FEW0225: High-efficiency, integrated reactors for sorbents, solvents, and membranes using additive manufacturing

NETL Carbon Capture Technology Program Review

August 13, 2018

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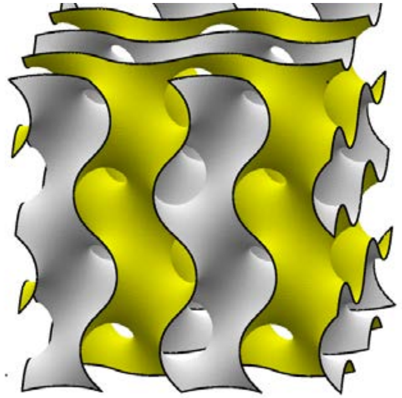
LLNL-PRES-XXXXX

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

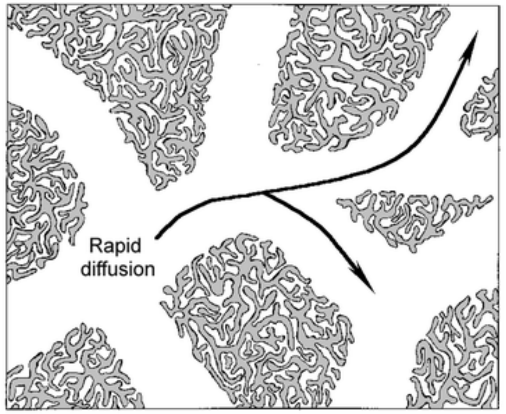
Lawrence Livermore National Laboratory

Goal: more efficient, lower cost reactors for CO_2 capture.

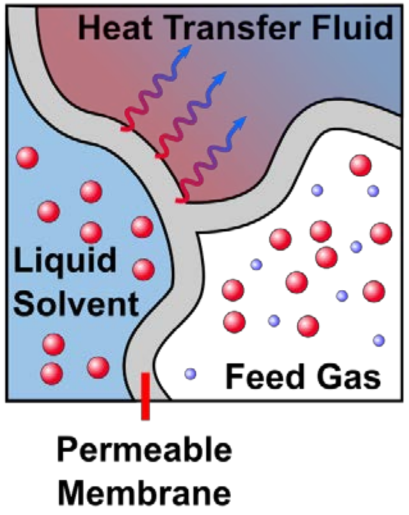
We focus on three design features:



Triply Periodic Minimal Surface (gyroid-like) structures



Hierarchical flow channels



Multifunctional Reactors

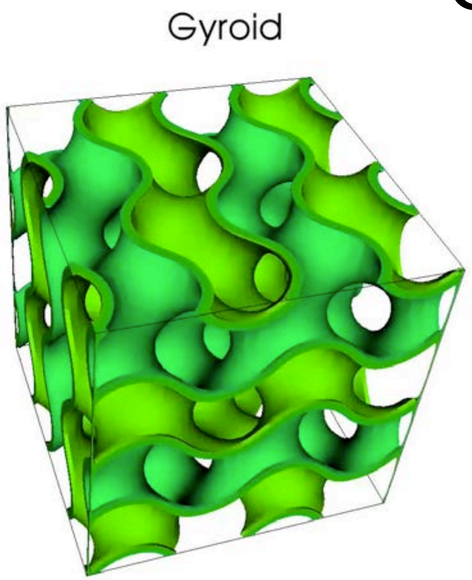
Project Plan

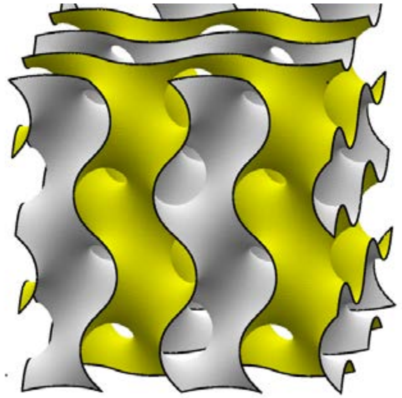
FEW0225: $3.8M over 4 years

	Year 1	Year 2	Year 3	Year 4
Theoretical Assessment	Downselect			
Fabrication Assessment	Proof of concept reactor			
Generation 1 Reactor		Design→ Bench-scale testing	Prototype demo→	
Generation 2 Reactor			Design→ Bench-scale test	Demo design

- 10 tasks in 3 tracks
- Downselect to two reactor concepts, developed in series
- Tech transfer targeted for middle of Year 4 for 1st-gen design

Gyroid reactors: now possible through additive manufacturing

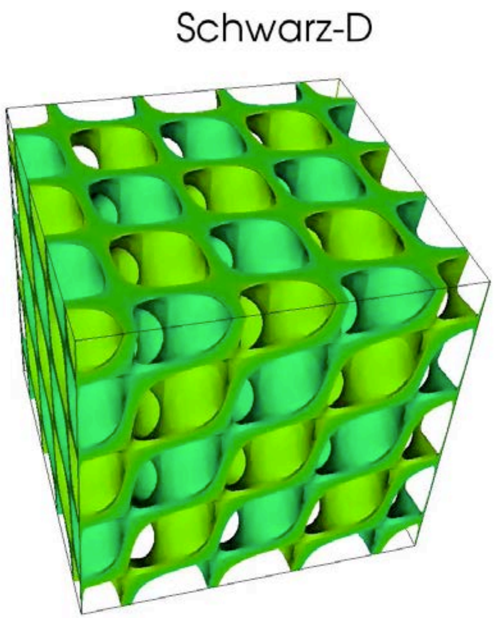


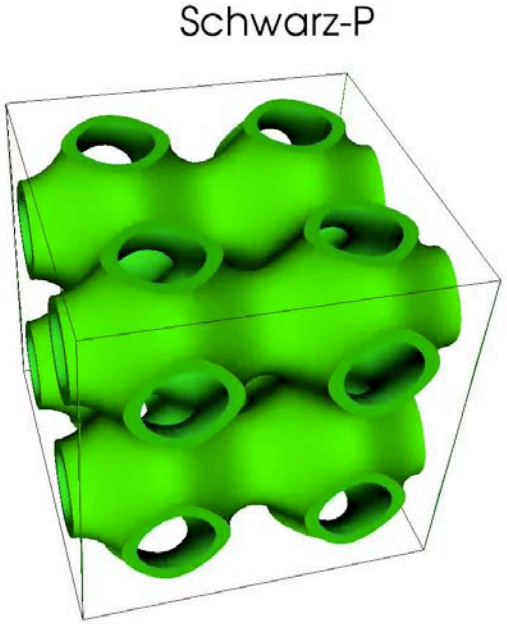


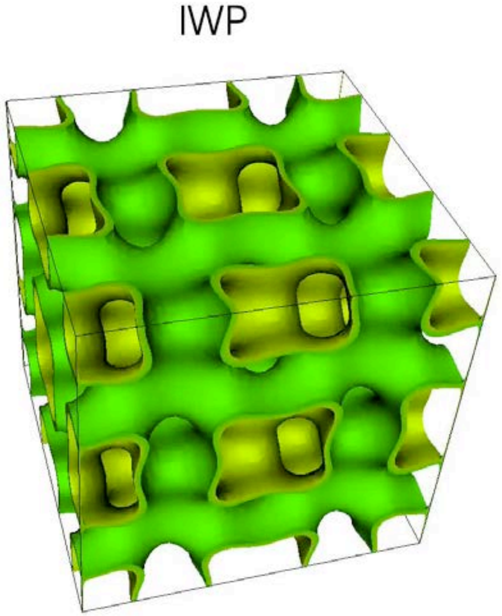
AKA: Triply Periodic Minimal Surfaces (TPMS)

Surface defined by, e.g.:

$$\sin\left(\frac{2\pi}{L}x\right)\cos\left(\frac{2\pi}{L}y\right)+\sin\left(\frac{2\pi}{L}y\right)\cos\left(\frac{2\pi}{L}z\right)+\sin\left(\frac{2\pi}{L}z\right)\cos\left(\frac{2\pi}{L}x\right)=t$$

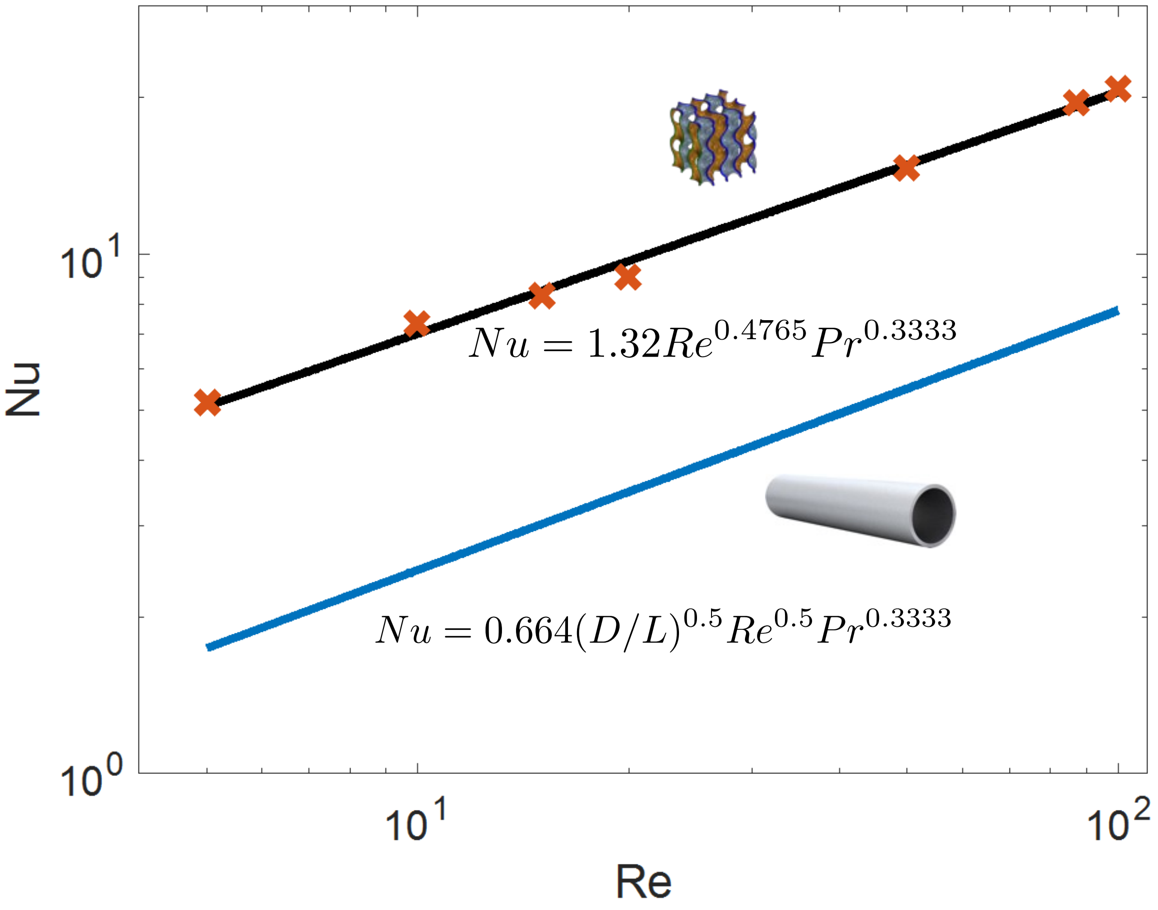






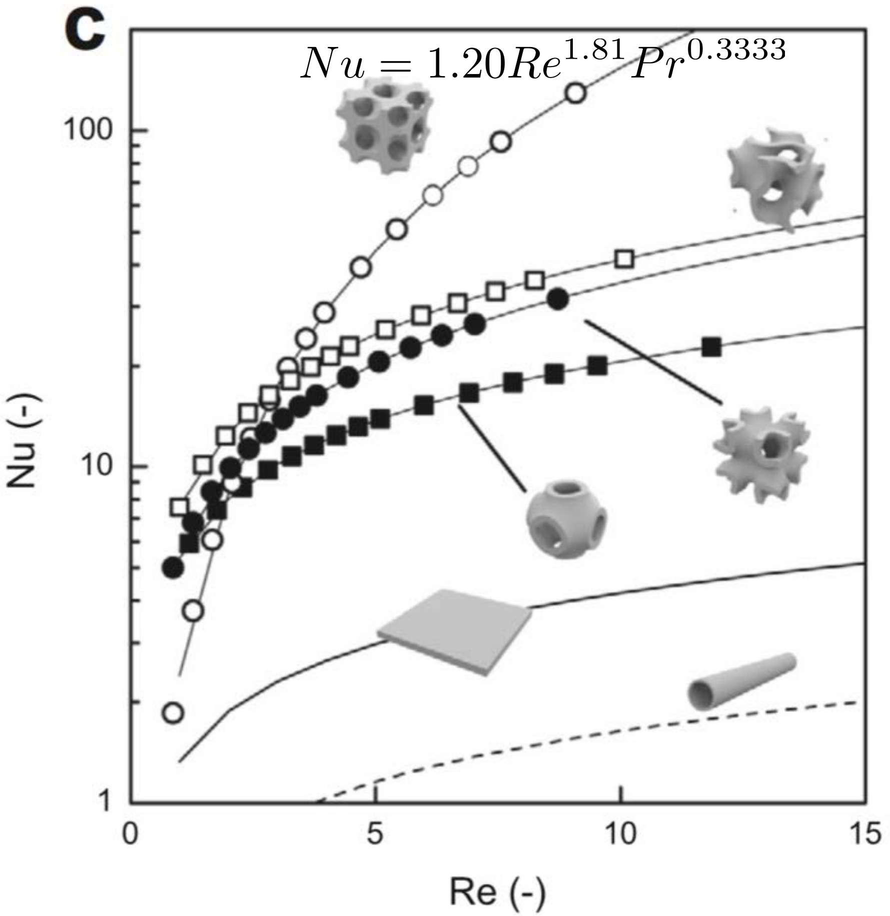
Order of magnitude improvement in heat & mass transfer vs tubes.

