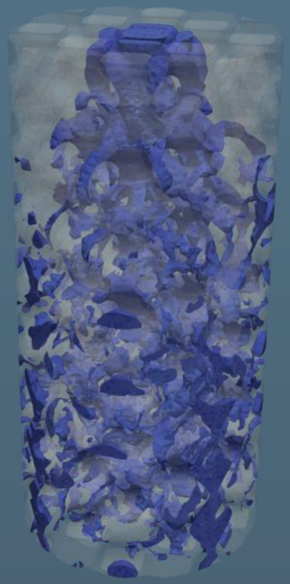
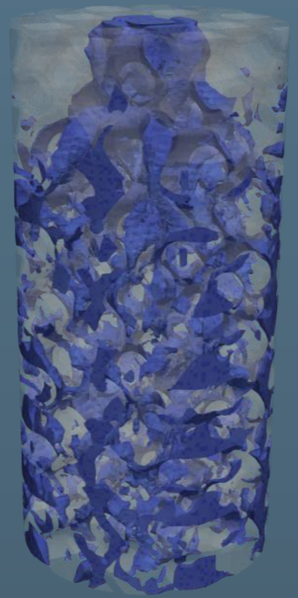
FEW0225: High-efficiency, integrated reactors for sorbents, solvents, and membranes using additive manufacturing

NETL Carbon Management and Oil and Gas Research Project Review Meeting
August 16, 2021

Du Nguyen



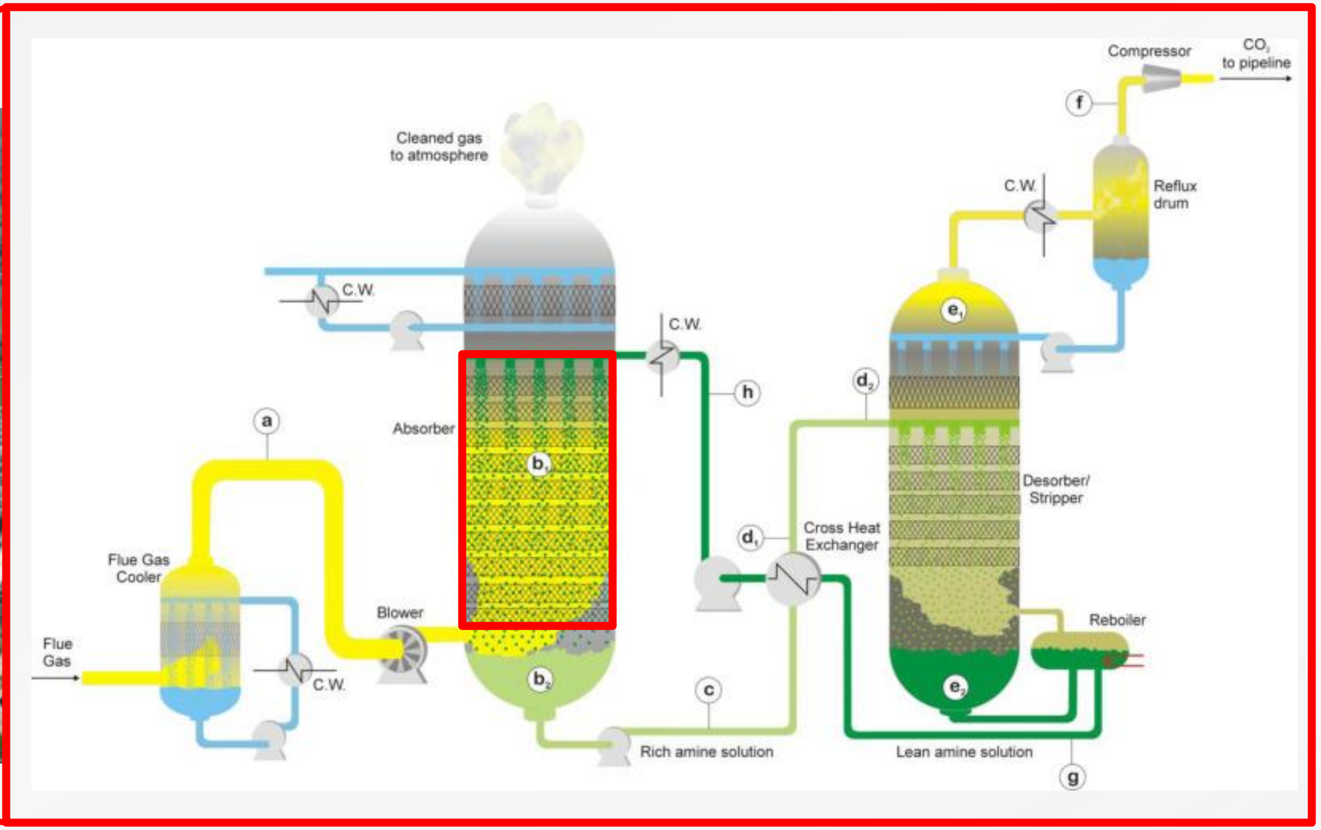


This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
LLNL-PRES-825446

Lawrence Livermore National Laboratory

Carbon capture, utilization, and storage technologies are driven by a need to improve efficiency

