CCSI²

Carbon Capture Simulation for Industry Impact

DOCCSS Support for LLNL Advanced Reactor Manufacturing

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Outline

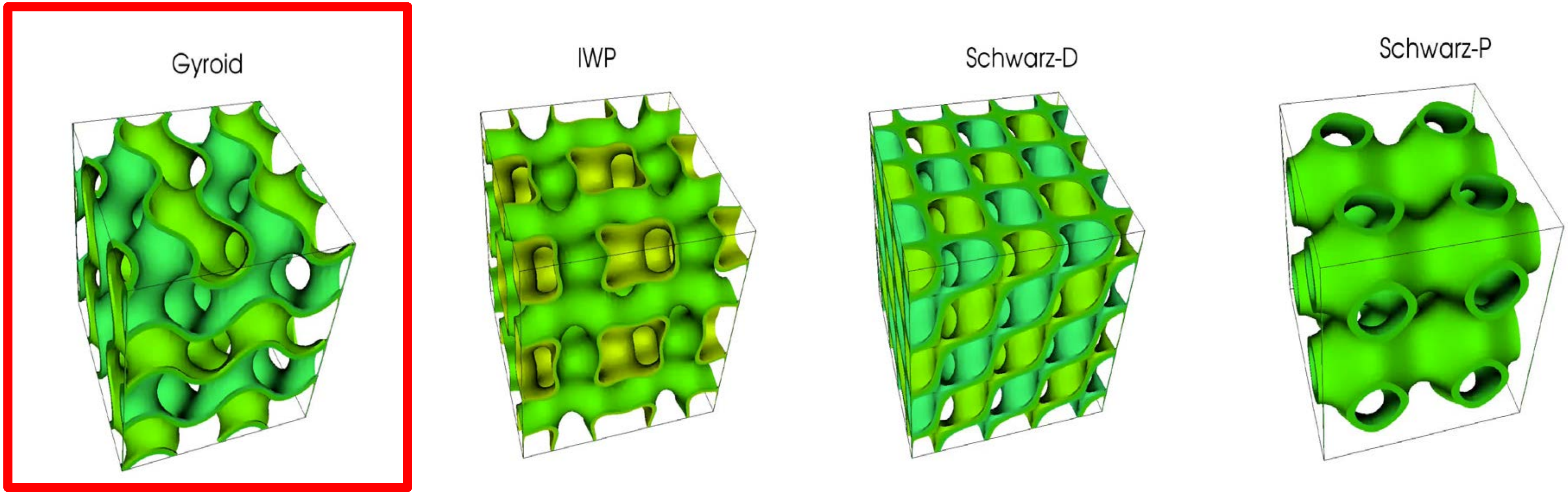
- Introduction of Gyroid Structure

- CFD models for countercurrent gas/solvent flow in Gyroid
  - Model validation using random rings packing
    - Model description
    - Mass transfer area (comp. with exp.)
    - Mass transfer coefficient (comp. with exp.)
  - Preliminary results for mass transfer area of Gyroid

- Conclusions

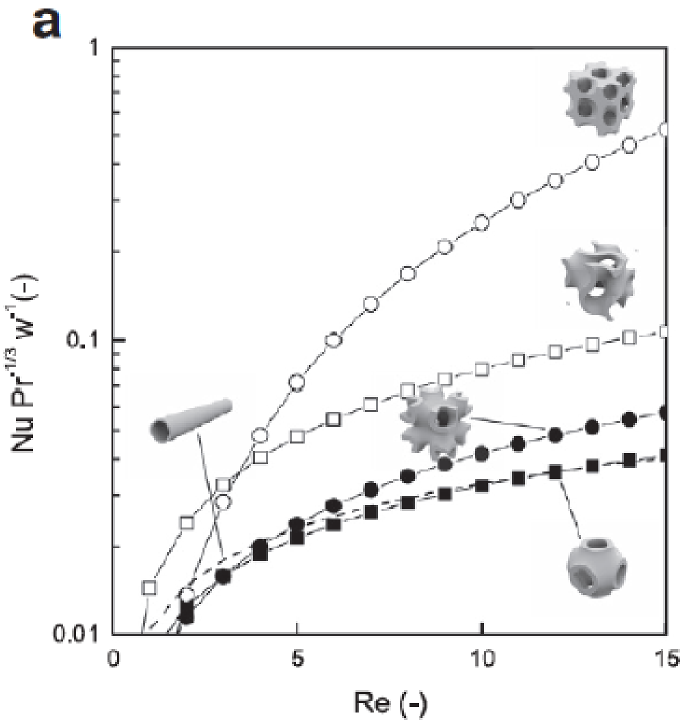
Introduction: Triply Periodic Minimal Surfaces (TPMS Structure)

- **Minimal surface**
  - Locally area-minimizing
  - Zero mean curvature

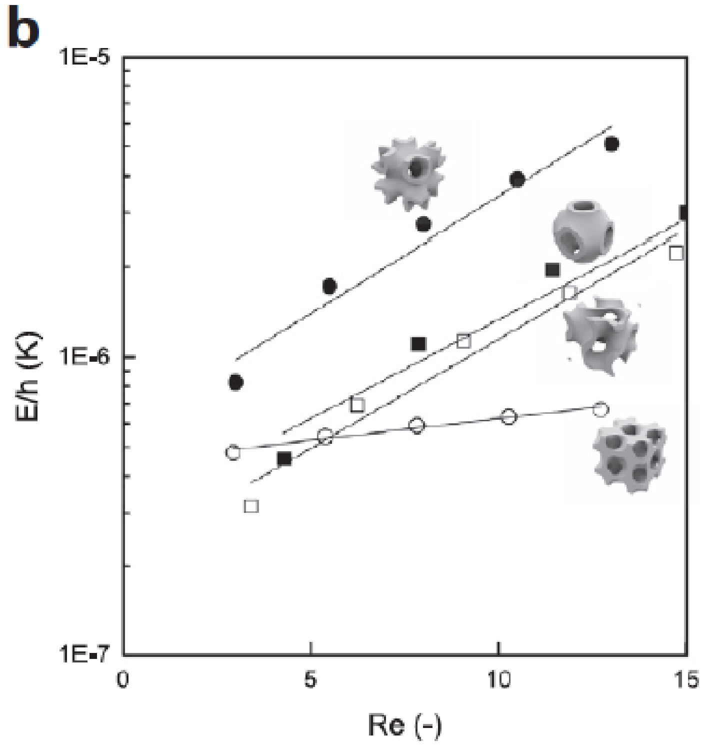


Introduction: Motivation for TPMS Geometry

- Triply periodic minimal surface (TPMS) structures
- Improved heat transfer (~10X)
- Less pressure drop than competing geometries (~1/10th)