Heat Transfer Correlation (our work)



$$Nu = \frac{hD}{k}$$

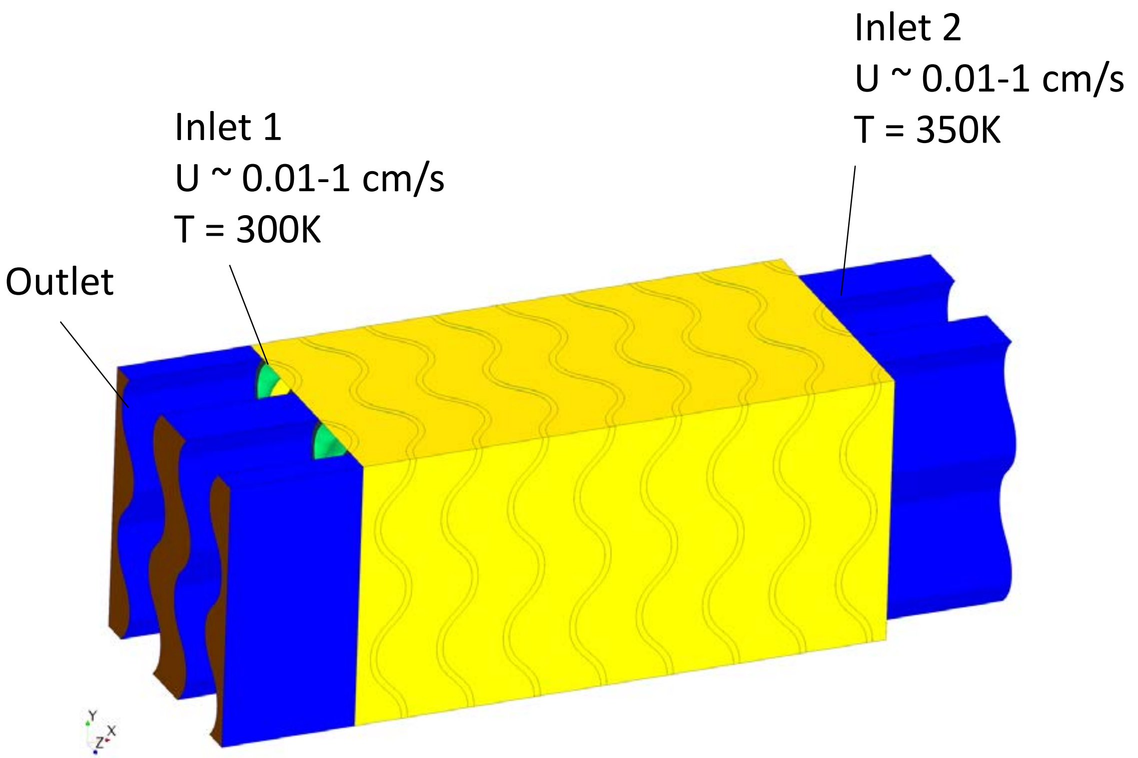
Experimental Correlation (literature)[1]



⇒ Need to understand mechanisms for optimal design.

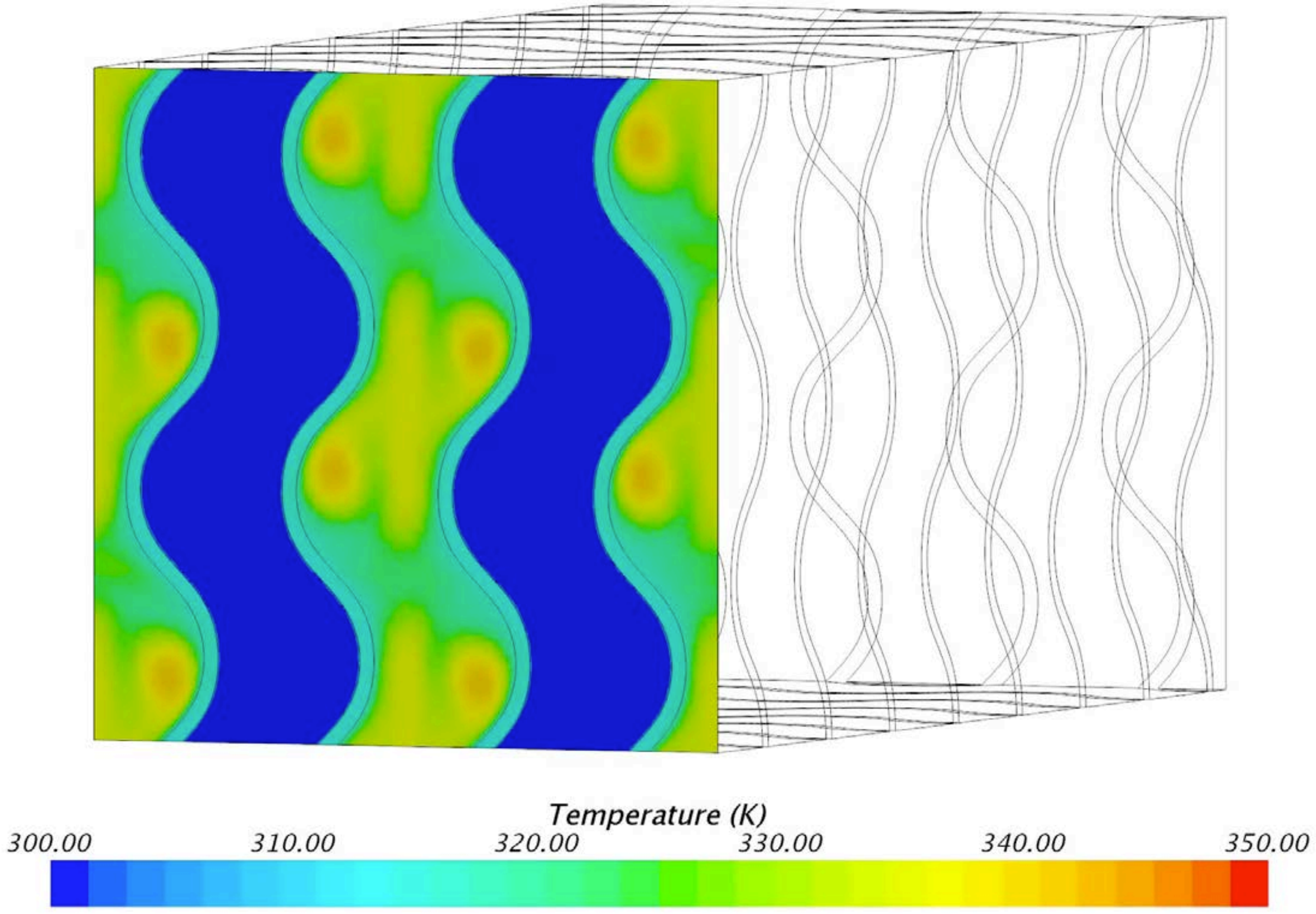
[1]Femmer et al. 2015

Fluid folding leads to improved heat exchange.



Water/water heat exchanger
(simulation in StarCCM)

Temperature in fluids at steady state



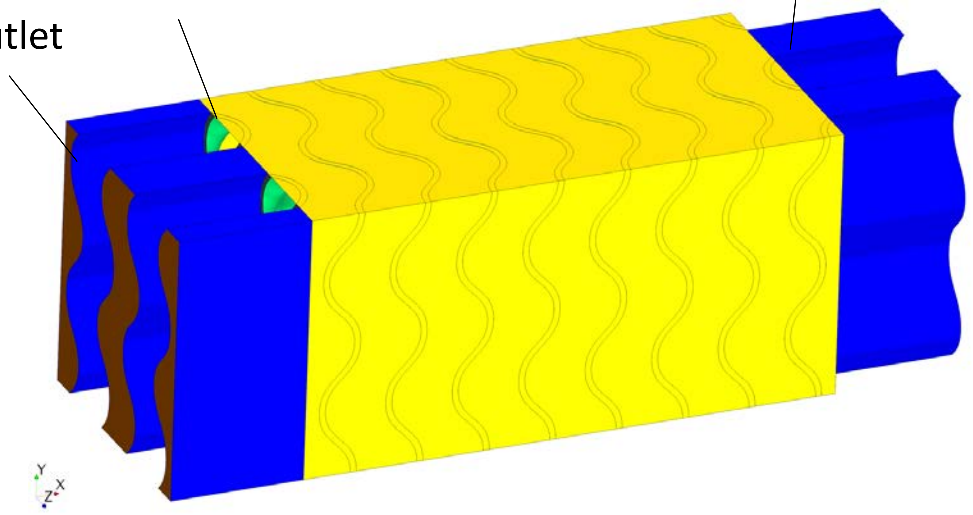
U = 0.01 m/s, *Re* = 87, *Pe* = 521

Fluid folding leads to improved heat exchange.

Inlet 2
U ~ 0.01-1 cm/s
T = 350K

Inlet 1
U ~ 0.01-1 cm/s
T = 300K

Outlet



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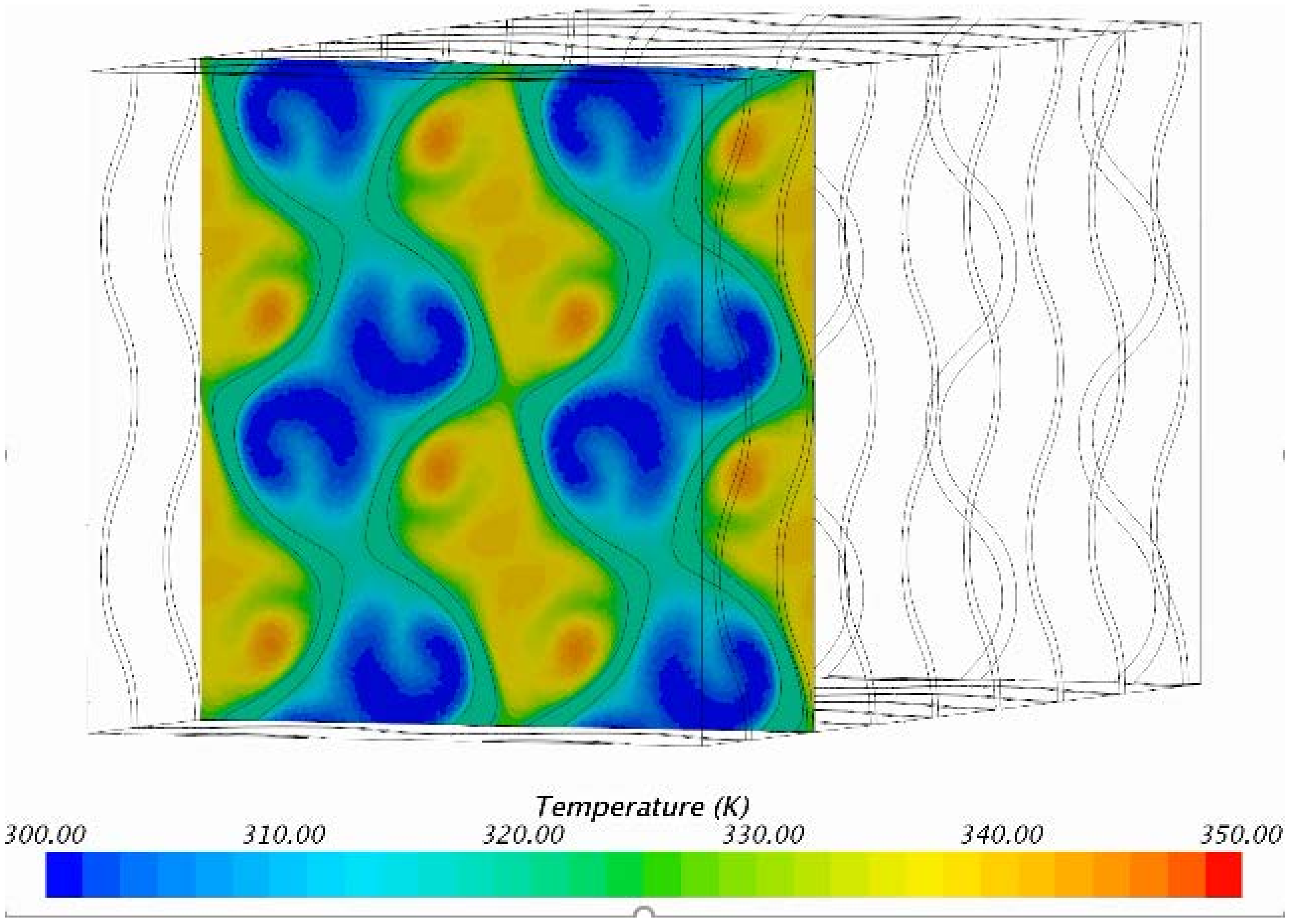