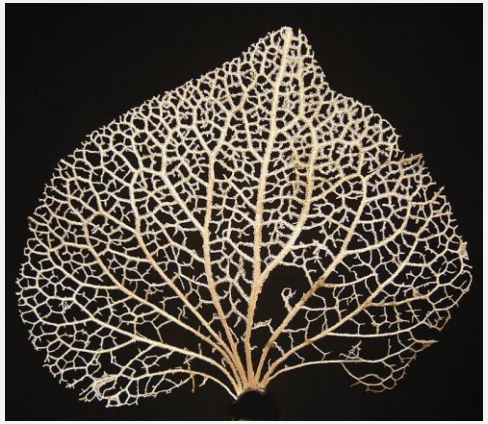
Petra Nova, a joint venture between NRG Energy and JX Nippon Oil & Gas Exploration



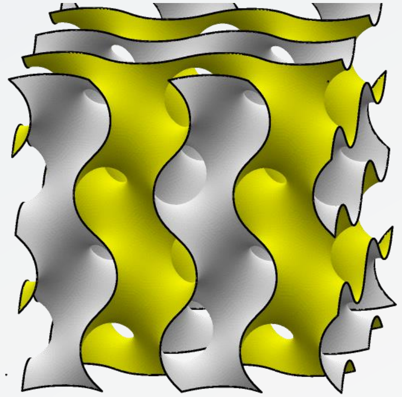
Krzemień, A.; Więckol-Ryk, A.; Duda, A.; Koteras, A. Risk Assessment of a Post-Combustion and Amine-Based CO2 Capture Ready Process. *Journal of Sustainable Mining* **2013**, *12* (4), 18–23. https://doi.org/10.7424/jsm130404.

What can advanced manufacturing bring to the table?

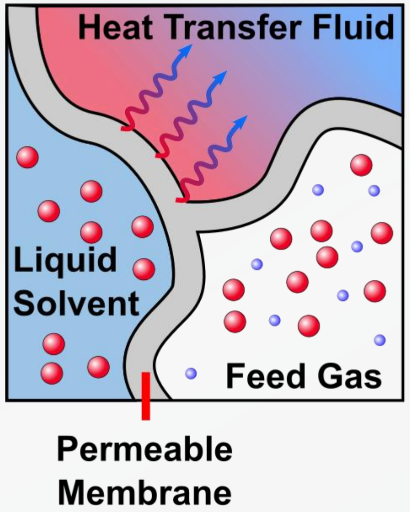
We focused on 3 design motifs



Hierarchical flow channels



Triply Periodic Minimal Surface structures



Multifunctional Reactors

Goal: More efficient, lower cost reactors for CO_2 capture

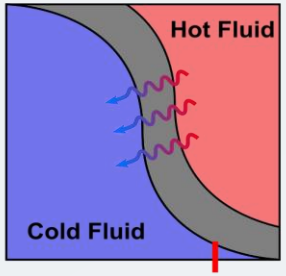
Project Plan

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

- 10 tasks in 3 tracks
- Downselected reactor design
- NCE requested until December 2021 due to COVID
- Tech transfer targeted for middle of Year 4 for 1st-gen design

Many reactor configurations possible with TPMS and additive manufacturing.