Heat transfer per unit surface area



Friction loss per unit heat transferred at ΔT=1∘C

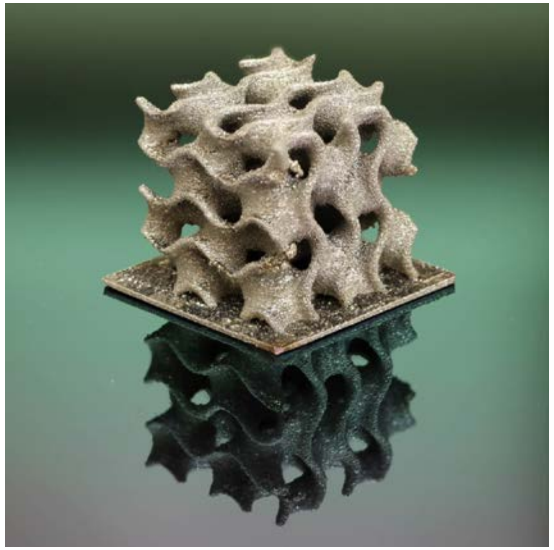
From: T. Femmer et al. *Chemical Engineering Journal* 273 (2015) 438–445.

Introduction: Gyroid TPMS Structure

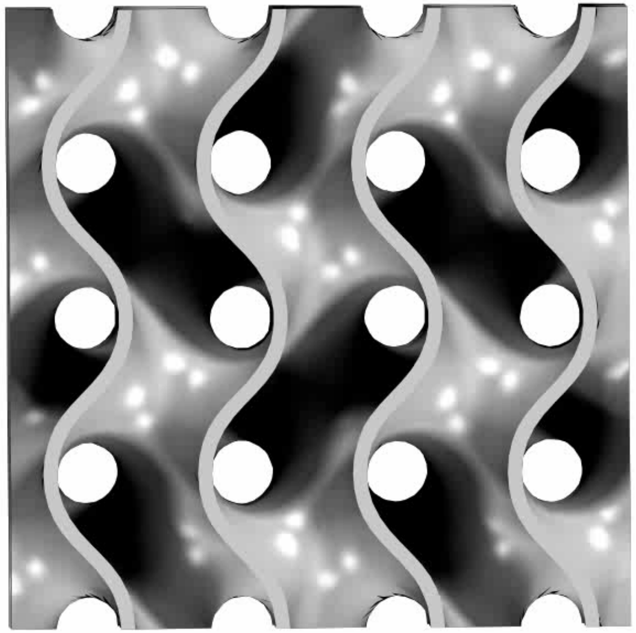
- Geometry
  - Triply periodic minimal surface (TPMS)
  - Can be approximated by a short equation

$$\sin x \cos y + \sin y \cos z + \sin z \cos x = 0$$

- 3D printed Gyroid @ LLNL



- For carbon capture
  - Mass transfer coefficients?
  - Mass transfer areas?
  - Highly viscous solvent?



- Objective: CFD modeling for the gas/solvent flow in Gyroid

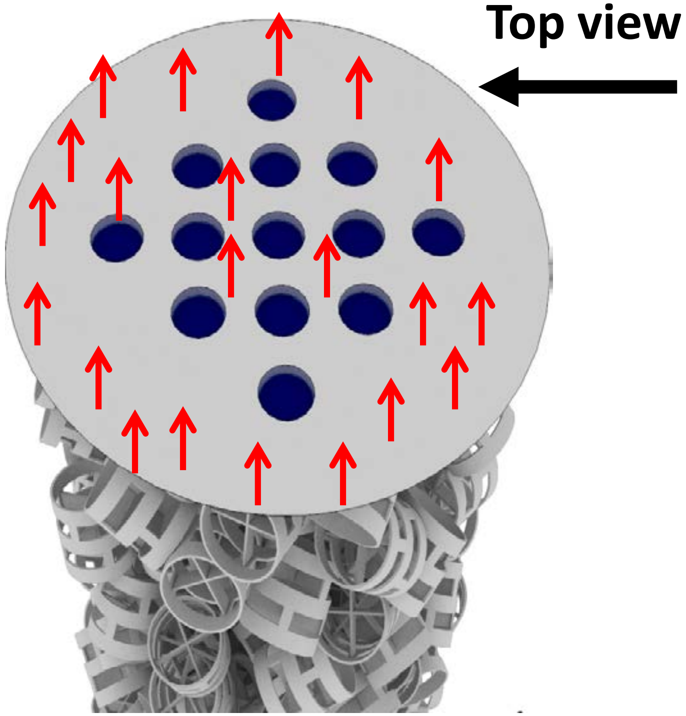
Model Validation: Model Description

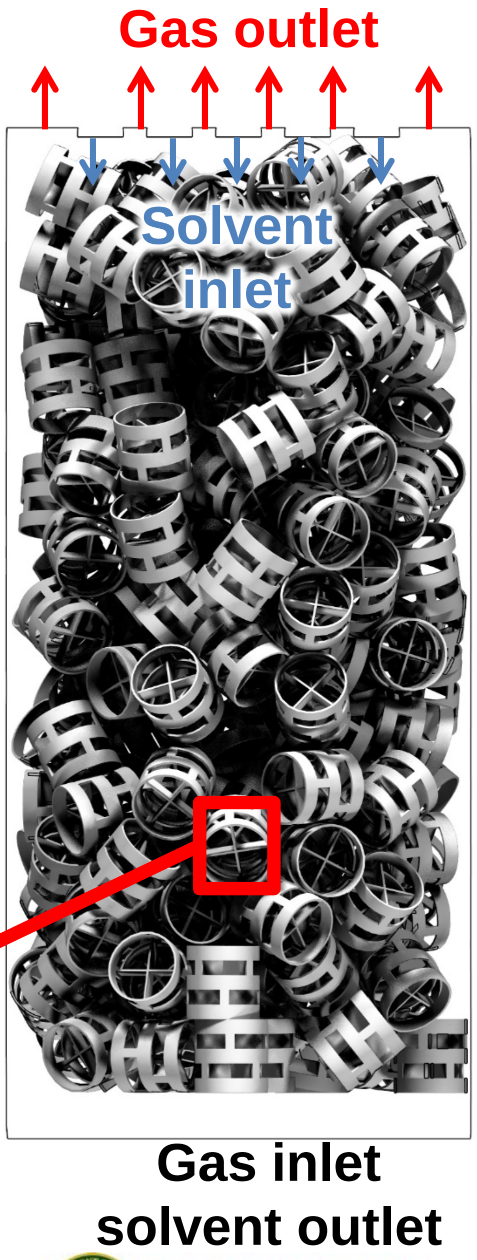
Modeling Method

Volume Of Fluids (VOF) for countercurrent multiphase flow

Packed column

- Column diameter: 100 mm
- Column height: 200 mm
- Number of Pall rings: 160





Boundary conditions

- 13 solvent dripping inlets (10 mm diameter)
- No slip ring surface
- Prescribed gas flow rate at outlet