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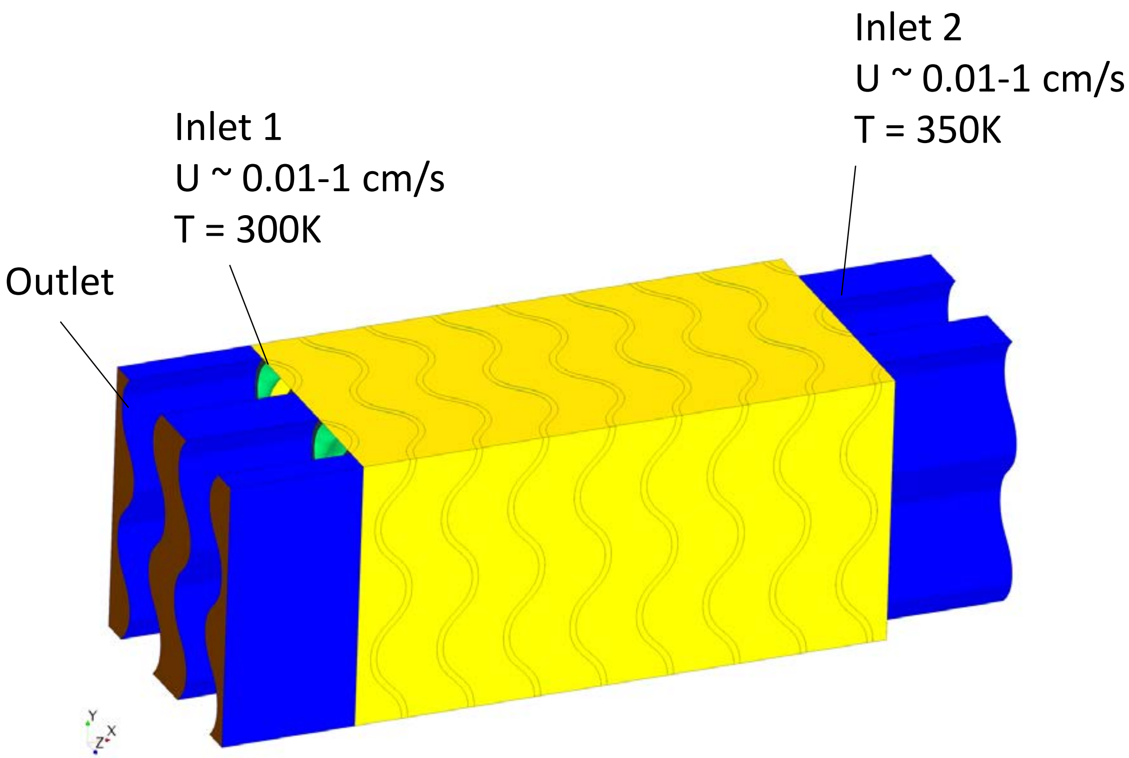

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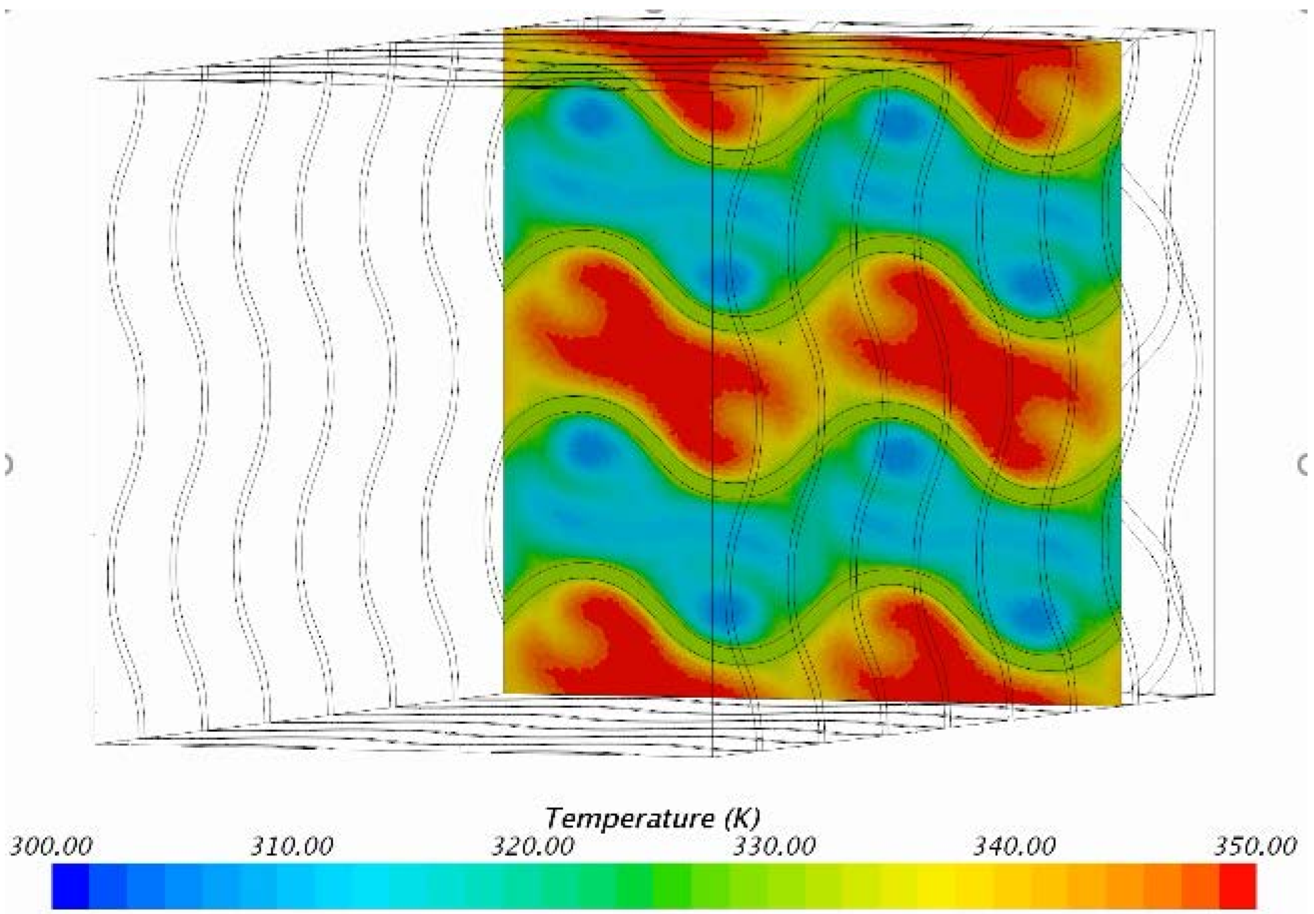
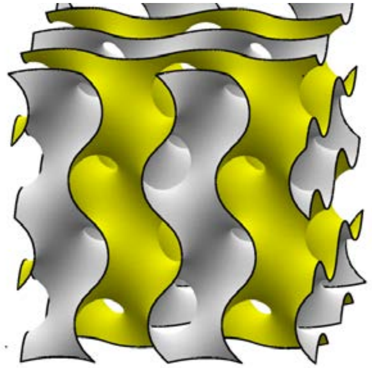
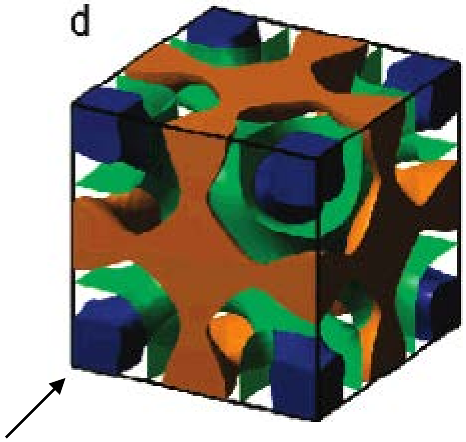


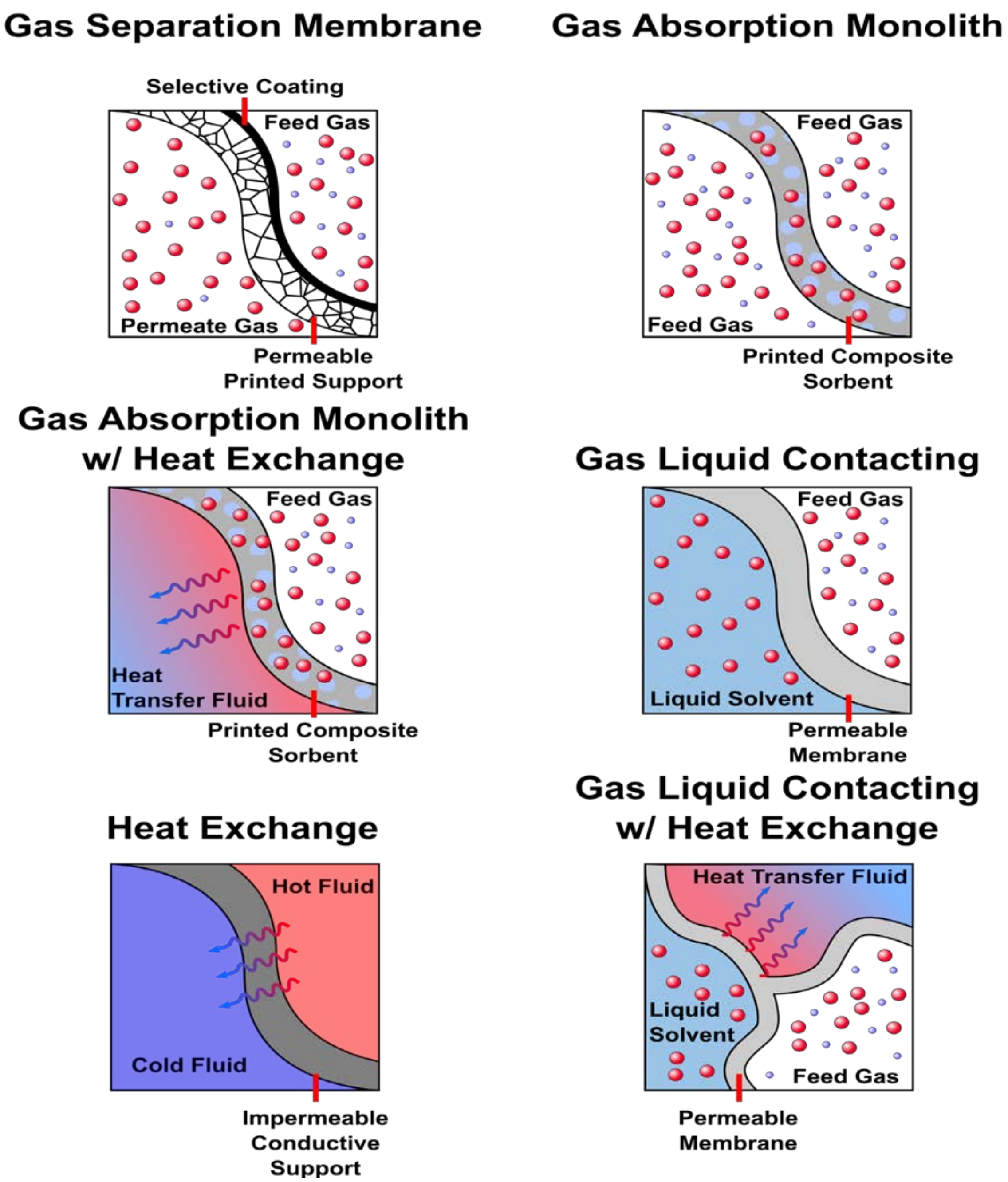
U = 0.01 m/s, *Re* = 87, *Pe* = 521

Many reactor configurations possible with additive manufacturing.