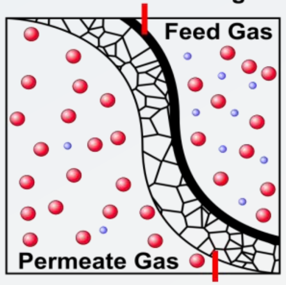
Heat Exchange



Impermeable Conductive Support

→ Active projects

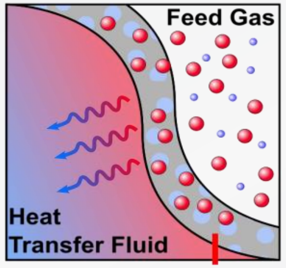
Gas Separation Membrane



Permeable Printed Support

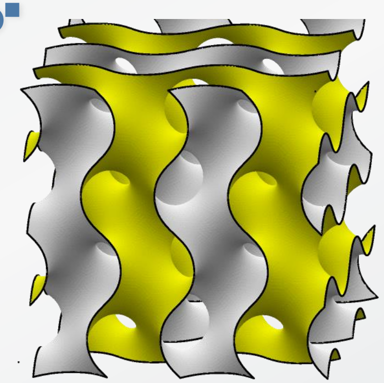
→ Unclear advantage

Gas Absorption Monolith w/ Heat Exchange



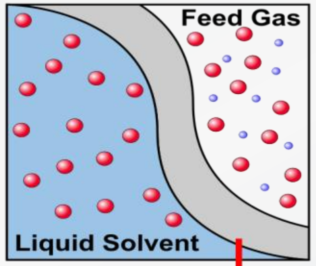
Printed Composite Sorbent

→ Unclear advantage



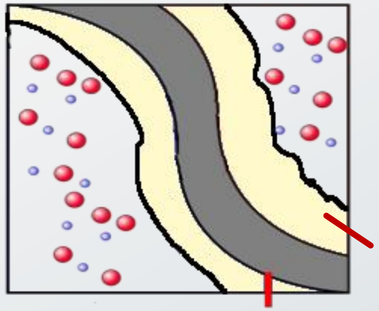
Active projects

Membrane Contactor



Permeable Membrane

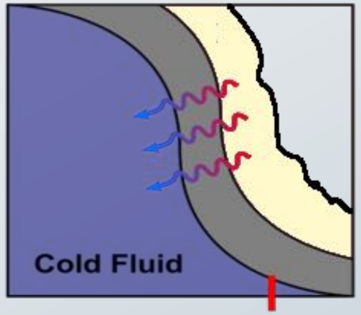
Conventional packing



solvent

Impermeable Conductive Support

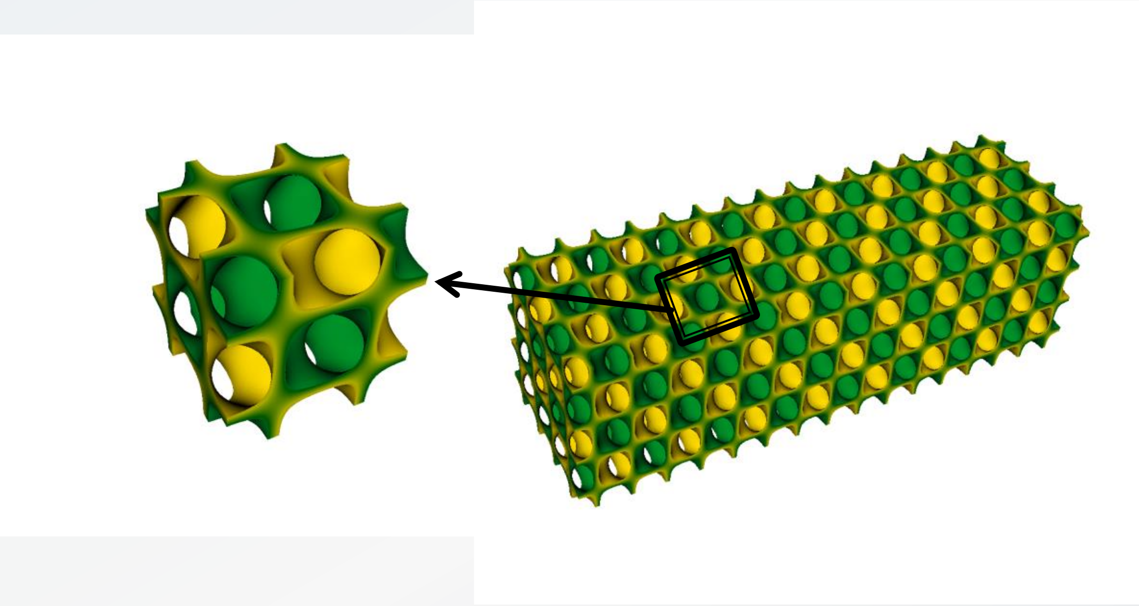
Heat exchange packing



Impermeable Conductive Support

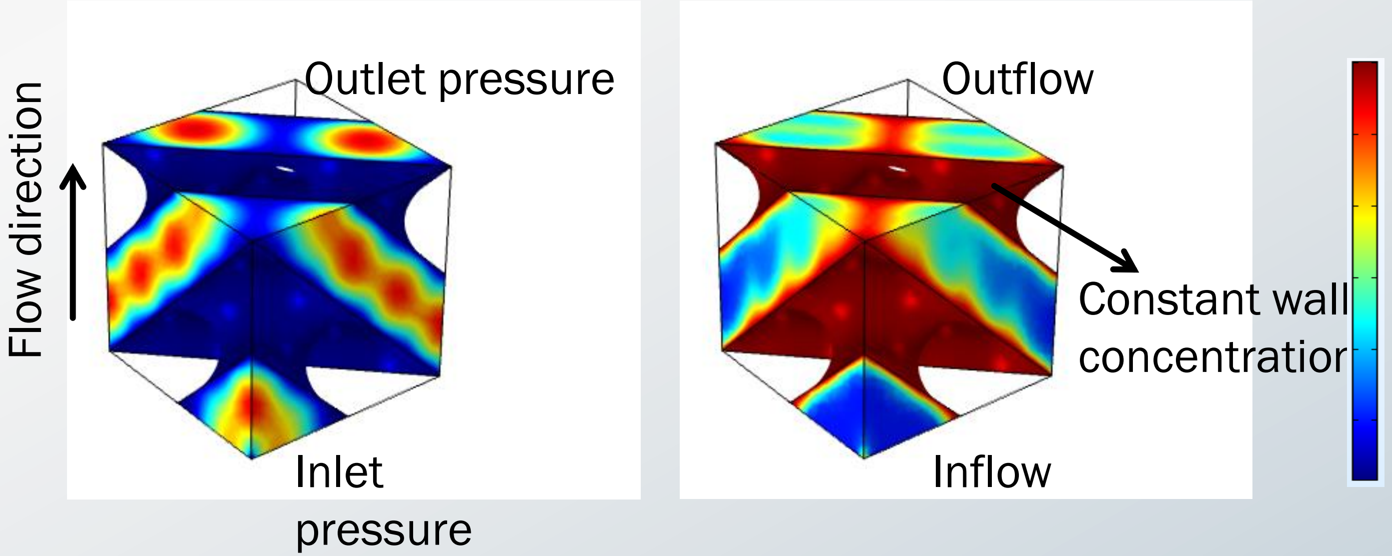
Mass transfer simulations inform TPMS reactor design

- Geometric properties
  - Void volume per unit cell
  - Surface area per unit cell
  - Hydraulic diameter
- Flow properties
  - Friction factor
- Mass transfer properties
  - Sherwood number