Design of pall ring

- Diameter: 16 mm
- Height: 16 mm
- Thickness: 0.5 mm
- Specific Area: 282 m^2/m^3

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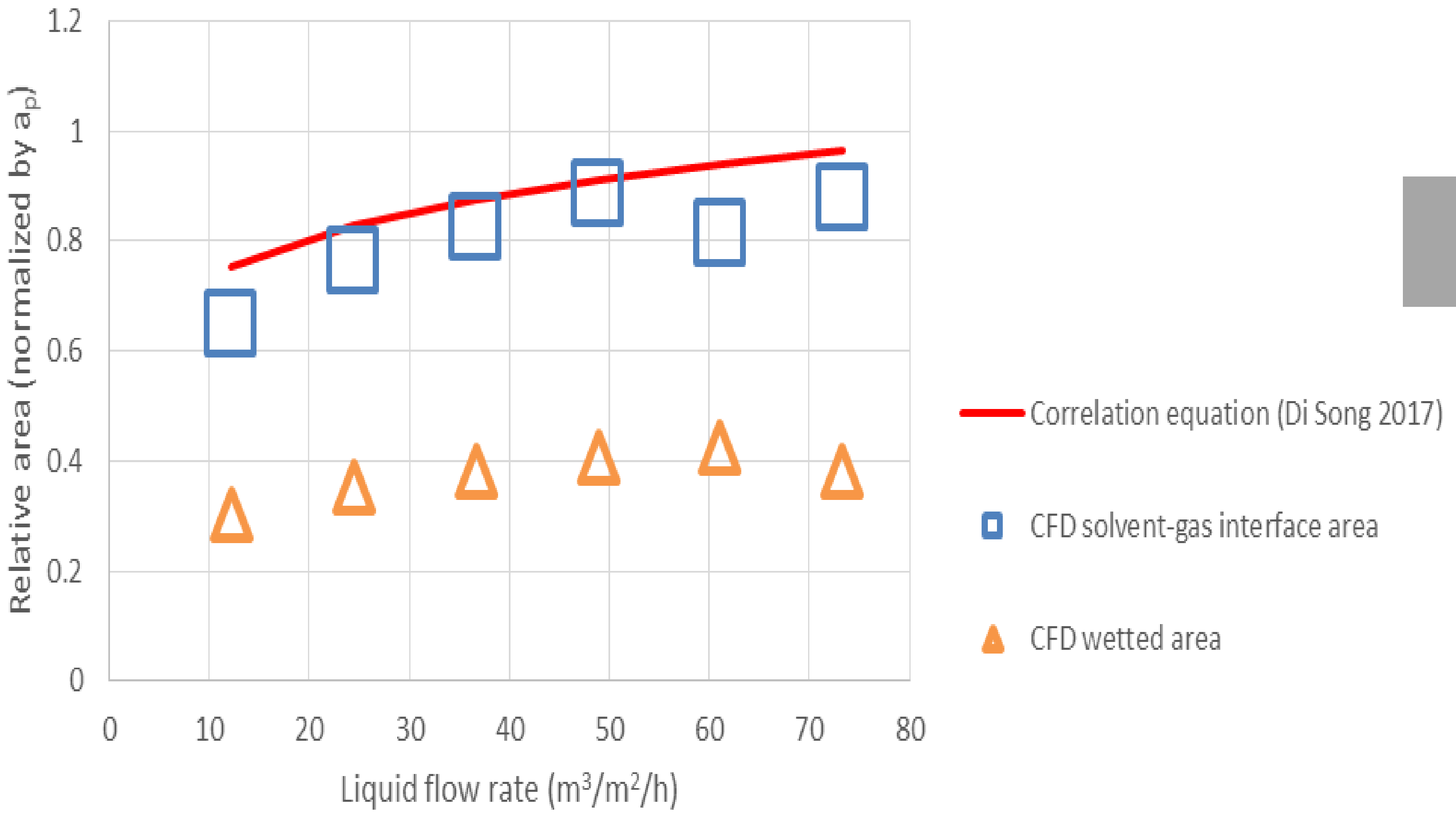
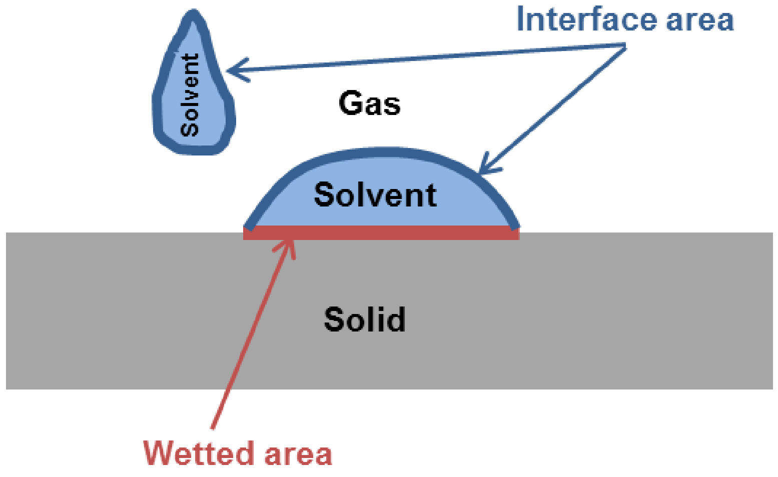
Model Validation: Mass transfer area





Distinguish three areas

- Interface area (CFD)
- Wetted area (CFD)
- Effective mass transfer area (Exp.)

Model Validation: Mass Transfer Coefficient

- **Mass transfer coefficient** k_L

Wetted Wall Exp. (flat): $k_L = 1.15\, u_L^{1/3} \nu_L^{-1/6} g^{1/6} a_P^{-1/6} D_L^{0.5}$

Column Exp.(vigorous): $k_L = 0.12\, u_L^{0.565} \nu_L^{-0.4} g^{1/6} a_P^{-0.065} D_L^{0.5}$

Song et.al. (*Ind. Eng. Chem. Res. 2018, 57, 718−729*)