from Toombes et al., Macromolecules 40(25):8974-8982, 2007



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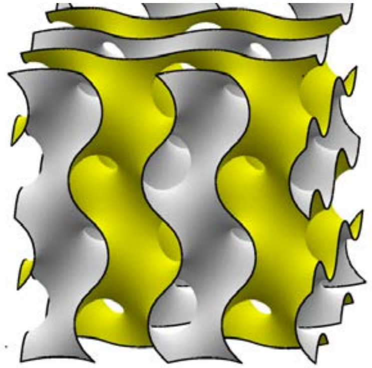

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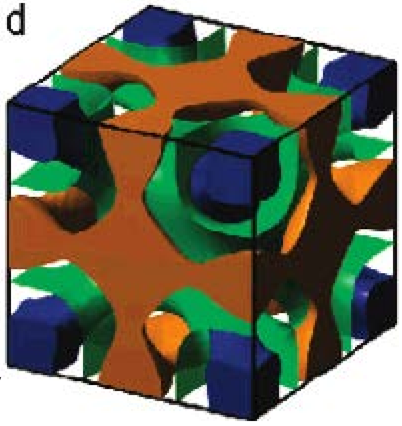

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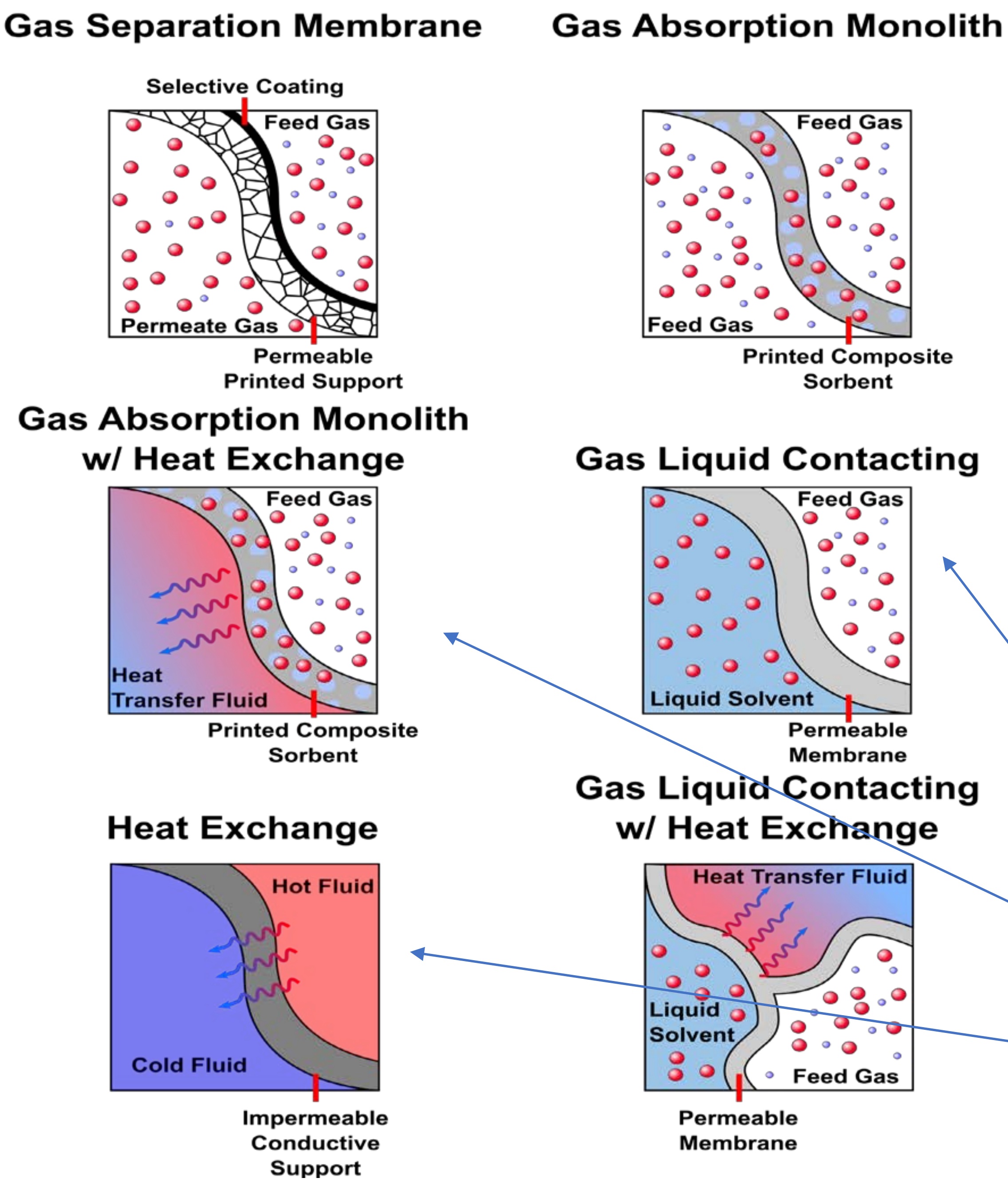
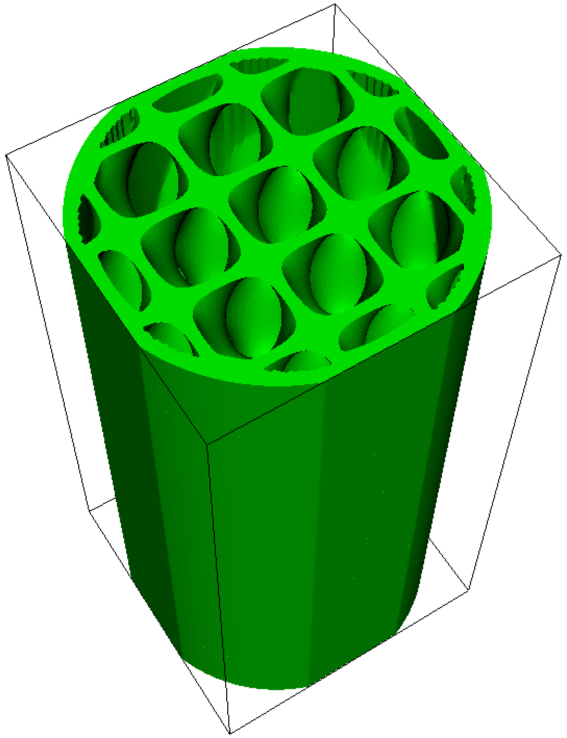
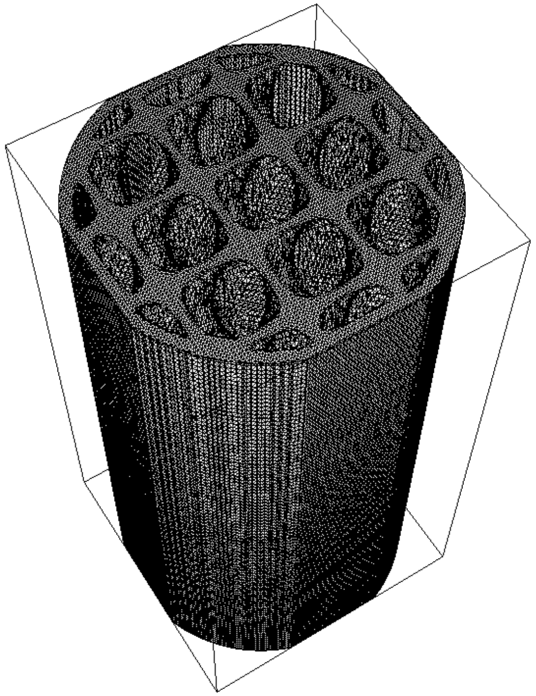


We've focused on three.

Work Flow: From design concept to 3D printing



Schwarz-D structure generated by in-house Level Set code (TransFort)



STL file generated by Visit

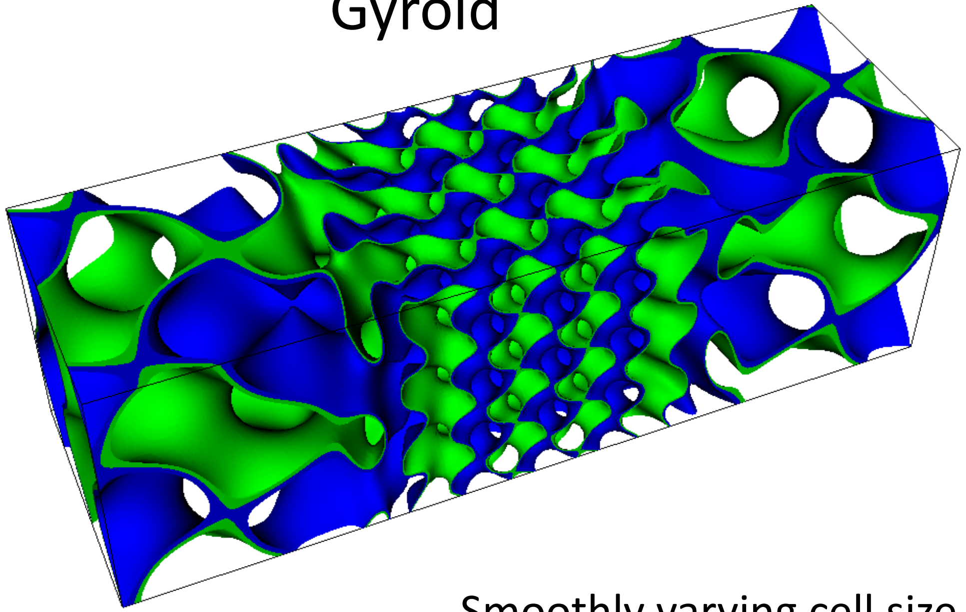
3D printed Schwarz-D using PDMS

Challenges for gyroid reactor design:

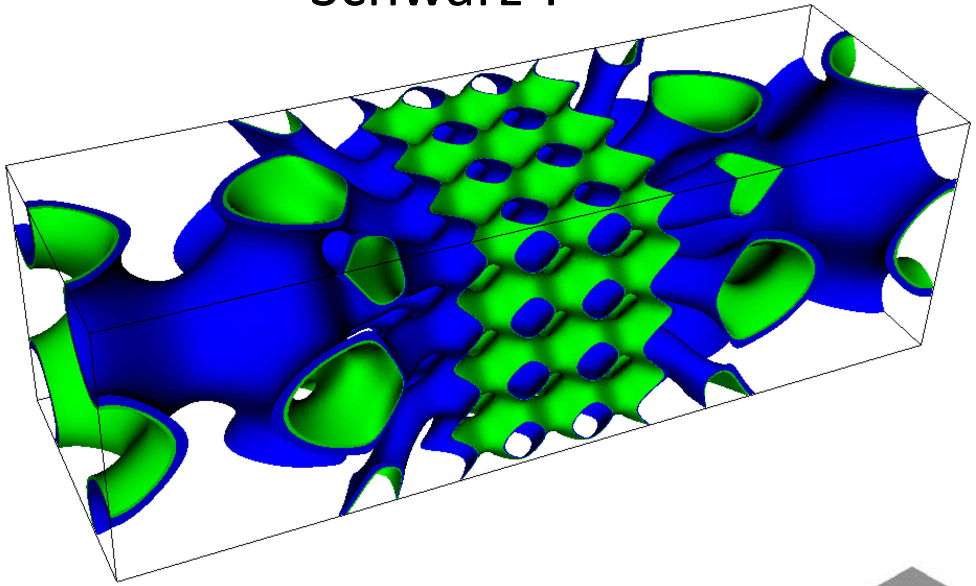
1. How to manifold the structure to connect fluids and distribute flow
2. How to maintain strength with small features
3. How to choose best geometry for the application