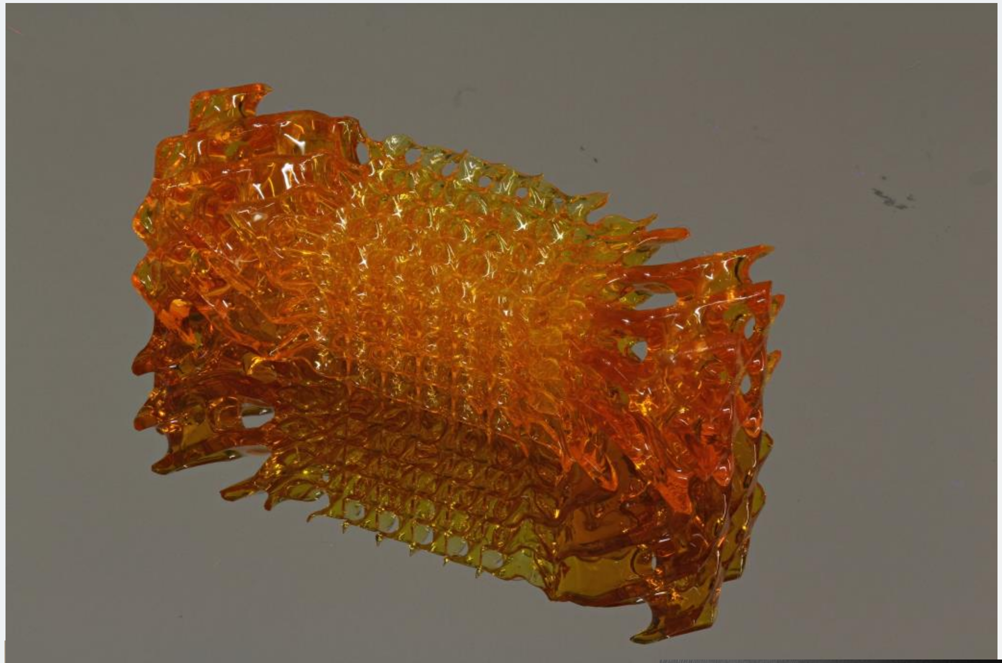
Flow simulation

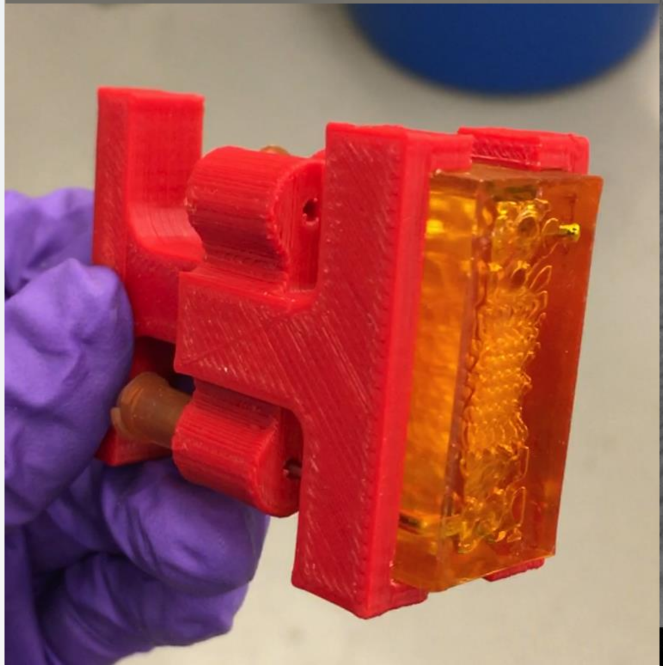
Mass transfer simulation