- **Proposed Mechanism: film flow with rolling waves**

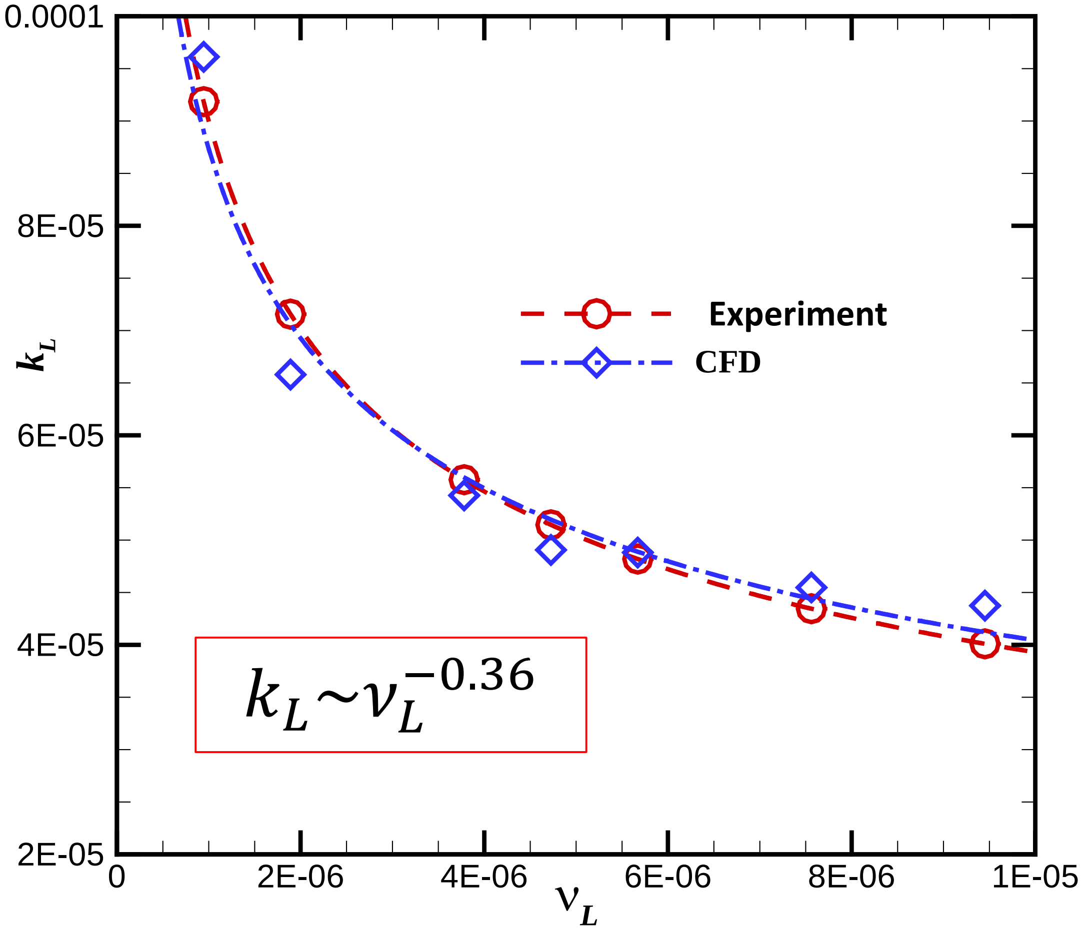
Theory (Hydrodynamics + eddy diffusion)

Theory + CFD →

$$k_{Le} = 1.15 C^{1/2} \mathbf{u}_L^{0.625} \mathbf{v}_L^{-0.36} g^{0.19} \left(\frac{a^{0.625}}{L^{0.5}}\right)\left(\frac{\sigma}{\rho}\right)^{-0.07} D_L^{1/2}$$

Rolling Waves (small ν_L) → **Eddy diffusion** → **Enhanced mass transfer**

Gyroid?