Size hierarchy can solve connection & distribution

Gyroid

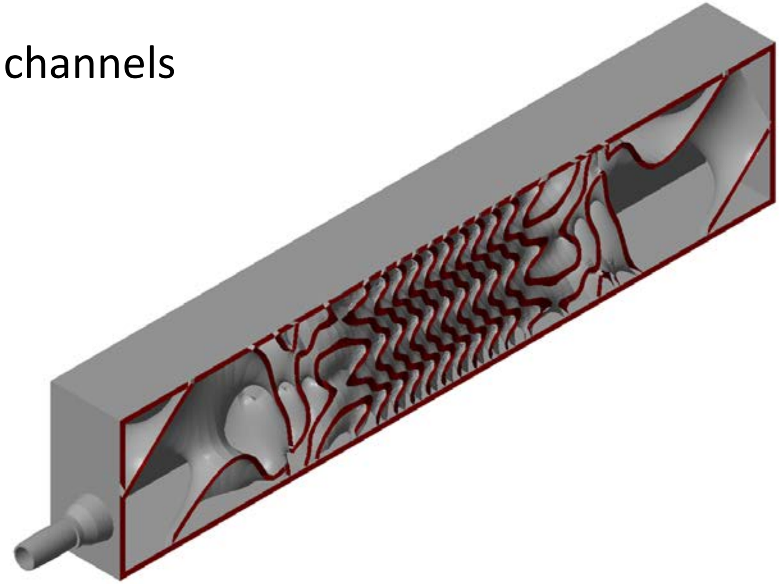


Schwarz-P



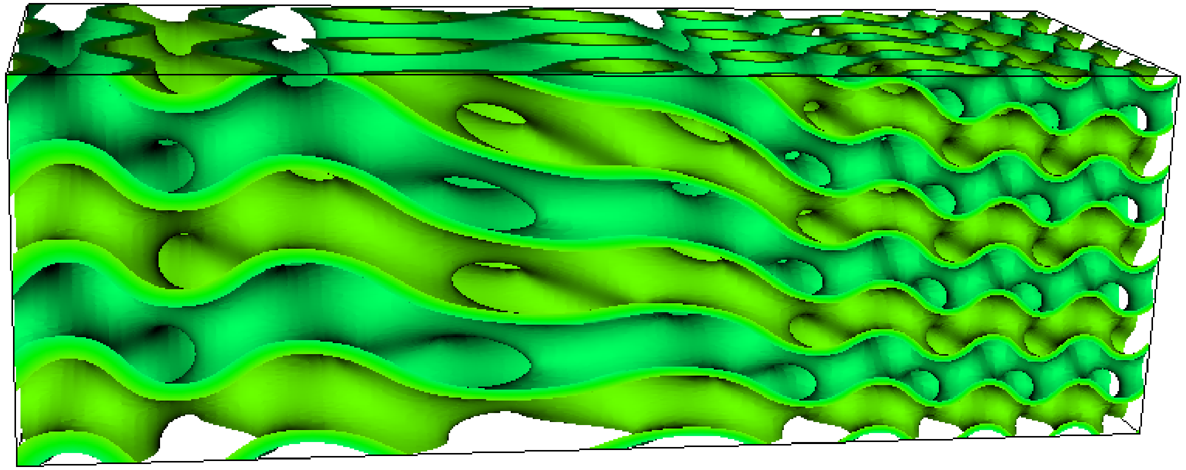
Smoothly varying cell size to link large & small channels

Large cells at ends make for easy fluid connections:

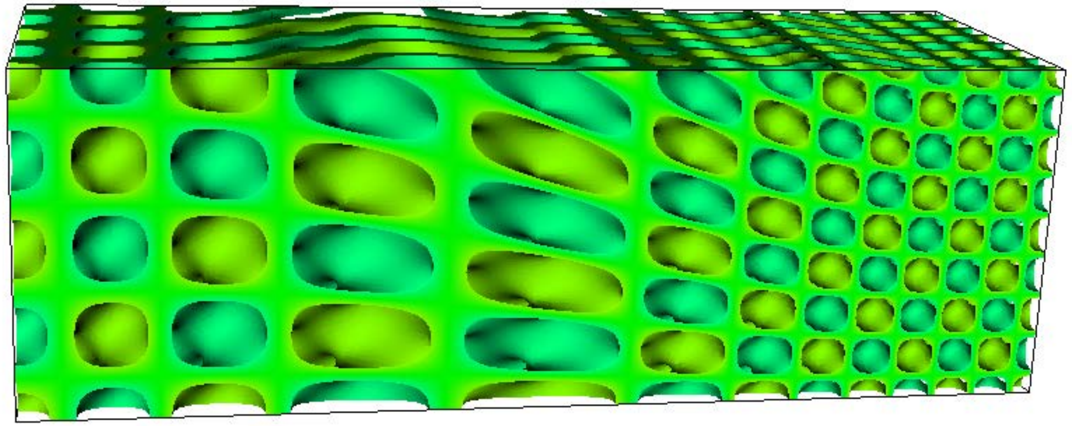


Varying wall thickness improves structural strength and robustness

Gyroid



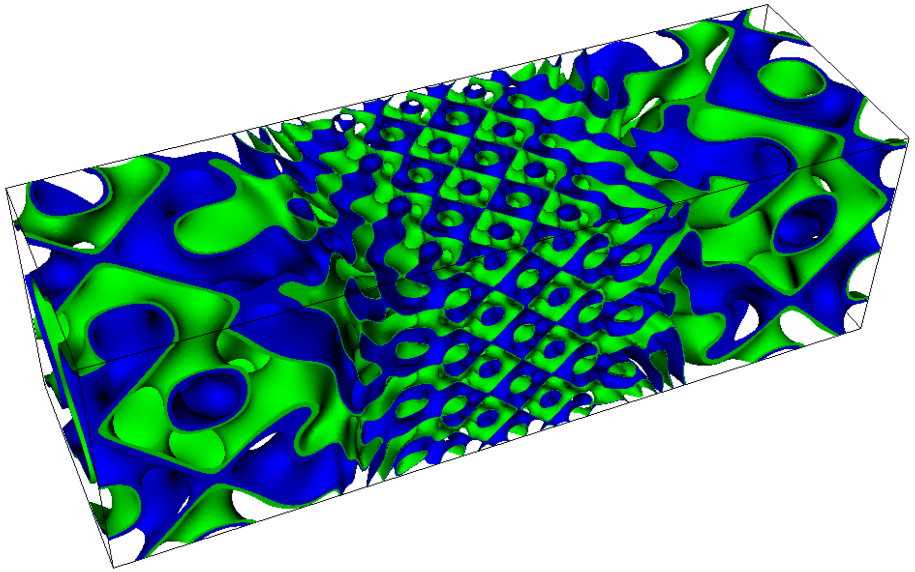
Schwarz-D

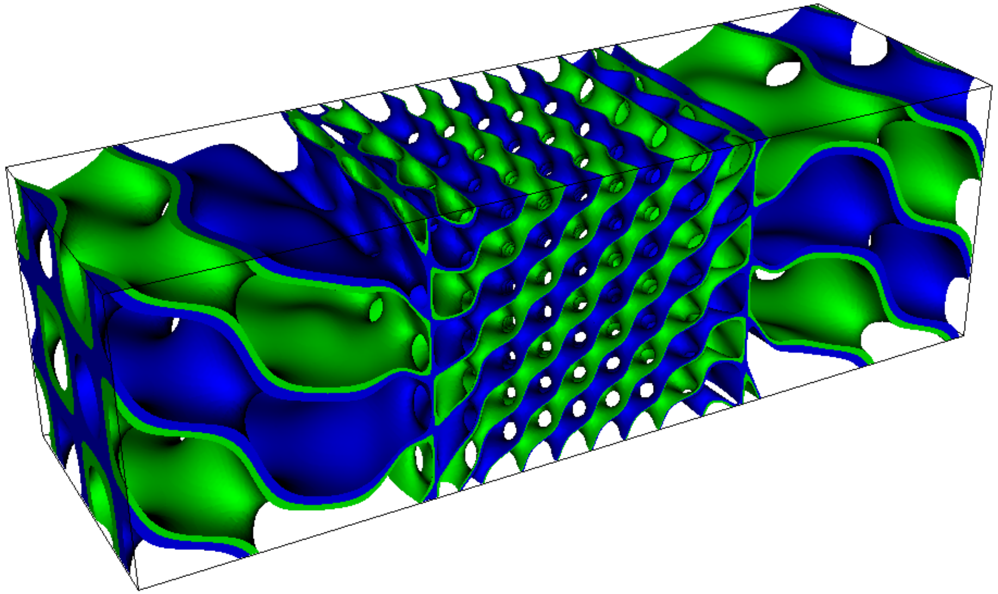


Otherwise large cells with thin walls are weak points.

New geometry candidates discovered through recent literature review

- Schoen-G or Gyroid[1]
- Schwarz-D[2]
- Schwarz-P[3]
- Schoen I-WP
- Fischer-Koch
- Schwarz-CLP
- Schwarz-transverse-CLP[4]



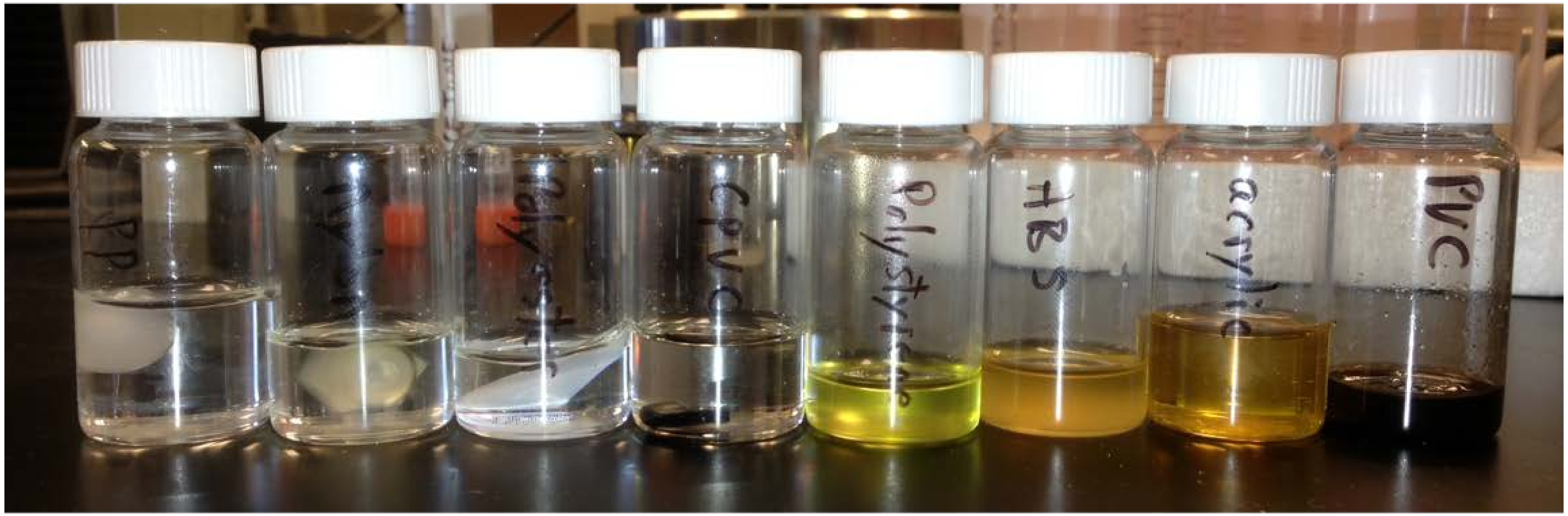


[1,4] High mass transfer in filtration and membrane distillation (Sreedhar et al., 2018, Thomas et al. 2018)
[2] High heat transfer using water (Femer et al. 2015)
[3] High mass transfer during CO_2 transport (Femmer et al. 2015)

Goals for reactor fabrication

1. Identify compatible, printable materials
2. Adapt fabrication techniques for gyroid reactors
3. Build & test reactor prototypes

Low-cost 3D-printed packings in plastic?