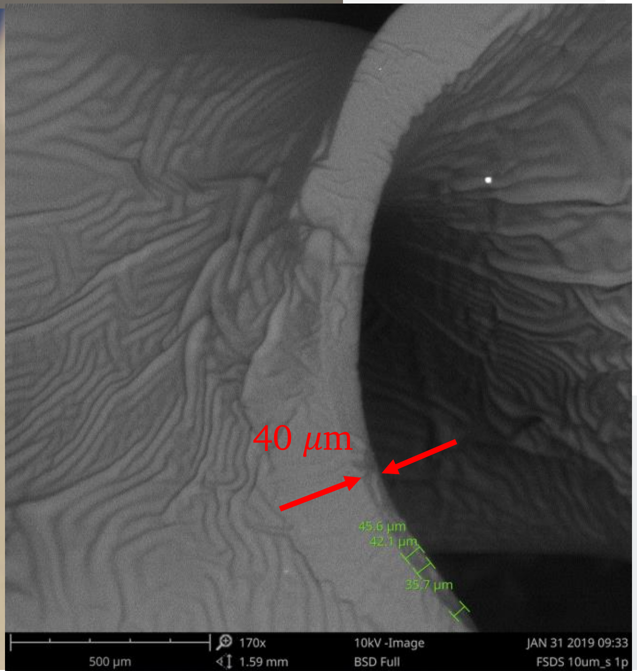


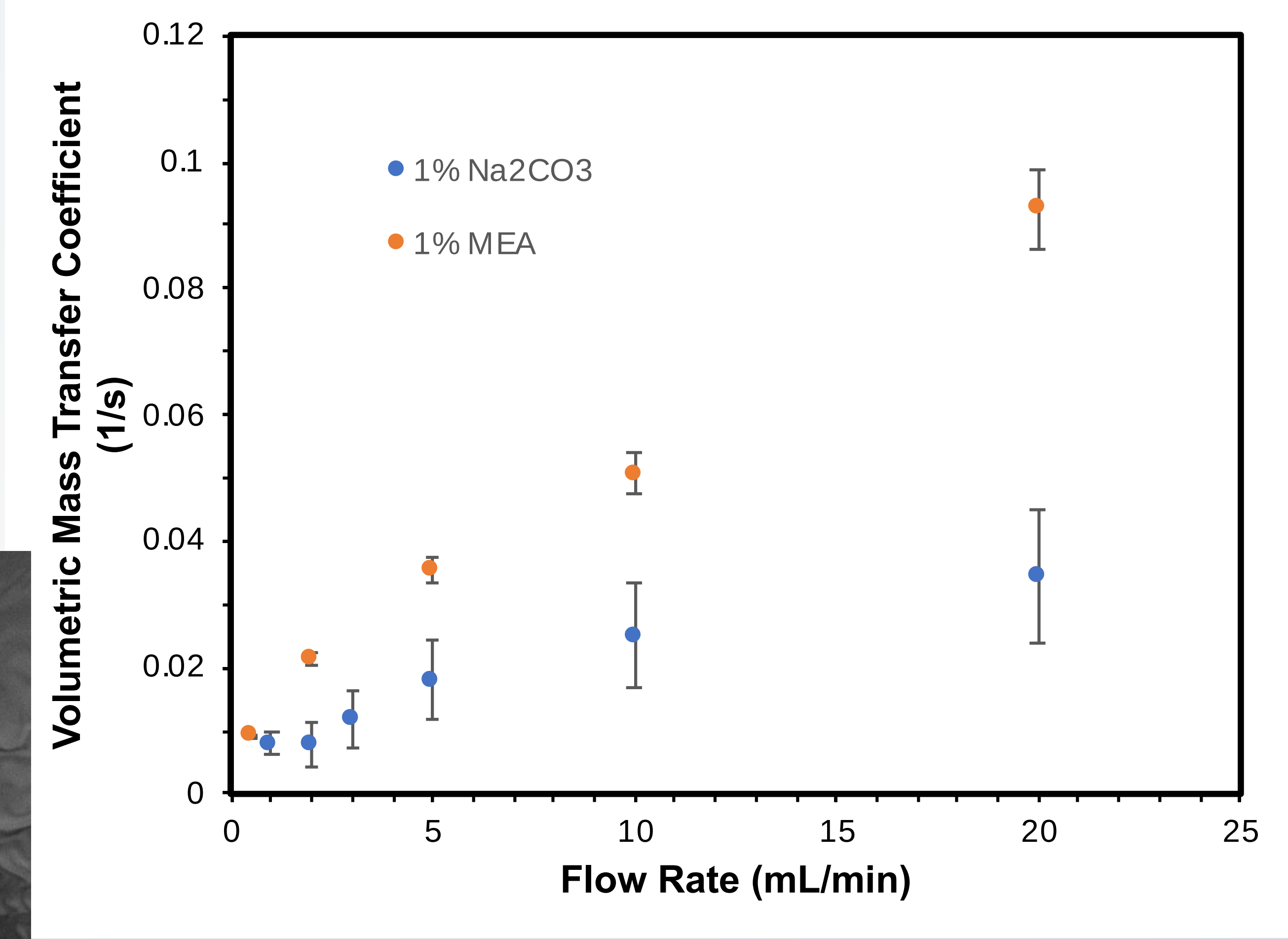
Periodic boundary conditions in all other directions