Variation of k_L with ν_L

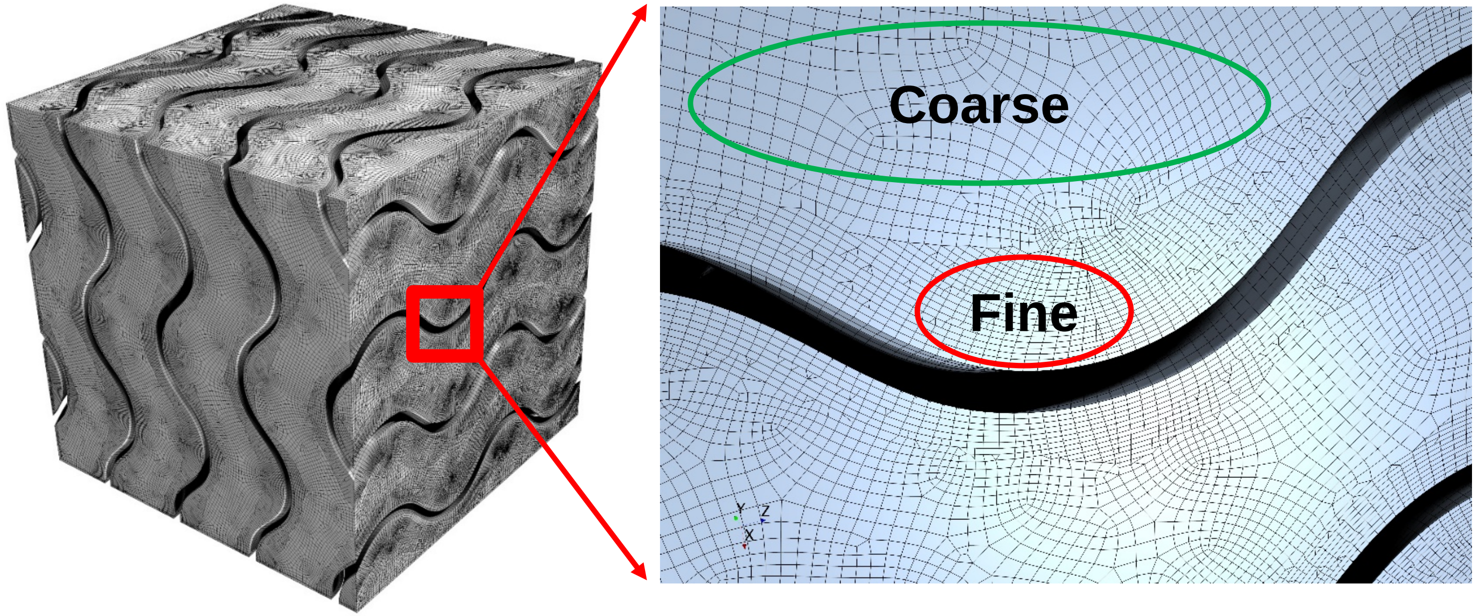
Model Setup: Geometry & Meshing

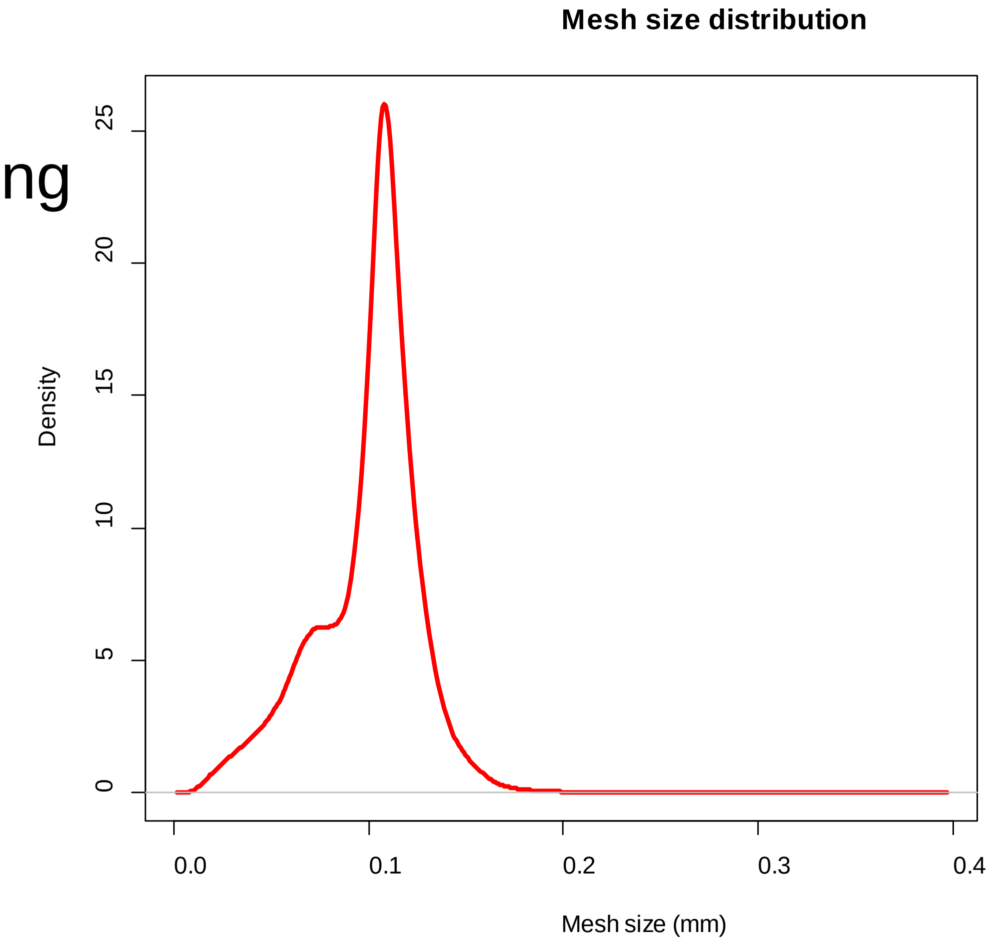
Original gyroid geometry

- 2cm X 2cm X 2cm
- Periodic in 3 directions

Meshing

- Advancing layer meshing
- 5.8 million meshes





Distribution of Mesh size

Model Setup: Gas/solvent Countercurrent Flow

Boundary conditions

− Periodic for flow

Initial conditions

− Solid initially wrapped with a thin layer of film (0.5-1.5mm)

− Initial thickness affects the final liquid flow rate

Body force

− Solvent driven by the gravity

− Gas driven by body force

Computational cost

− 96 cores on PNNL PIC HPC

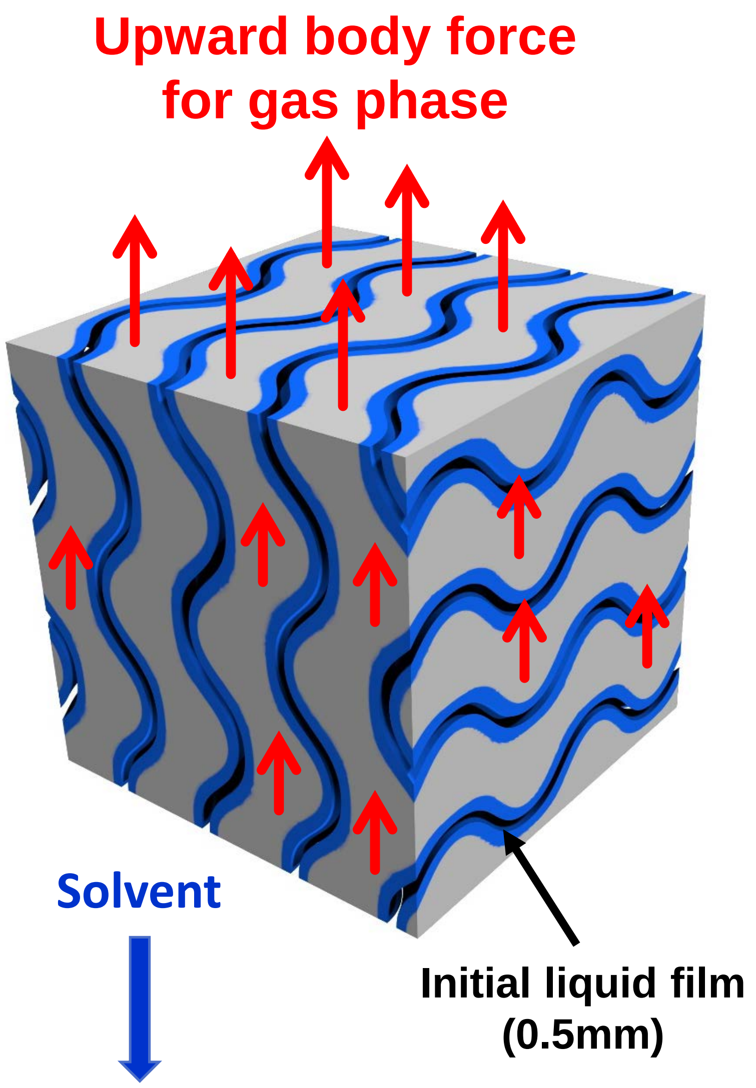
− 7-8 CPU hours for every 1s solution

Solvent Properties (30% MEA)

Physical Properties	
Density ρ (kg/m^3)	1000
Viscosity μ (cP)	2.5, 5, 10, 25
$D_{CO_2}[l]$ (m^2/s)	1.0×10^{-9}
Surface Tension (N/m)	0.065
Contact angle (°)	40

Gas Properties (Air)