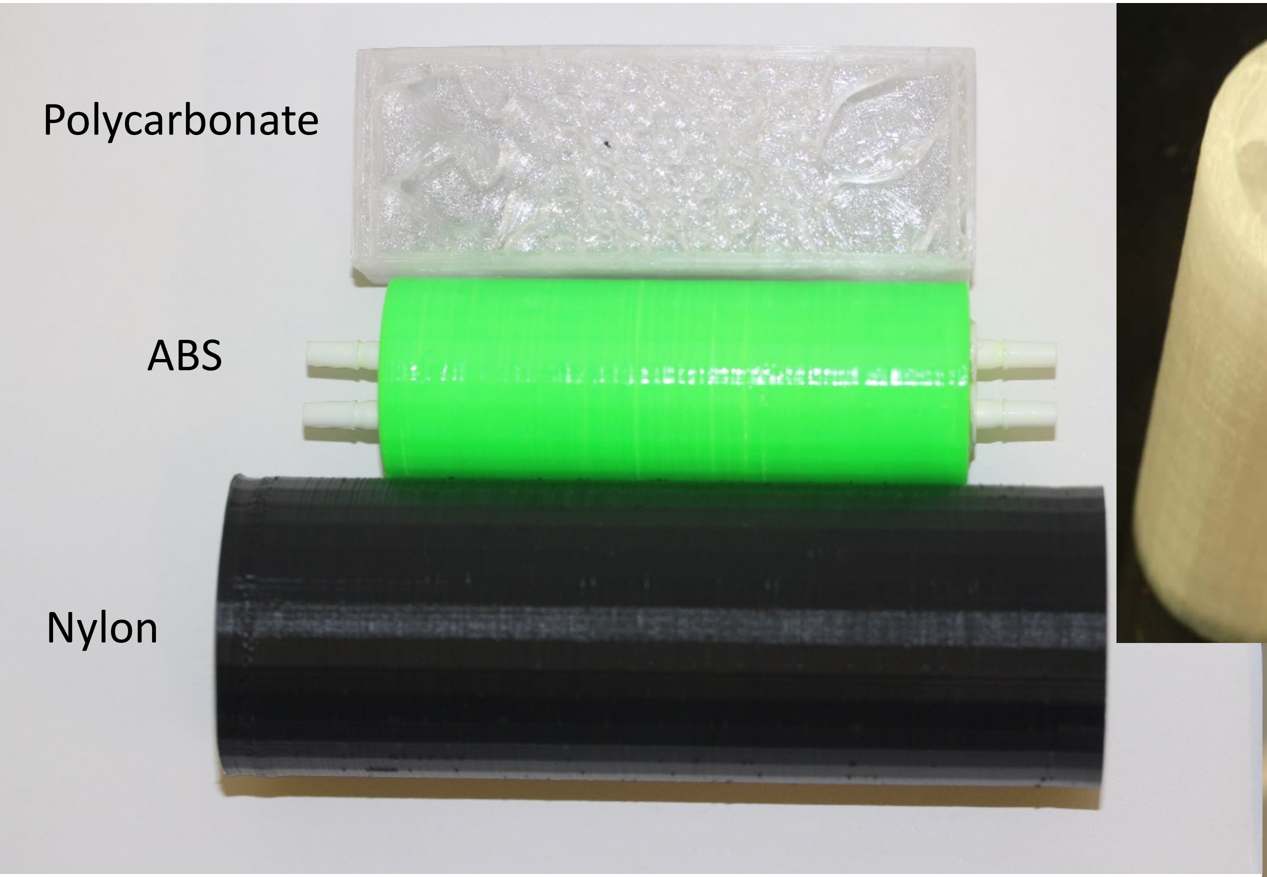
Compatible with CO_2-binding Organic Liquids:

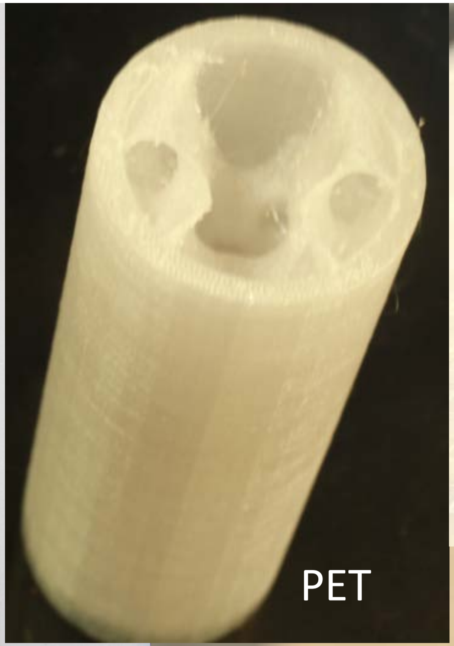
- Polypropylene
- Nylon,
- polyester (PET)
- CPVC

Compatible with diethanolamine:

- Nylon
- PET

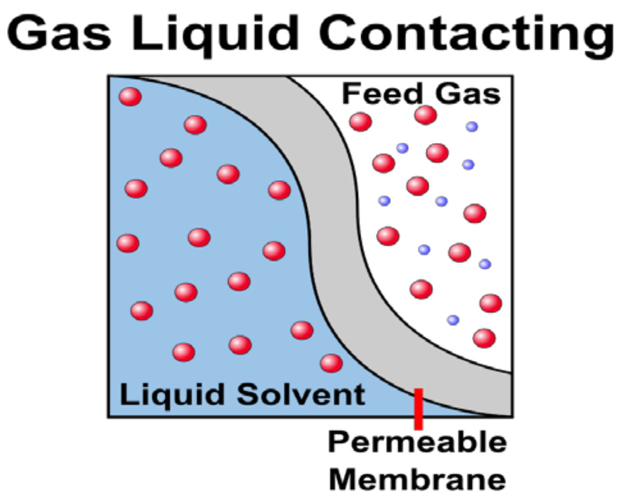
Multiple impermeable materials demonstrated.

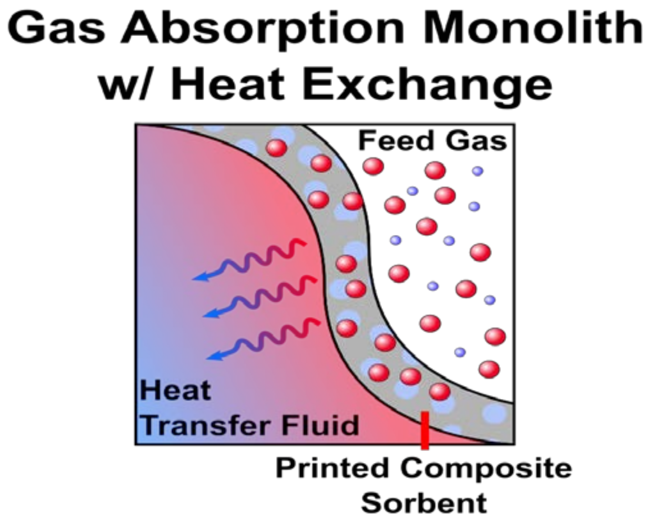




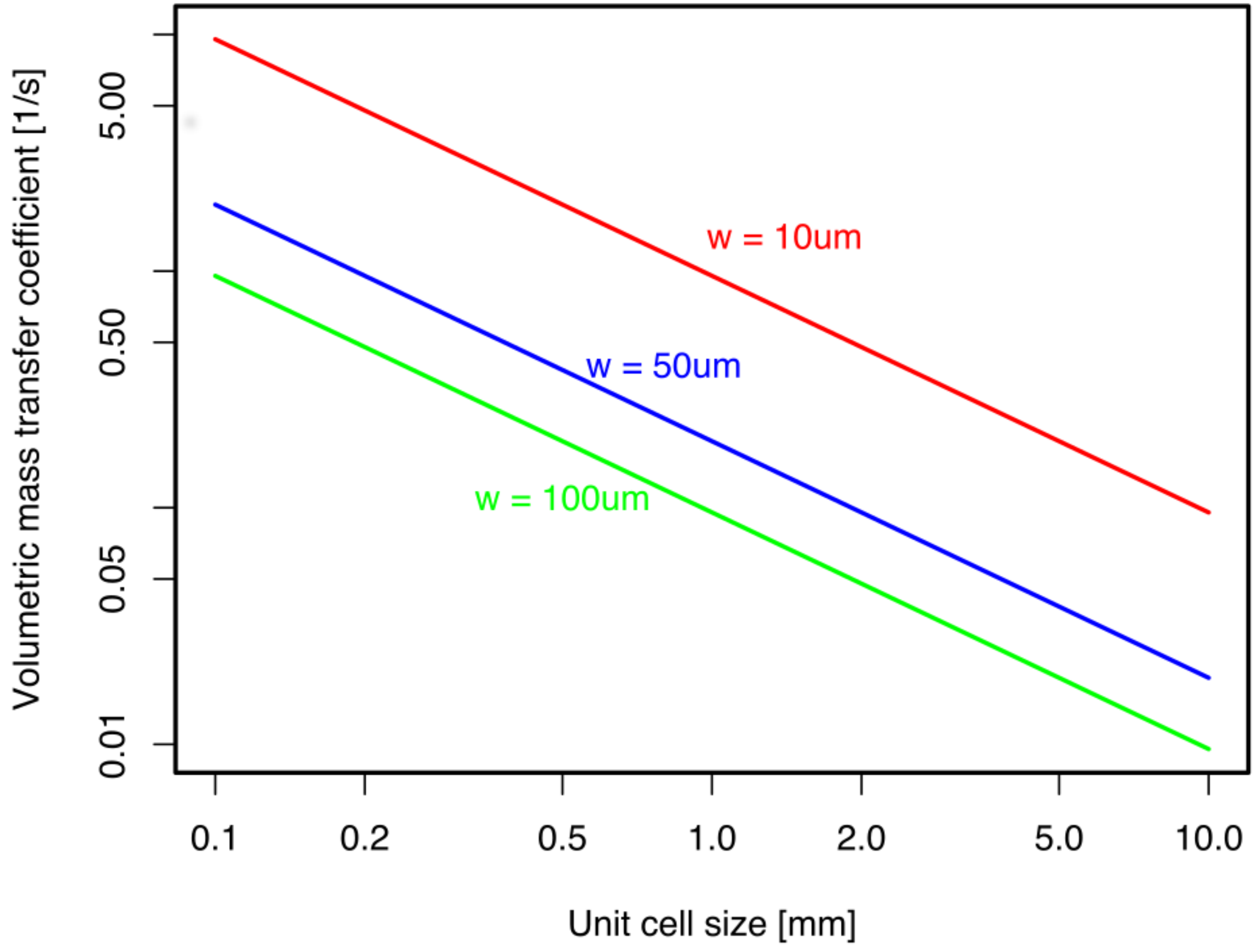
Many material options for heat-exchange based reactors.

Permeable materials would allow additional reactor types.