Silicone-based membrane reactors explored for intensified CO_2 absorption



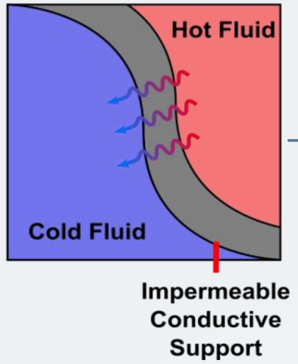






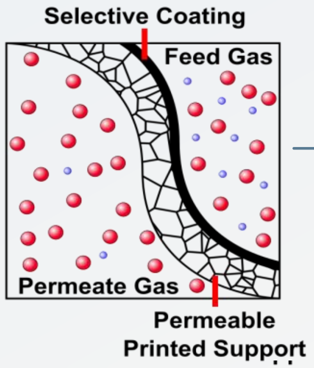
Many reactor configurations possible with TPMS and additive manufacturing.

Heat Exchange



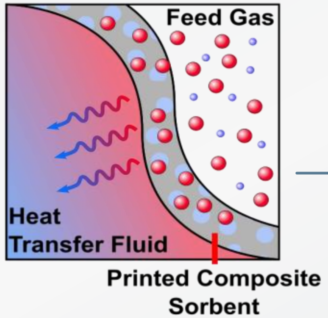
Active projects

Gas Separation Membrane

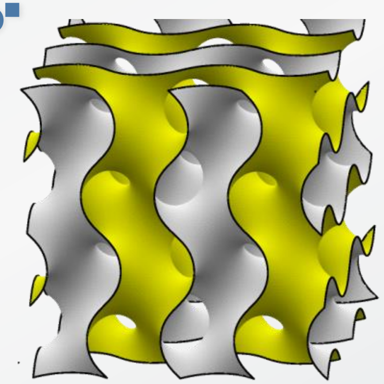


Unclear advantage

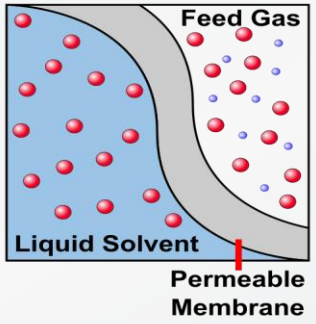
Gas Absorption Monolith w/ Heat Exchange