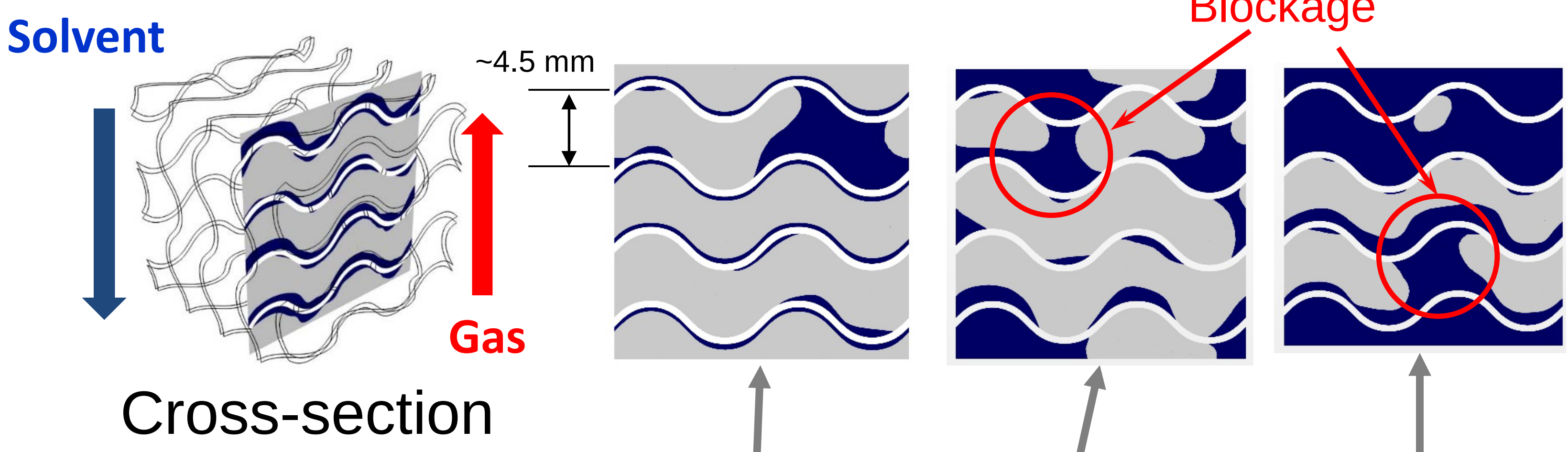
Physical Properties	
Density ρ (kg/m^3)	1.184
Viscosity μ (cP)	0.0186
$D_{CO_2}[g]$ (m^2/s)	1.0×10^{-5}

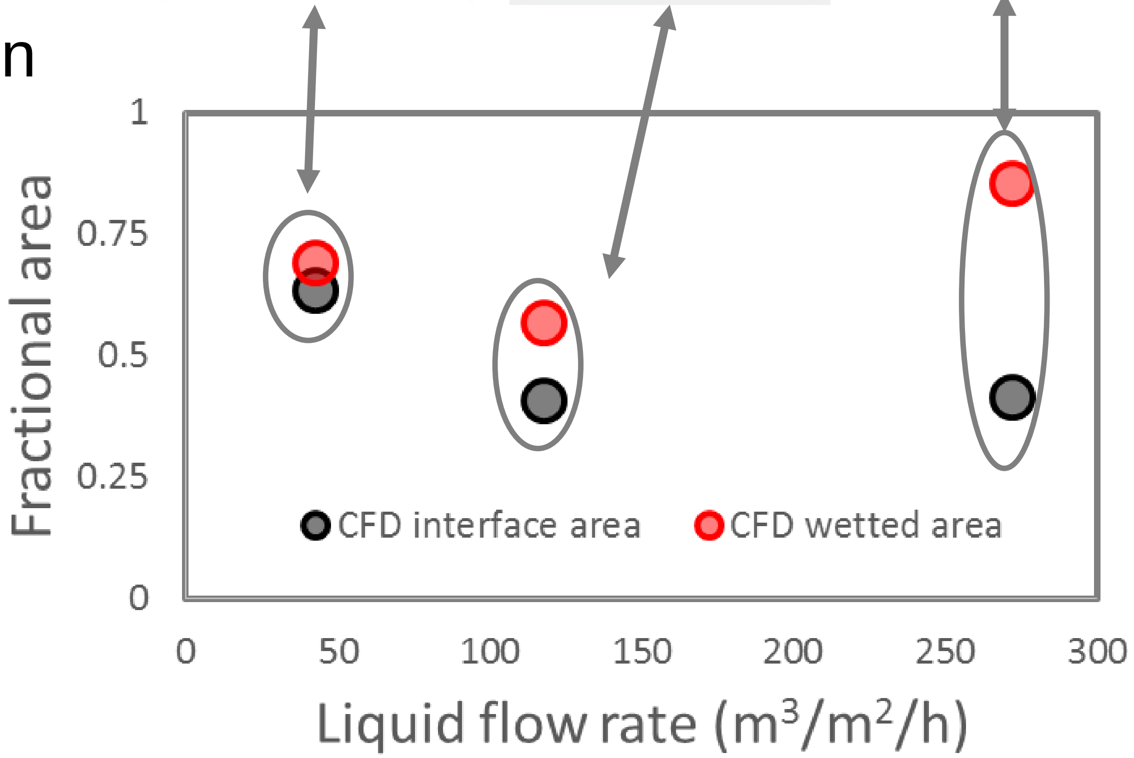


Results and Discussion

Original LLNL gyroid geometry

- 2cm X 2cm X 2cm
- Channel size: ~4.5 mm
- Surface/volume: 614 1/m
- Low viscosity solvent: 2.5 cp





Findings:

- Rivulet flow at low to medium flow rate
- Non-monotonic behavior
- Solvent blocks the channel (reduces interface area)
- May not be an ideal geometry for countercurrent liquid/gas flow

