetting”
> 90, “incompatible”
Guesses?



80 deg



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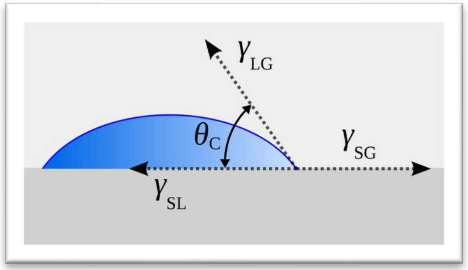
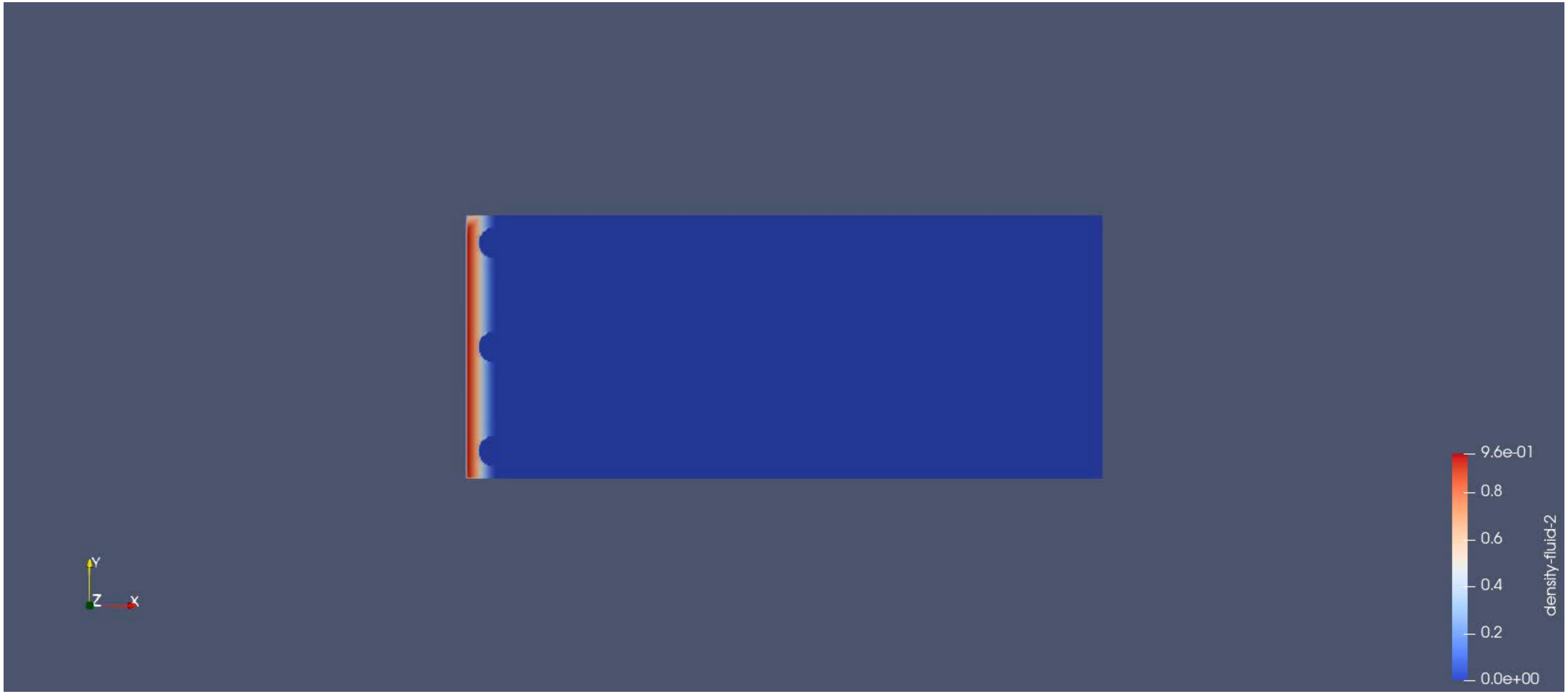
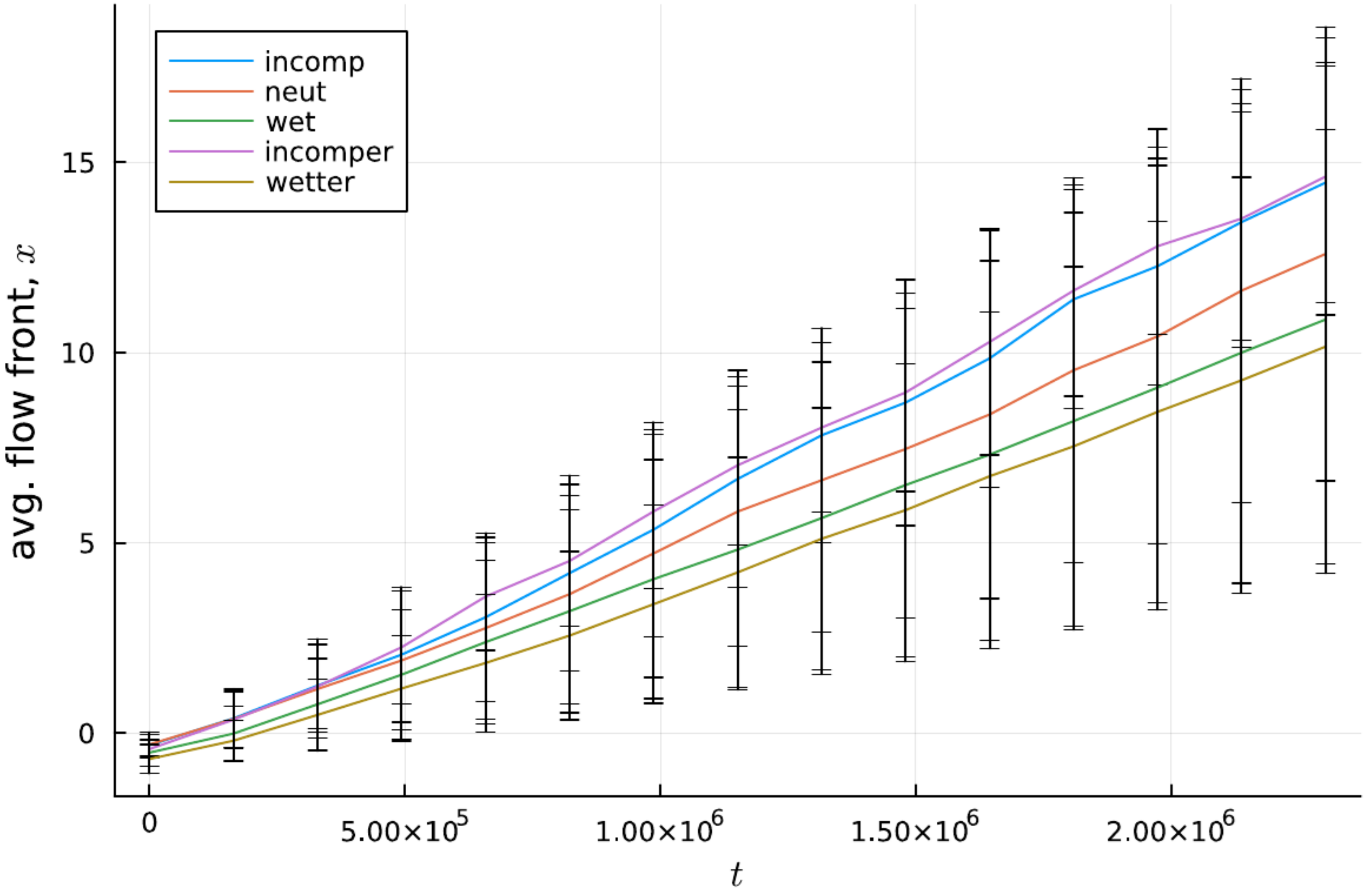