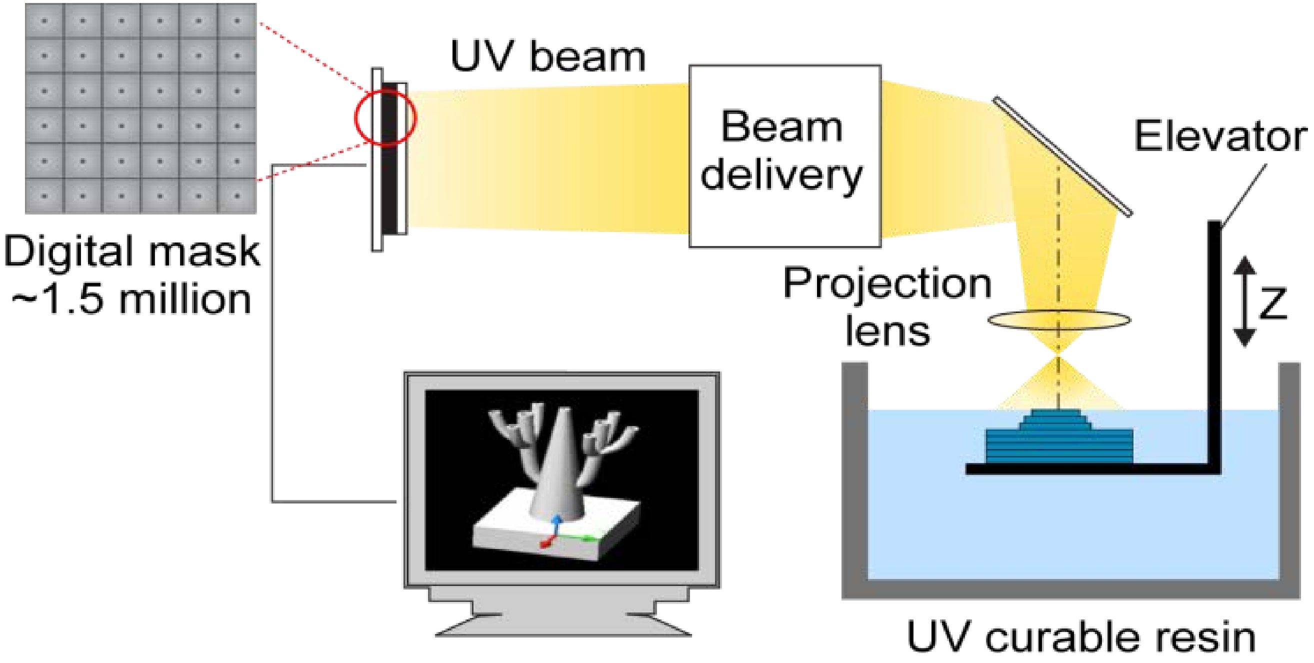




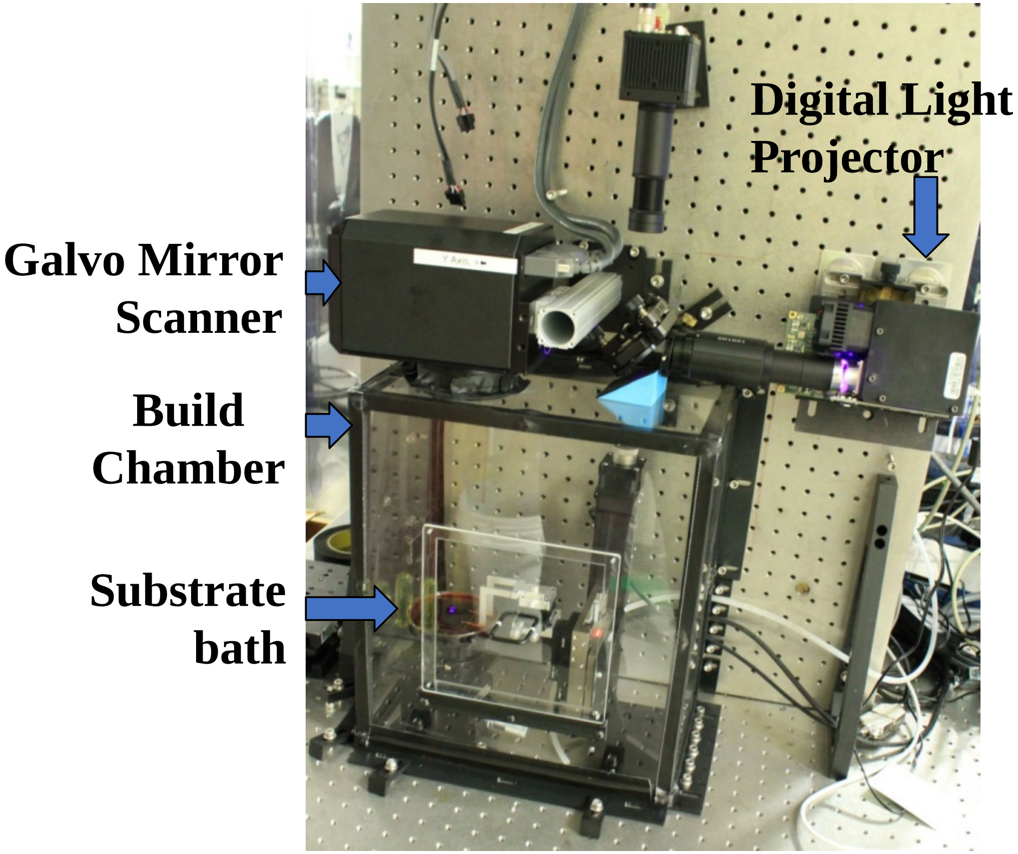
Calculated mass transfer in a silicone gyroid membrane reactor



Large Area Projection Micro Stereo-Lithography: 1 μm resolution on a 10 cm build



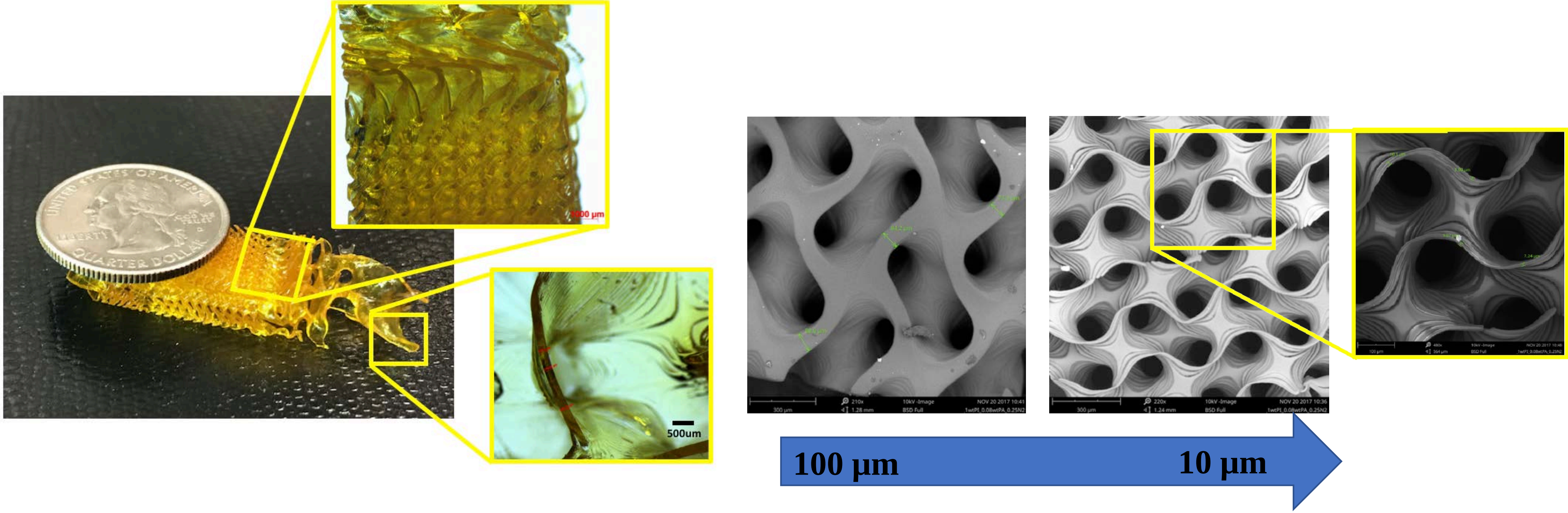
PμSL System



Large Area PμSL at LLNL

LAPµSL makes the high resolution gyroid reactors possible

CO_2-permeable silicone gyroids can now be printed in LAPµSL

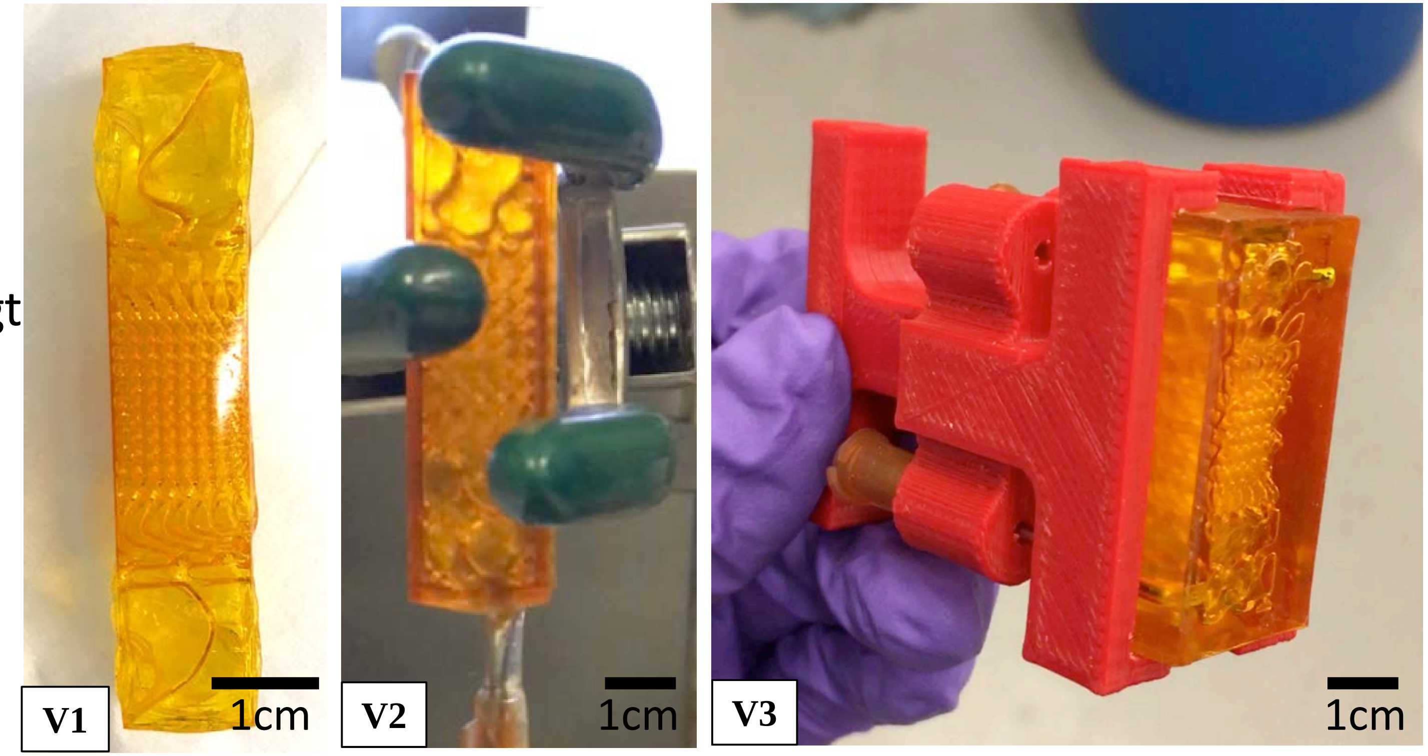


Required adjusting resin formulation and and print parameters.

Reactor designs are currently being refined

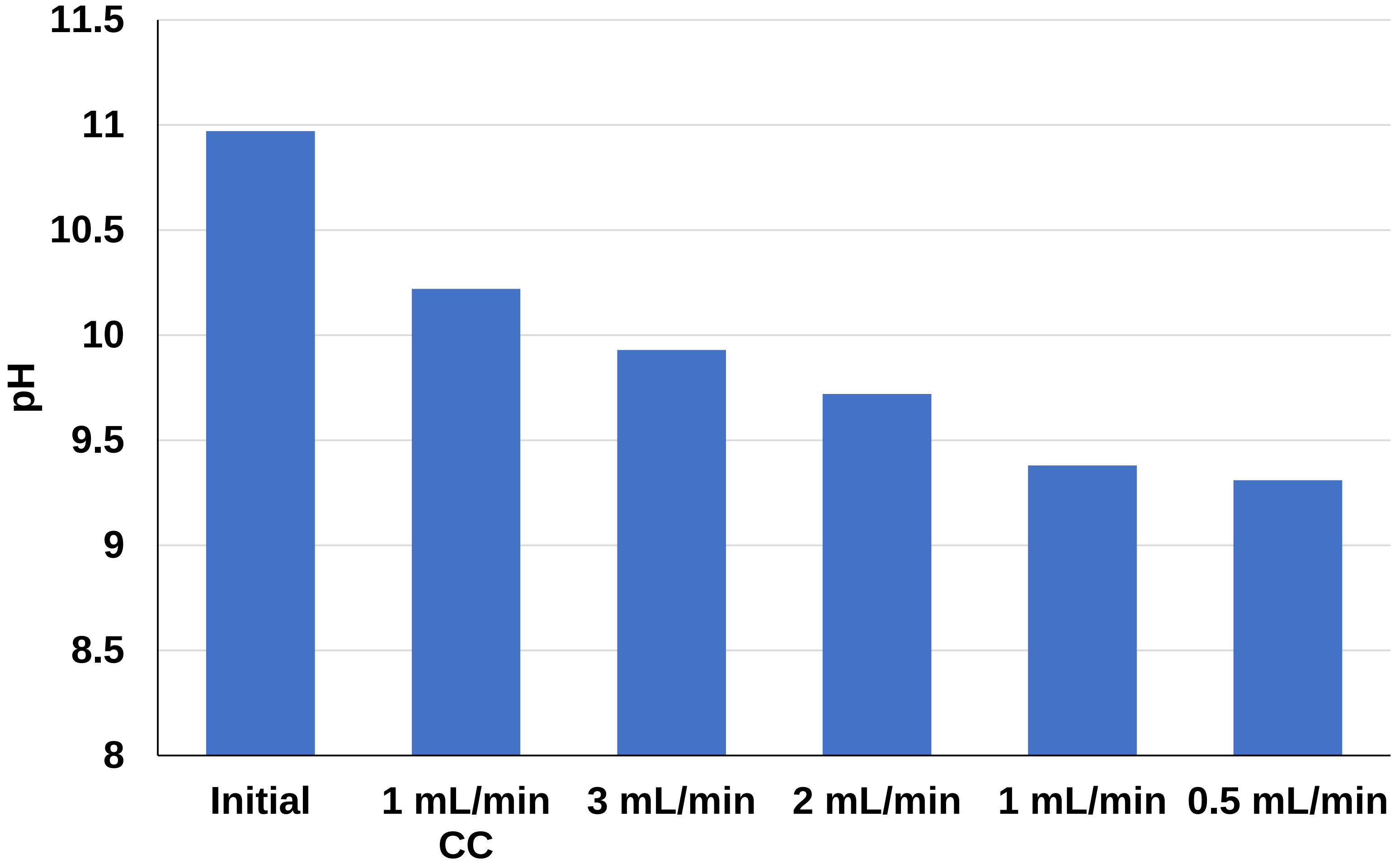
Design parameters:

- Flow geometry
- Inlet/outlet orientation
- Outer wall thickness for maximum strengt
- Cleaning methods
- Nozzle attachment mechanism