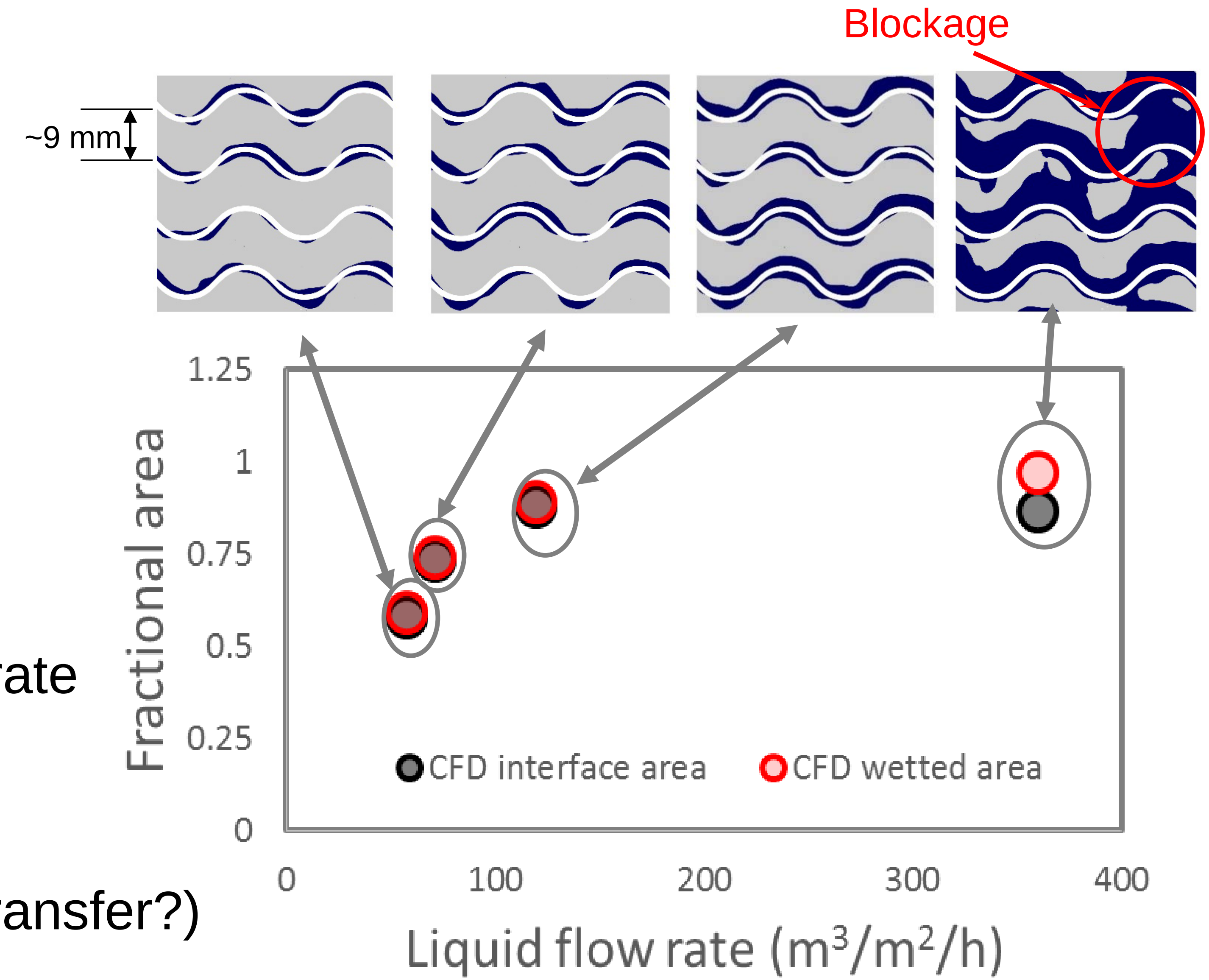
Results and Discussion

<u>Modified LLNL gyroid geometry</u>

- 4cm X 4cm X 4cm
- Channel size: ~9 mm
- Surface volume ratio: 307 1/m
- Low viscosity solvent: 2.5 cp

<u>Findings:</u>

- Rivulet flow at low flow rate
- Interface area increases with flow rate
- Blockage only at high flow rate
- Geometry induced film fluctuation (rolling waves ➡ enhanced mass transfer?)



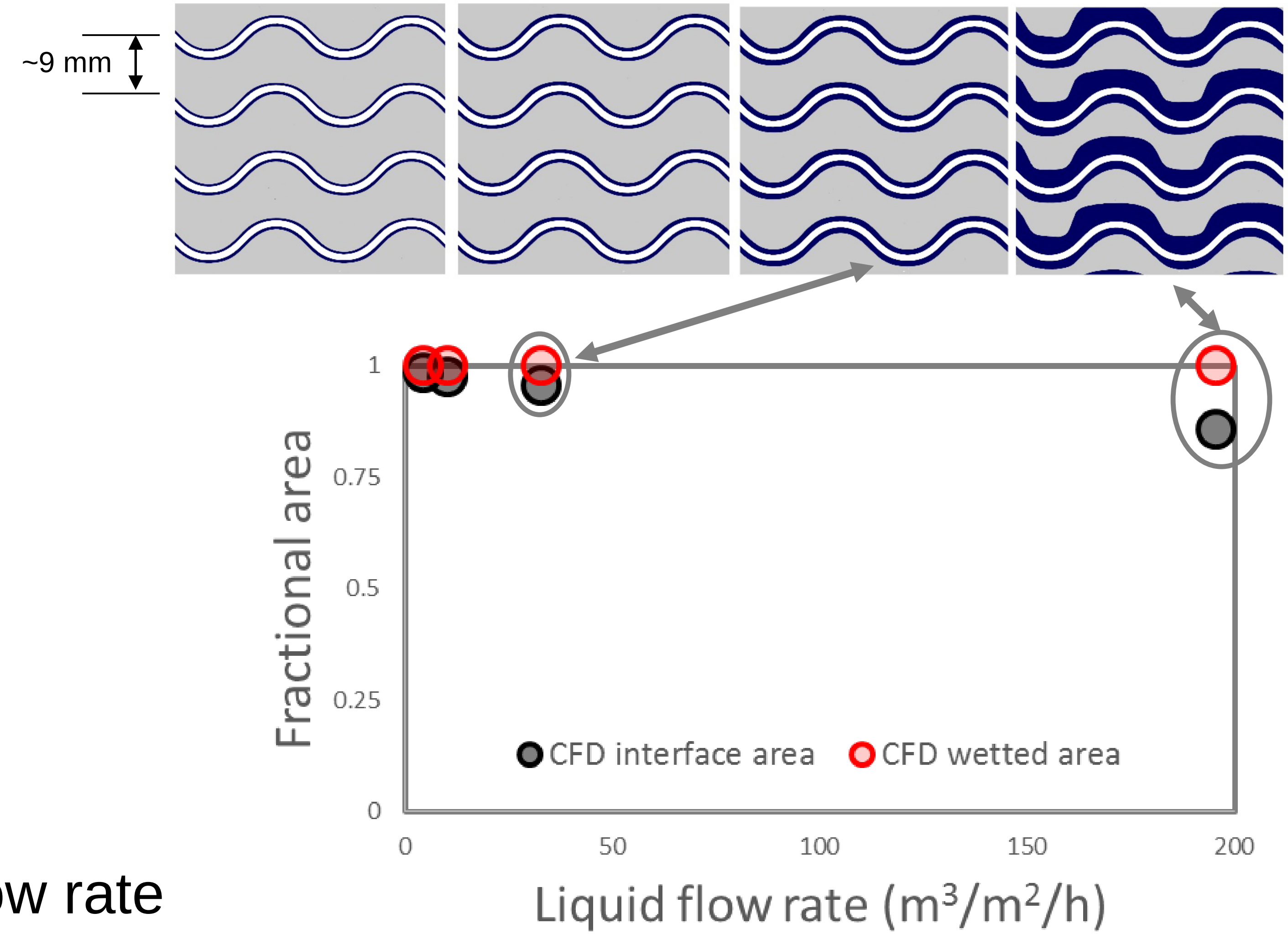
Results and discussion

Modified gyroid geometry

- 4cm X 4cm X 4cm
- Channel size: ~9 mm
- Surface volume ratio: 307 1/m
- Highly viscous solvent: 25 cp

Findings:

- Film flow only (No rivulet flow)
  good for mass transfer
- No solvent blockage observed
- Geometry induced film thickness fluctuation (waves) only at high flow rate