100 deg



"Permeability" depends on wettability

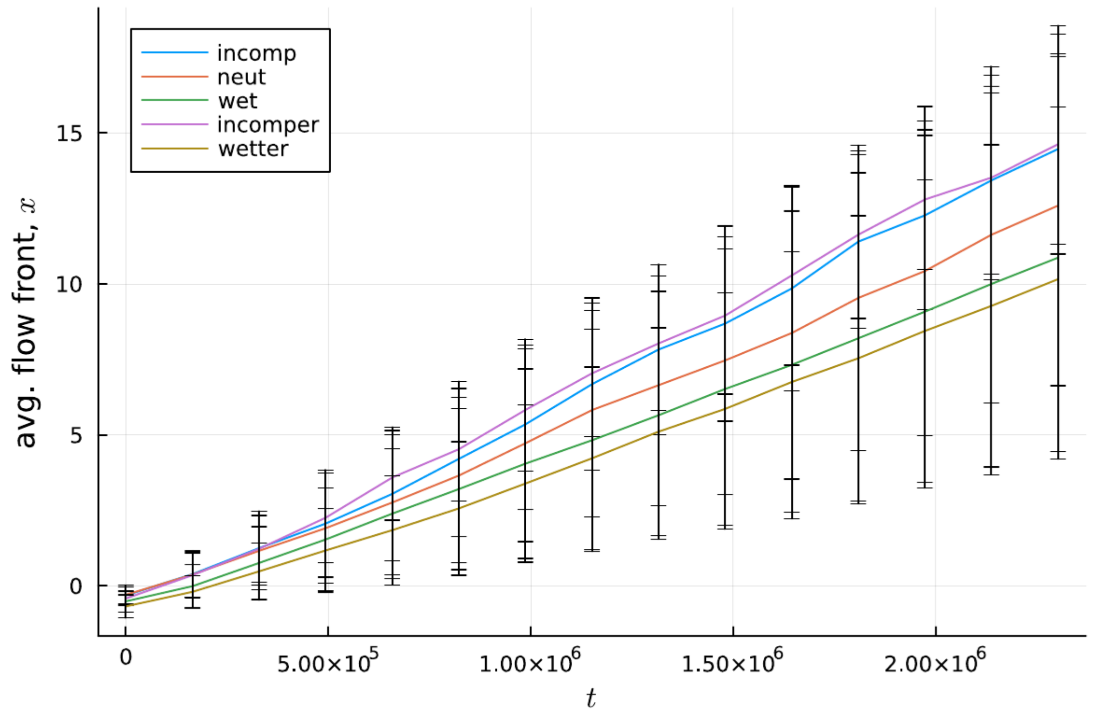


"incomper":	70 deg
"incomp":	80 deg
"neut":	90 deg
"wet":	100 deg
"wetter":	110 deg

“Permeability” depends on wettability

- Simulations reproduce expected scaling
  - Inversely proportional to viscosity
  - Proportional to pressure
  - Somewhat insensitive to surface tension
- Can we use simulations to inform capillary pressure?

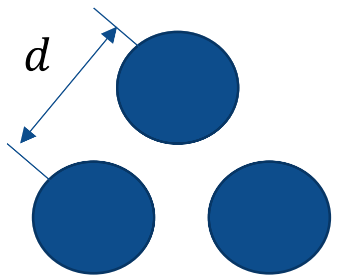
“Capillary pressure”



"Permeability" depends on wettability

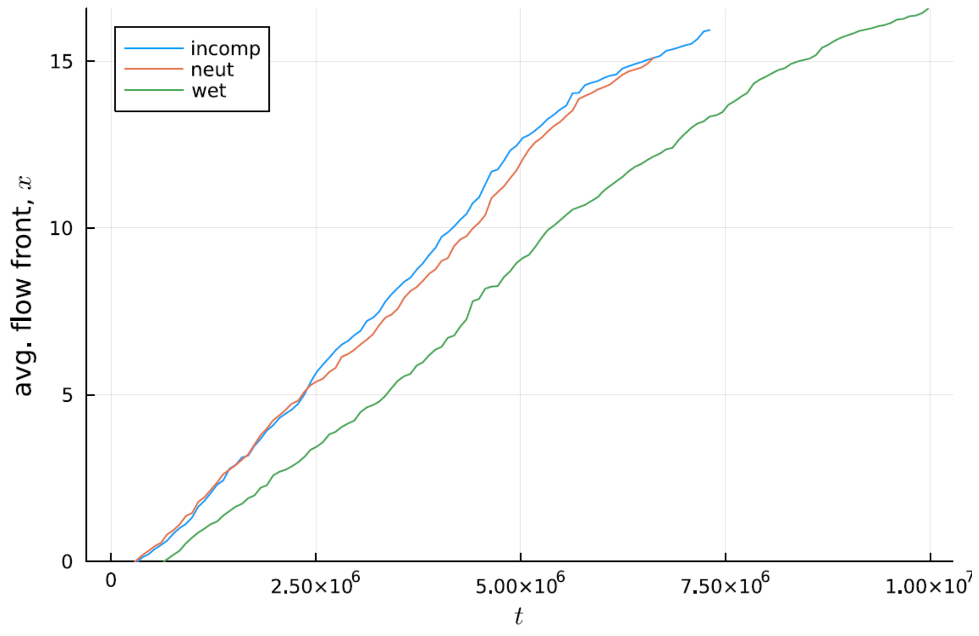
Looser pack => less sensitive to incompatibility