Unclear advantage

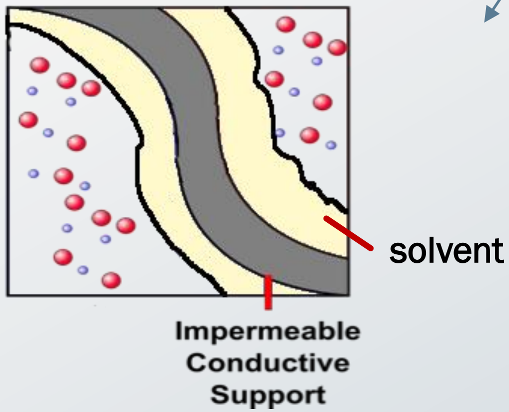


Membrane Contactor

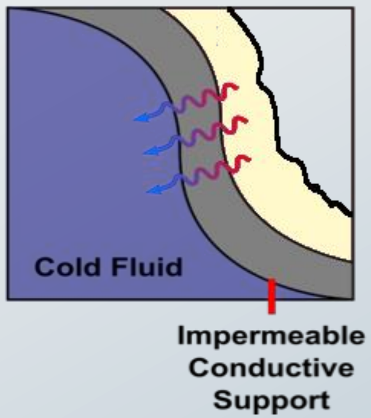


Active projects

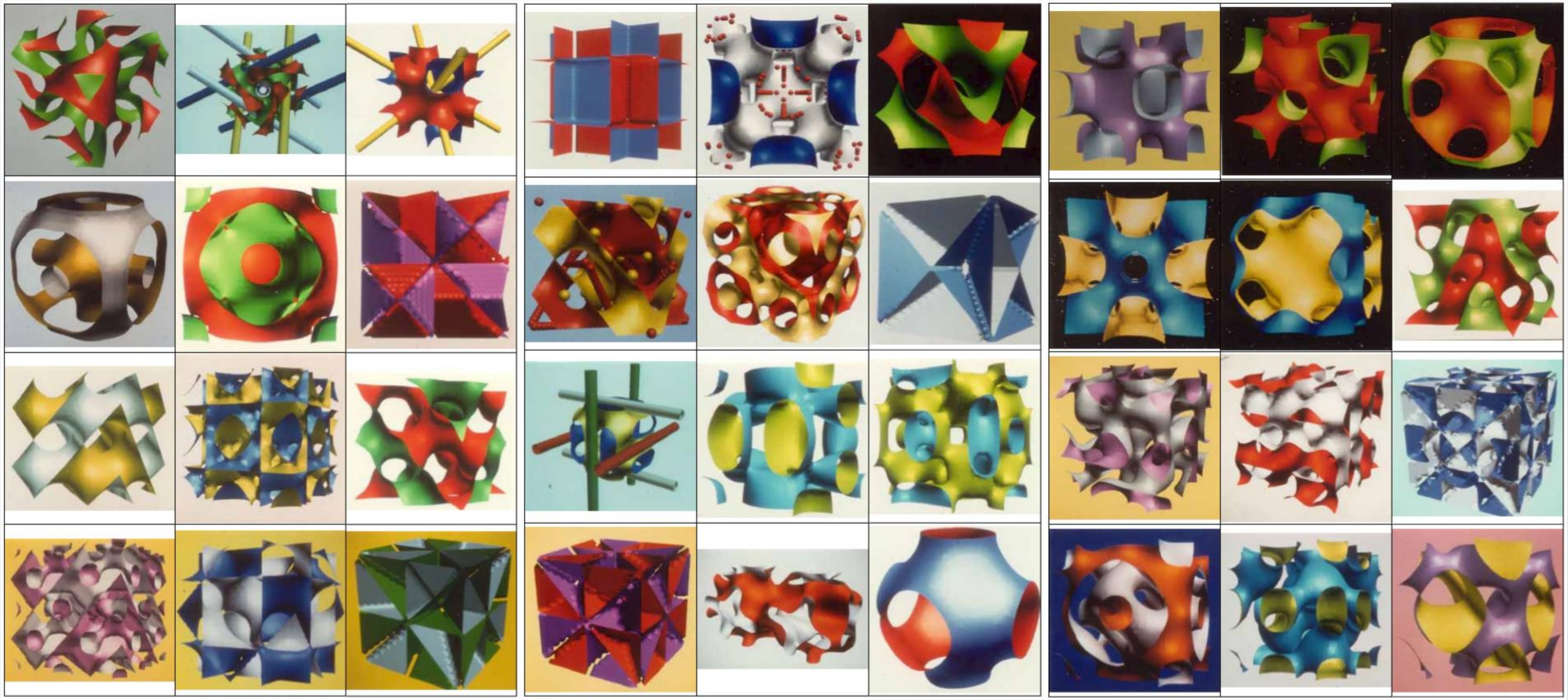
Conventional packing



Heat exchange packing

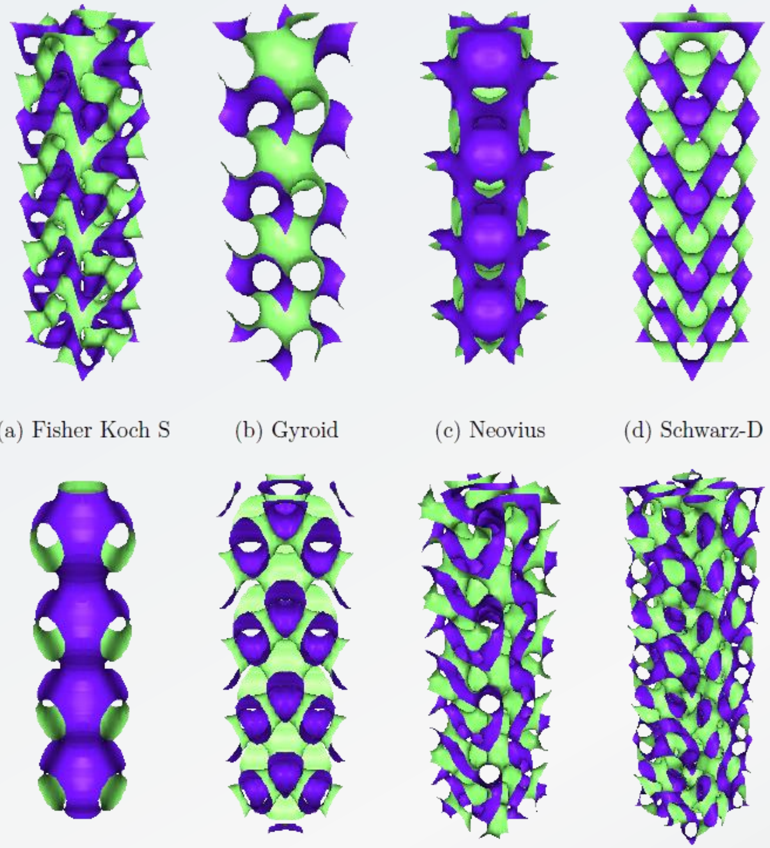