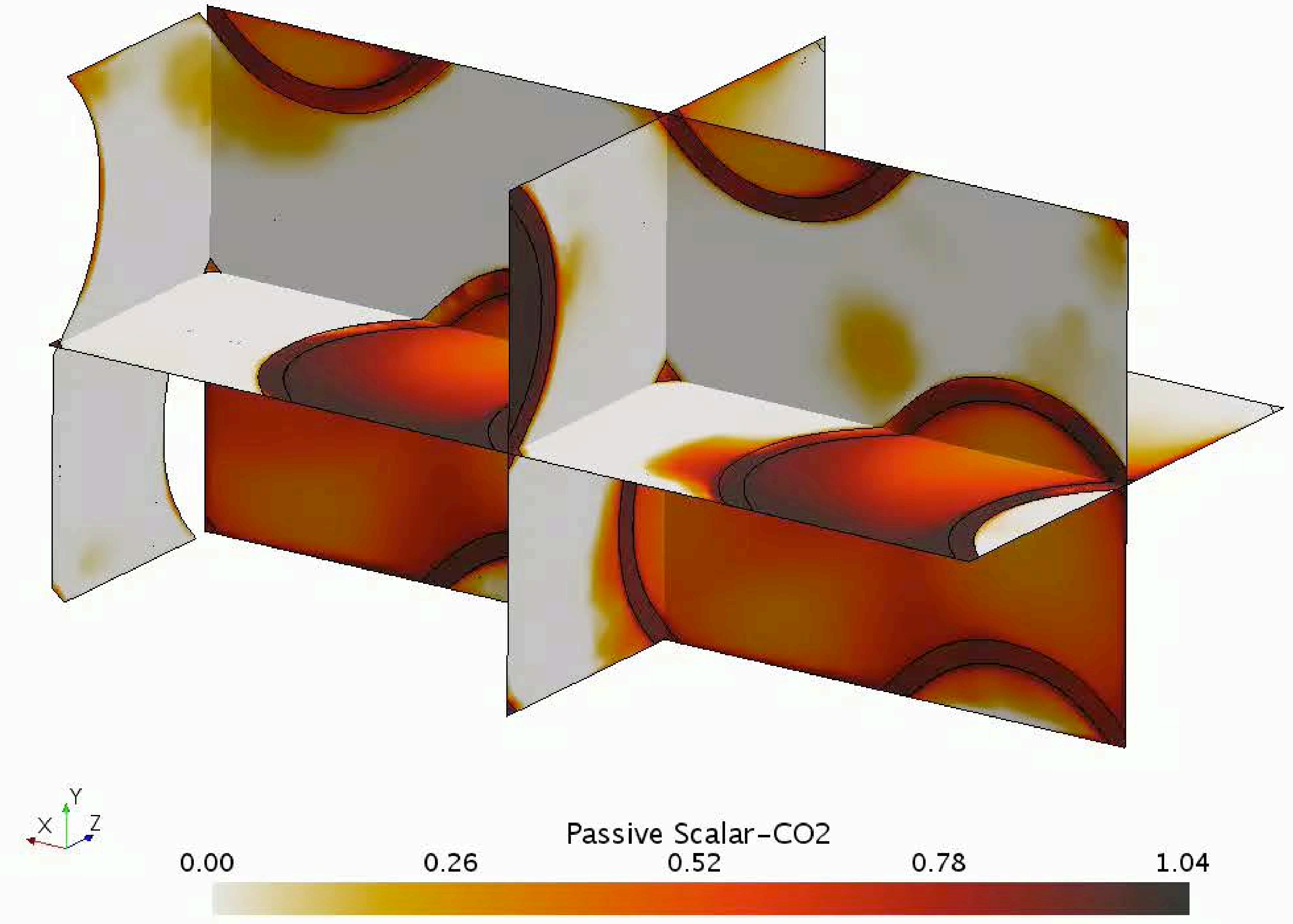
Through design iteration the reactor has become more robust

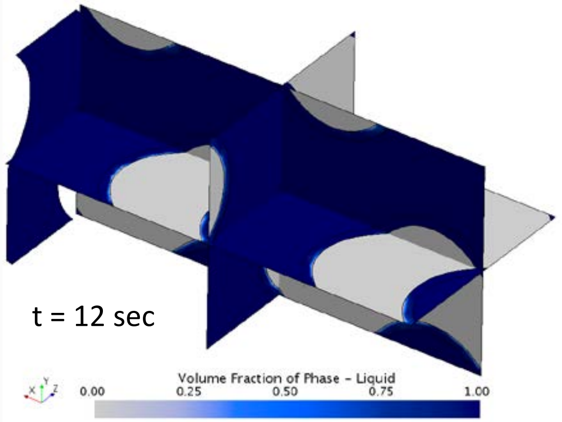
First mass transfer measurements in silicone-gyroid reactor



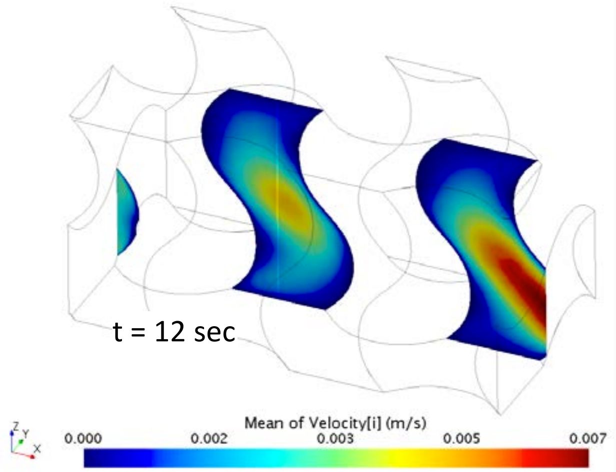
- 3% Na_2CO_3 solvent
- 0.47 L/min CO_2 flow rate
- Monolithic reactor configuration / CC: Countercurrent reactor configuration

Initial simulations of mass transfer in StarCCM

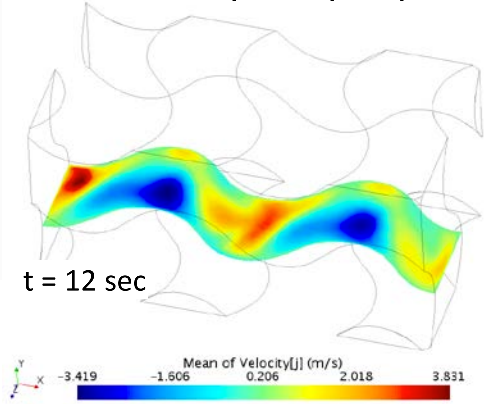




[Volume fraction]

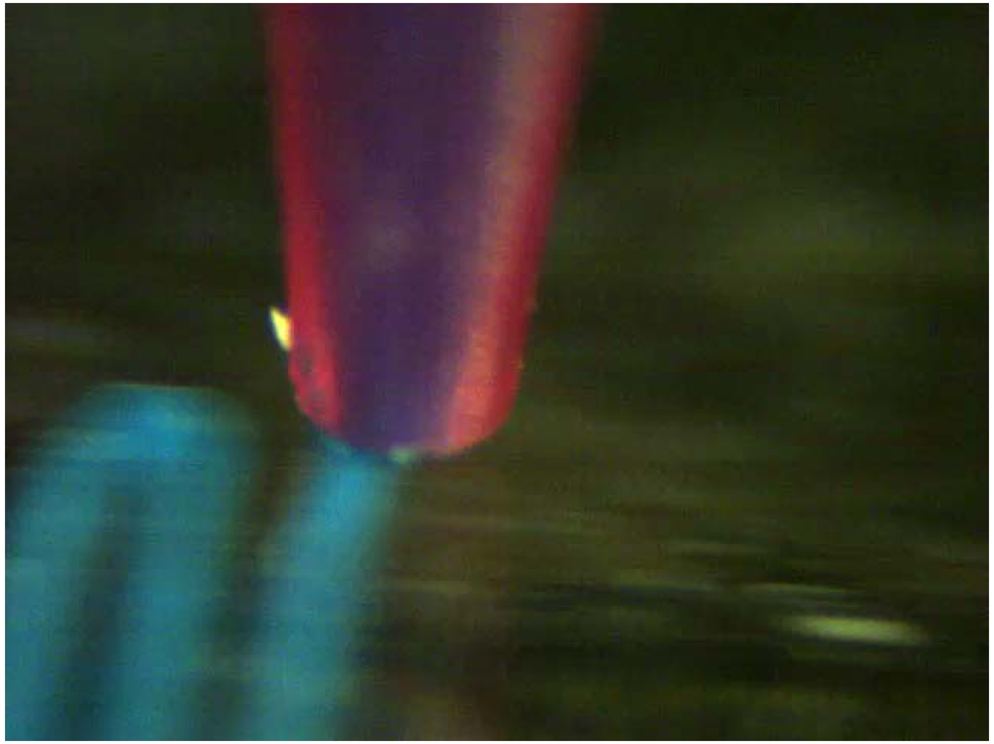


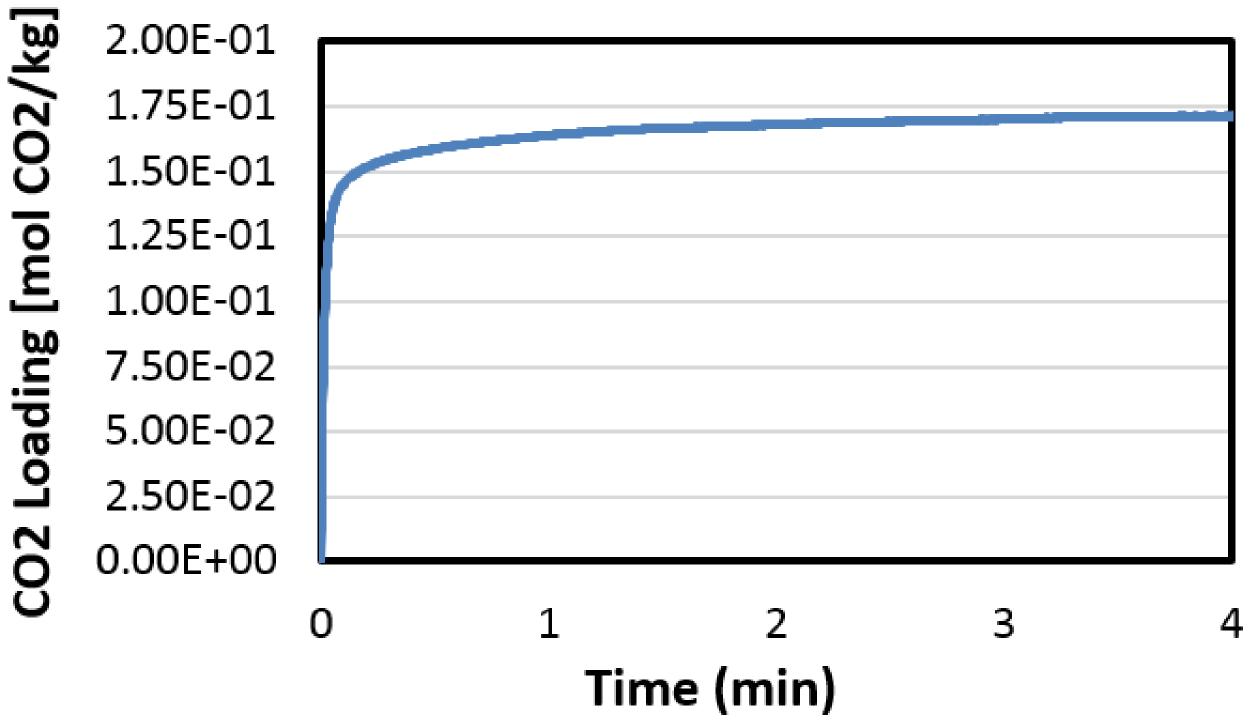
[Mean x-velocity of liquid phase]



[Mean y-velocity of gas phase]

First Silicone-MOF Printed Composite Sorbent tested.





- 30 wt% HKUST-1 Metal Organic Framework / 70% SE-1700
- 0.22 mmol/g loading
  - 80% expected loading
  - 50% loading within ~1s

Conclusions

- Hierarchical gyroids show great promise as next-generation reactor designs.
- Gyroids appear most useful to improve liquid-side heat transfer or mass transfer
- Candidate configurations for further development are:
    - Intercooled absorber packings
    - Gas/solvent membrane reactor
    - Sorbent scaffolds with integrated heat exchange

Project Team

Lawrence Livermore National Laboratory

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Samantha Ruelas, Matthew Worthington, William Smith,
Sarah E. Baker, James S. Oakdale

Acknowledgements

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NATIONAL ENERGY TECHNOLOGY LABORATORY

Andy Aurelio
Lynn Brickett

Questions