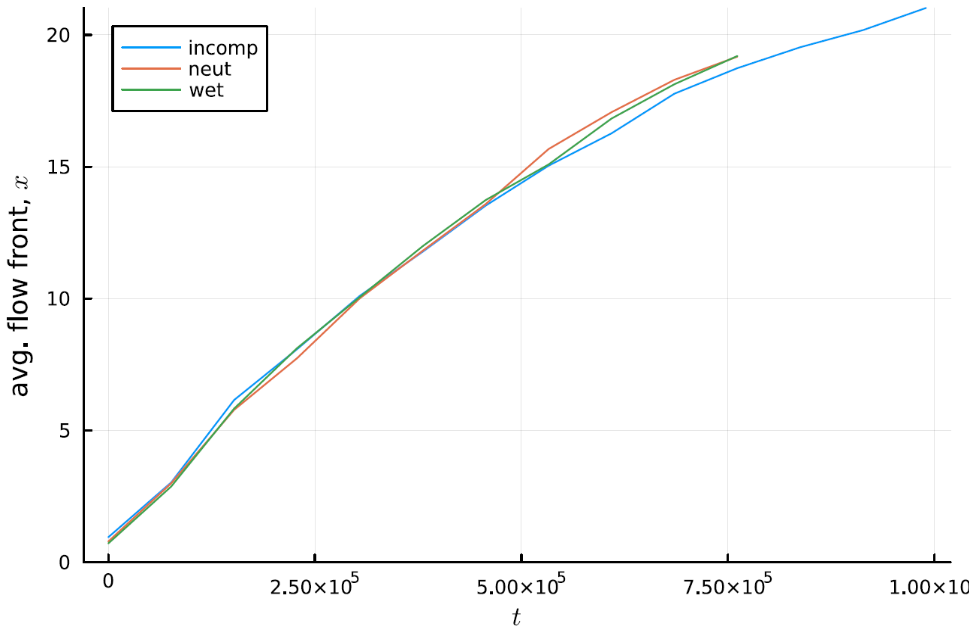
$d = 2.25r$



Looser still => invariance

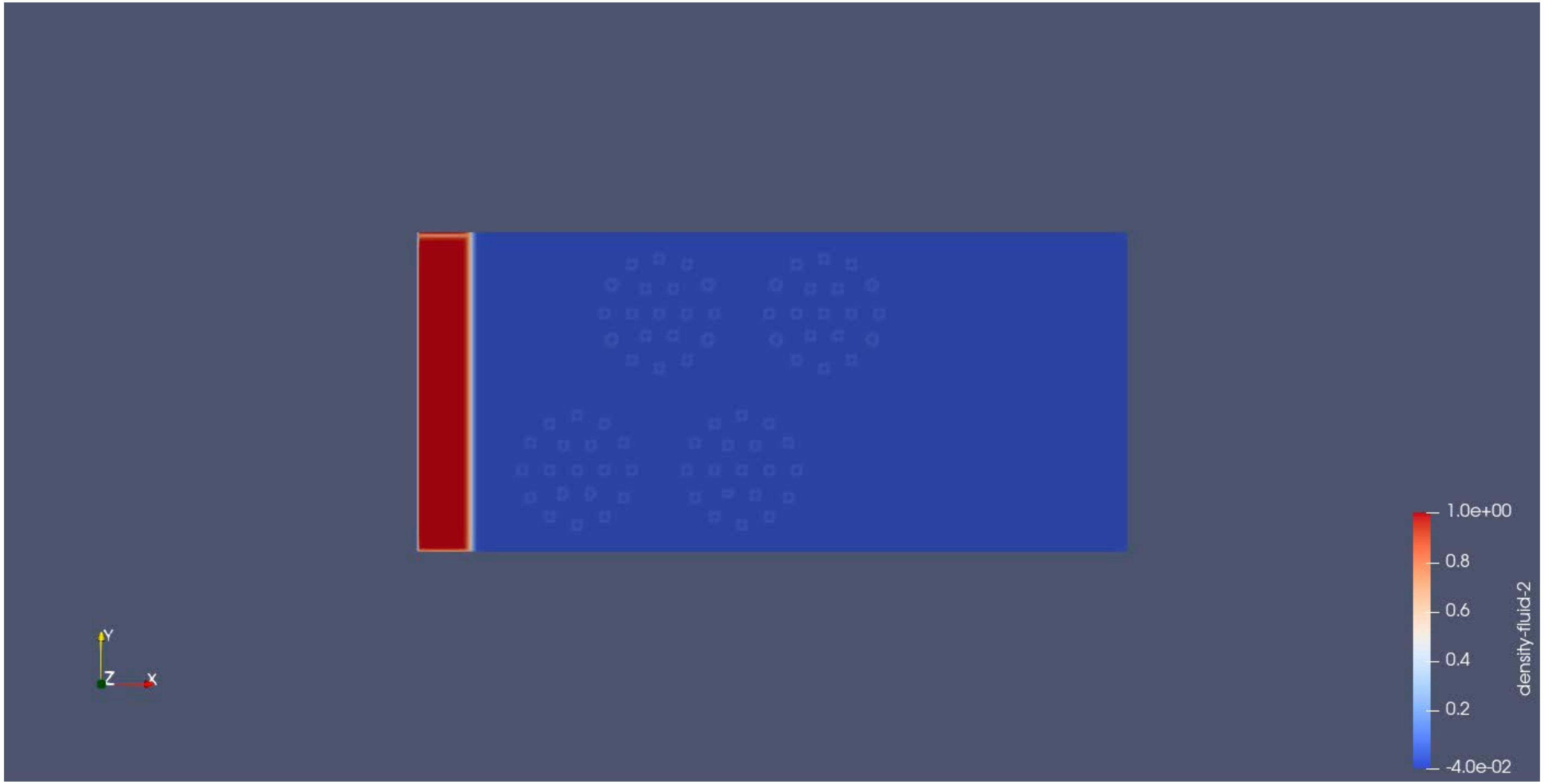
$d = 2.75r$