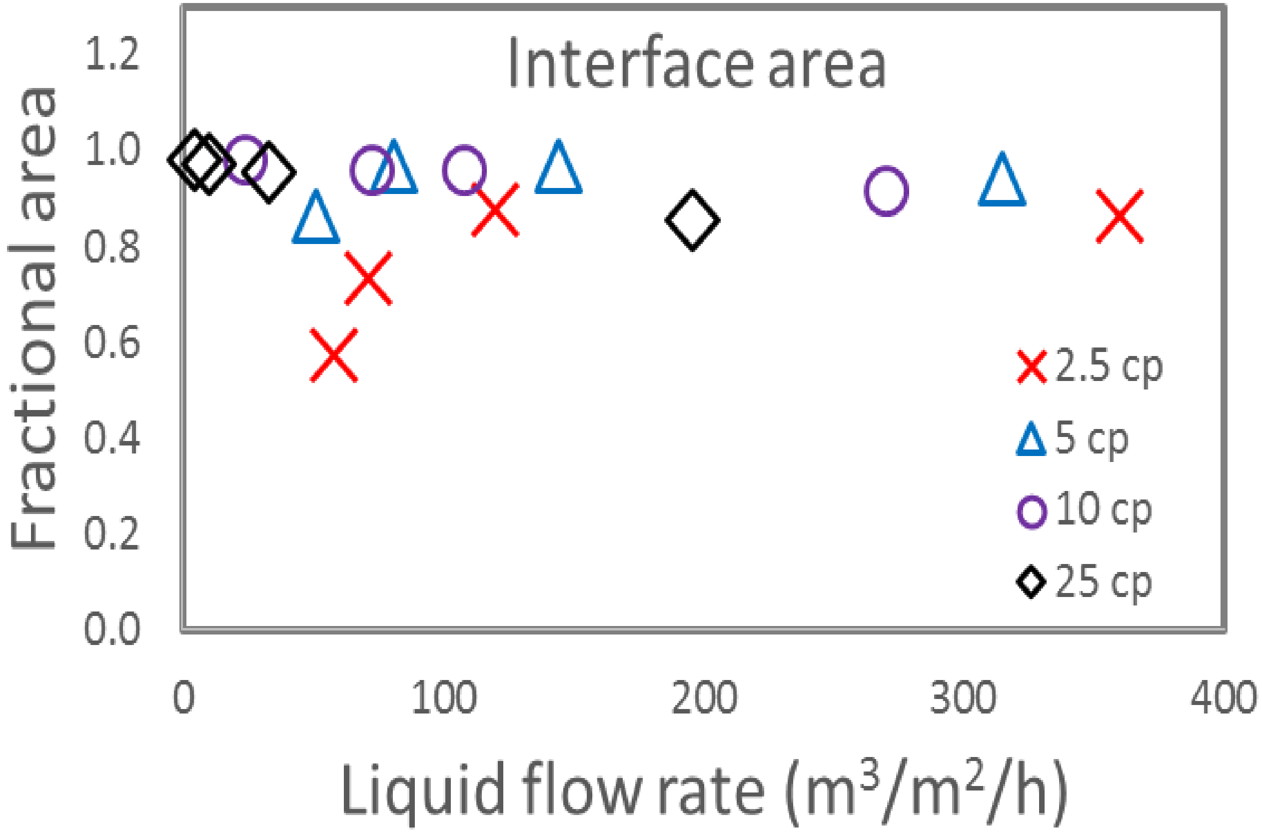
Results and Discussion

Modified gyroid geometry

- 4cm X 4cm X 4cm
- Channel size: ~9 mm
- Surface volume ratio: 307 1/m
- Viscosity: 2.5, 5, 10, 25 cp

Findings:

- For viscosity <= 5cp, interface area increases with flow rate (rivulet flow regime)
- For viscosity >=10cp, constant interface area (film flow regime)



Interface area varying with Solvent flow rate

Conclusions

- Original LLNL gyroid size might be too small to allow an efficient countercurrent gas/solvent flow due to the solvent blockage.

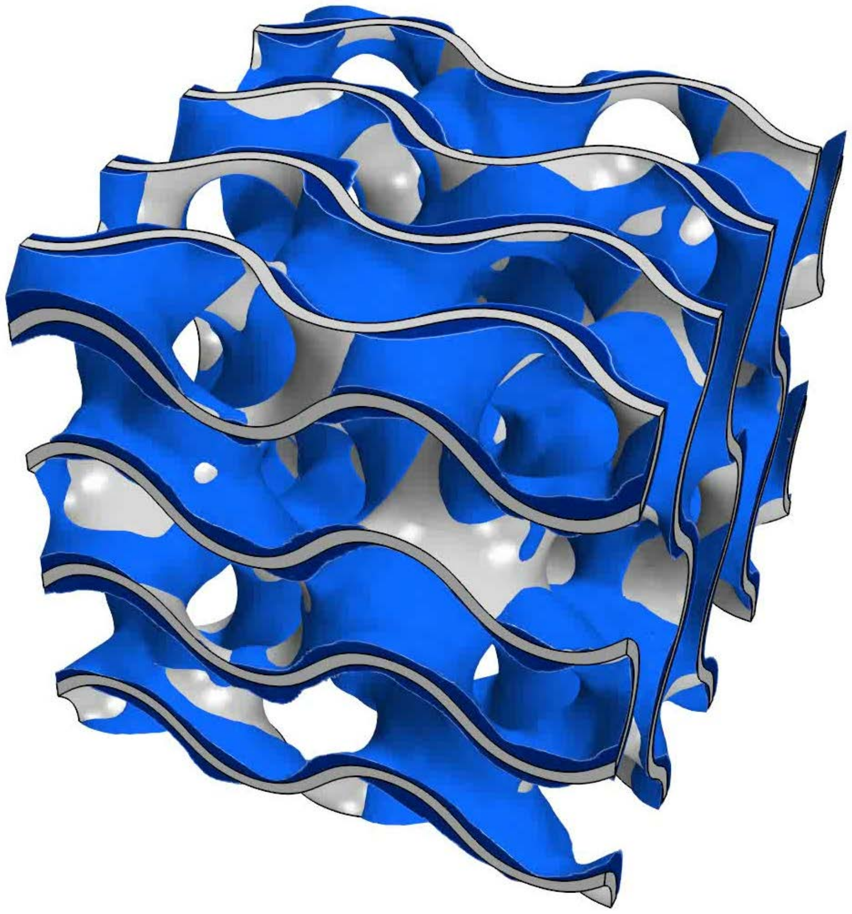
- Solvent viscosity affects the interface area at different flow rates
− For viscosity ≤ 5cp ➡ rivulet flow

  Interface area increases with flow rate

− For viscosity ≥ 10cp ➡ film flow

  Constant interface area

- Geometry induced film thickness fluctuation (waves)
- Also dependent on surface tension & contact angle



Rivulet Flow & Fluctuation

Acknowledgments

Carbon Capture Simulation for Industry Impact (CCSI^2)

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