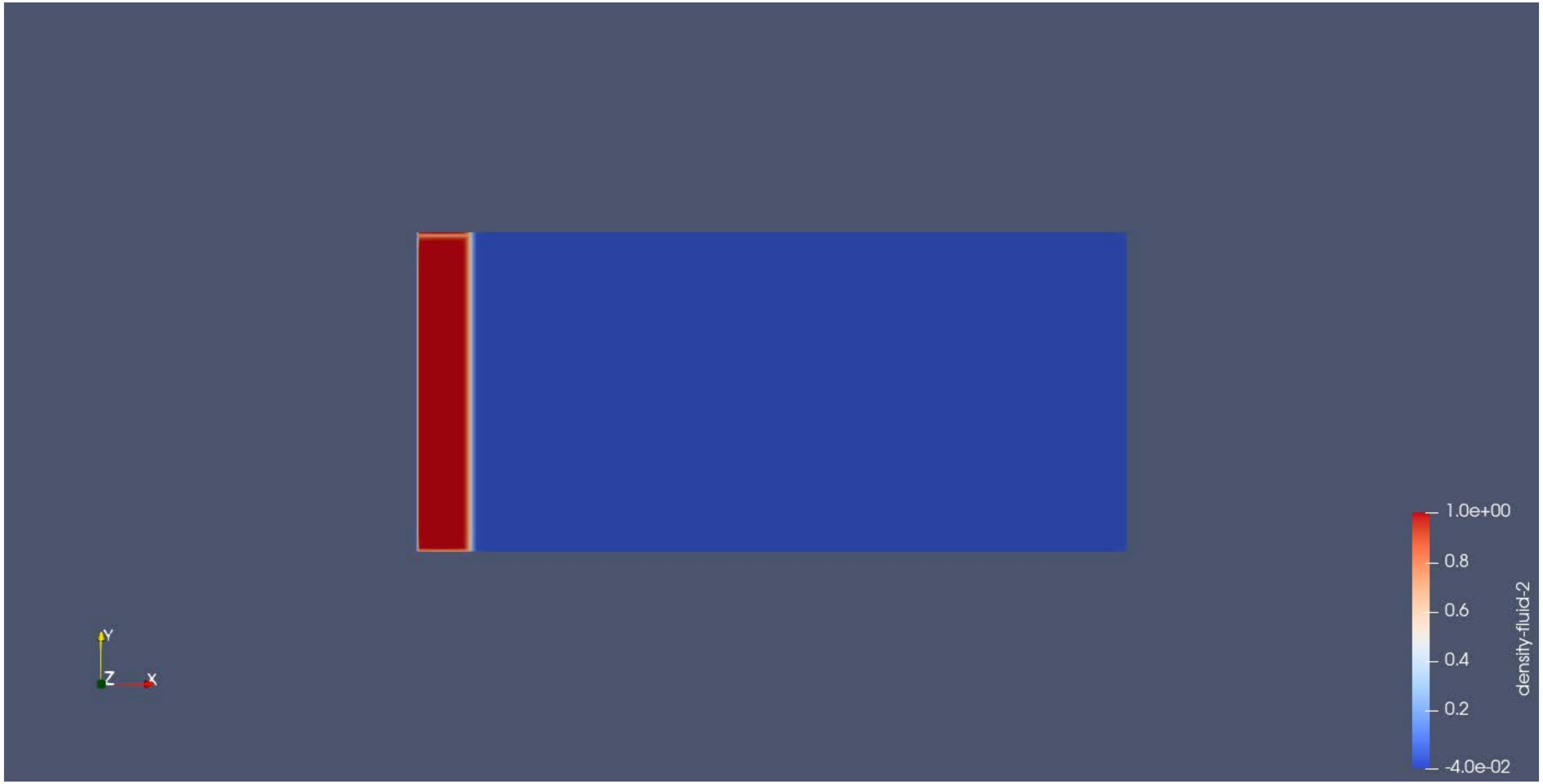
Void formation: where and why

80 deg, incompatible



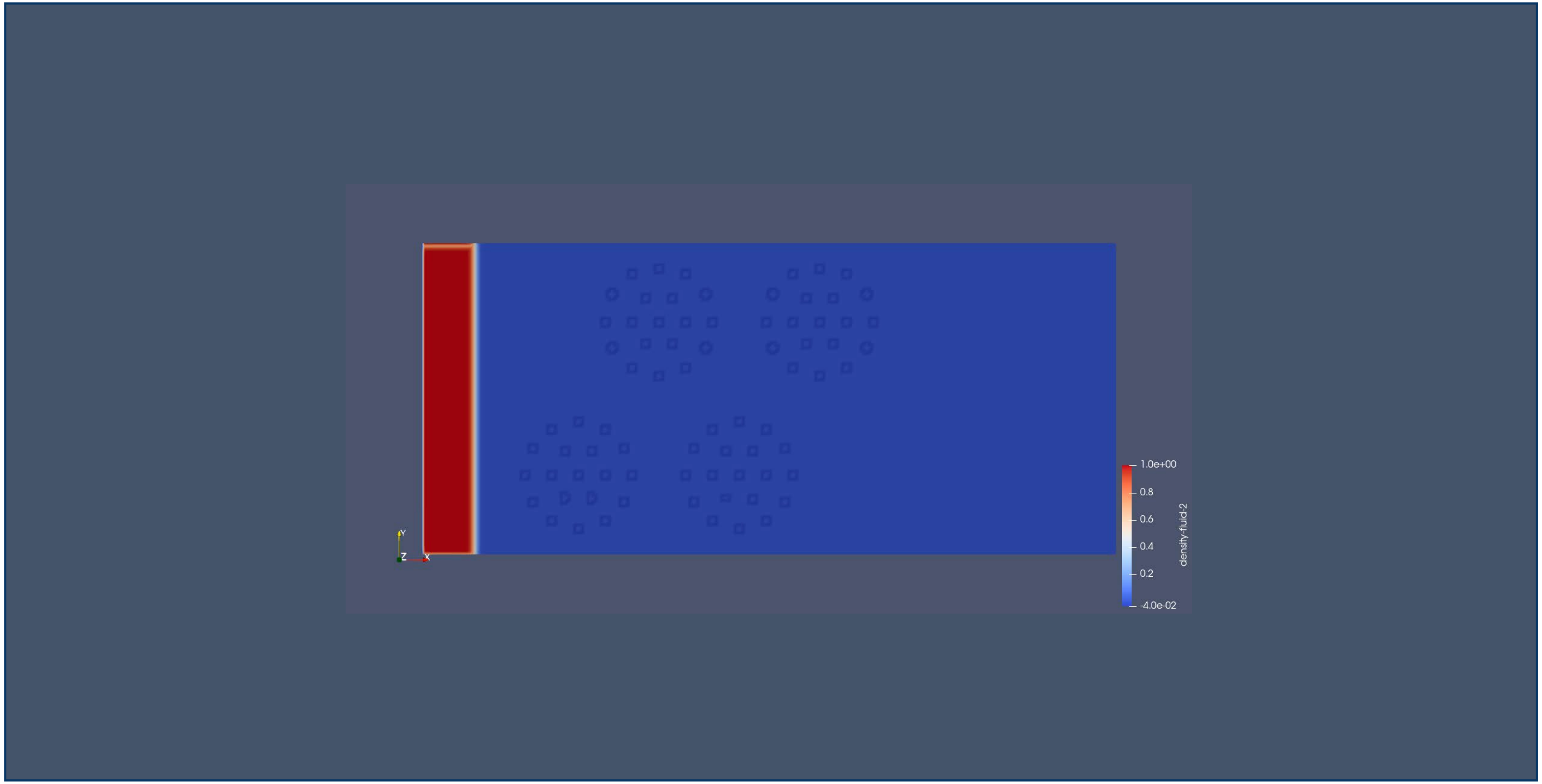
Void formation: where and why

90 deg, neutral



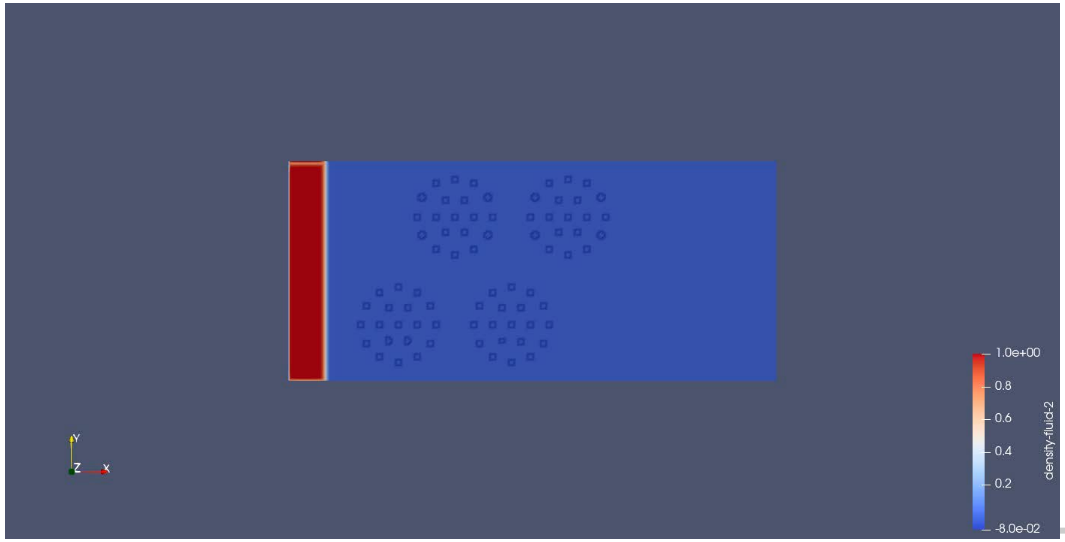
Void formation: where and why

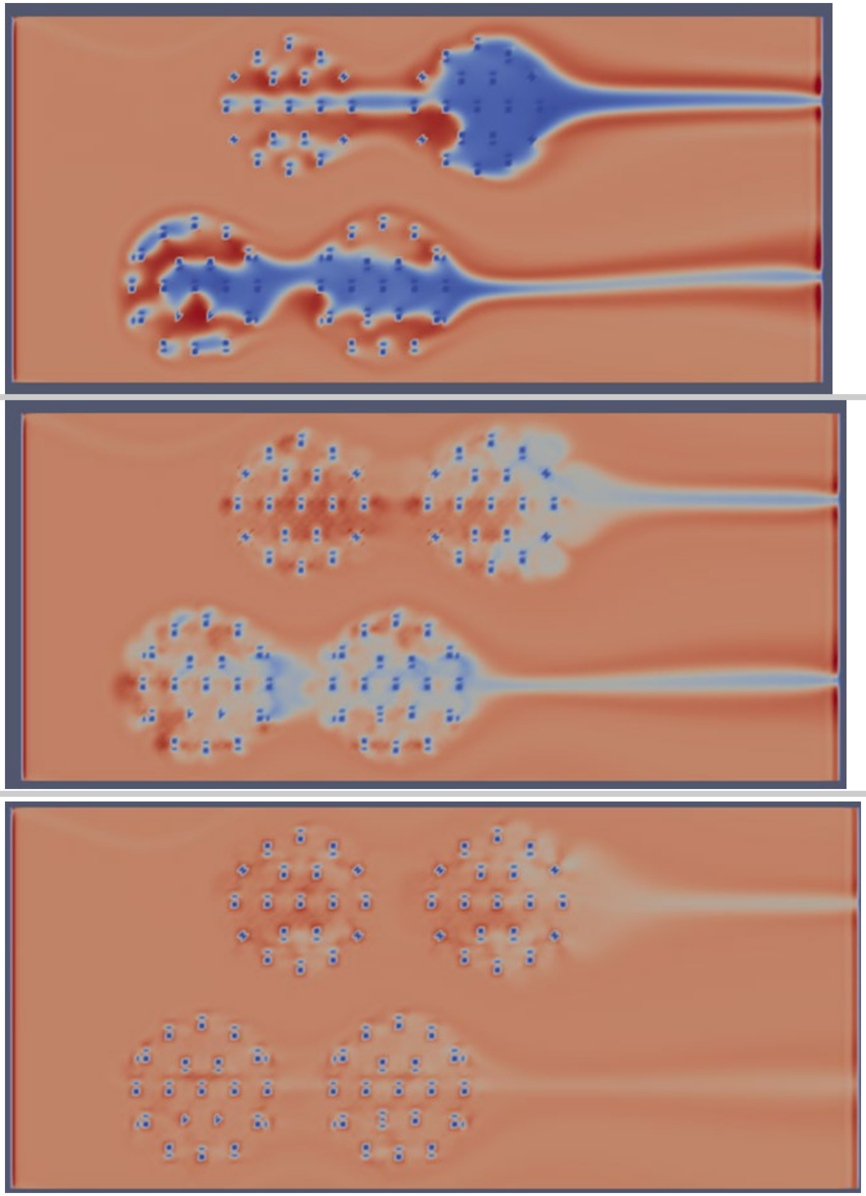
100 deg, wetting



Surface tension and its interplay

“RTM-6”, but what about surface tension?





80 deg

90 deg

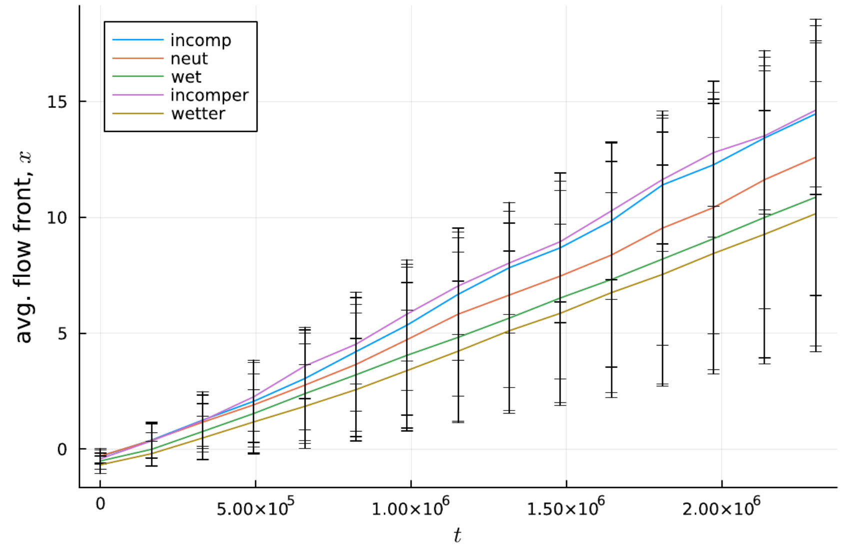
100 deg

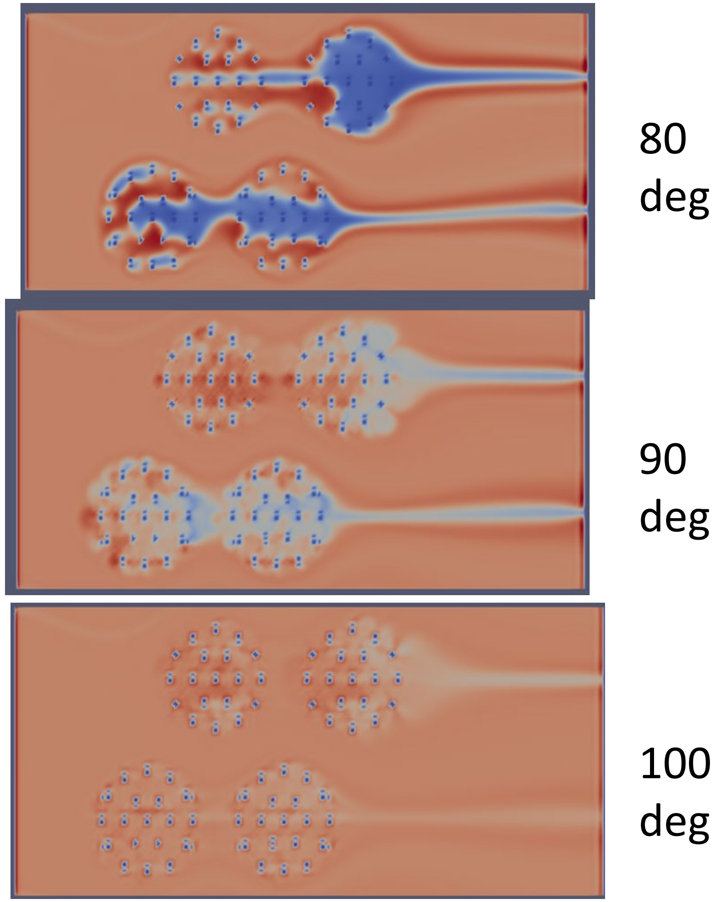
Outlook

- Realistic fluid parameters, fiber volume fraction, boundary conditions
- Unstable for high density ratio + high viscosity ratio + high volume fraction
  - Mesh refinement
  - “Free surface” idealization
- Extend to 1) non-Newtonian fluids (e.g. shear thinning) and
  2) electrowetting
  - Carbon fibers are conductive; apply voltage difference?
  - Electrowetting is underexplored for modifying surface interactions during processing
  - May require micromechanical models to determine electrical response of resin
    - Polarization and electrostatic Coulomb forces
    - Surface tension

Acknowledgements / questions

- Thanks, Air Force Research Laboratory





Matthew Grasinger
email: matthew.grasinger.1@afrl.af.mil

Feel free to reach out about internships, fellowships, collaborations, etc.
Students: HPC Internship program; NDSEG and SMART fellowships
Postdocs: NRC & other opportunities