A wide range of TPMS and periodic nodal surface structures exist



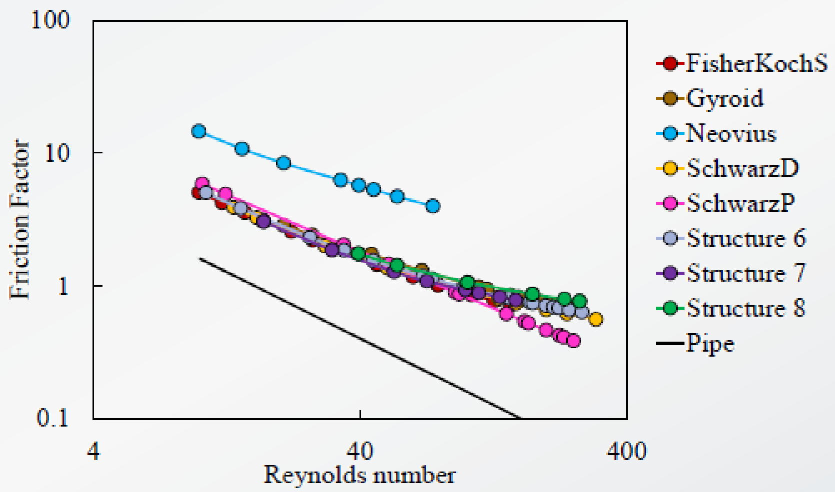
Which ones would be the best performing structures?

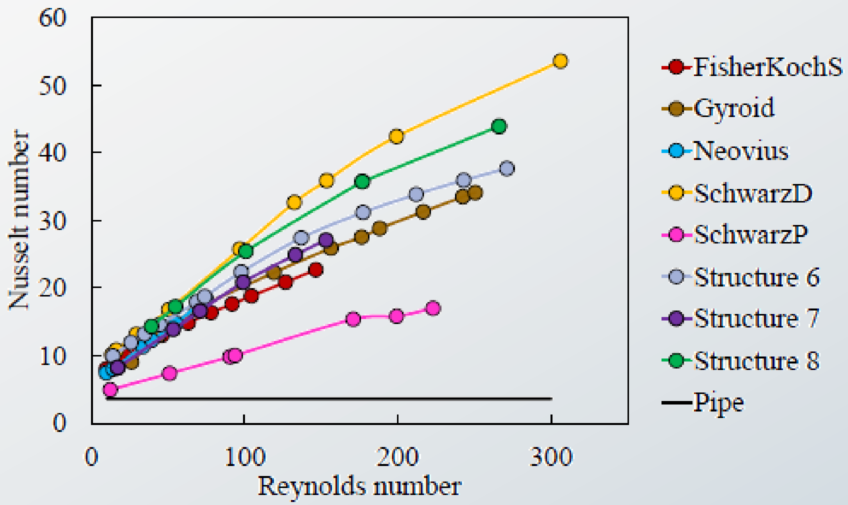
We have explored the heat transfer characteristics of a wide range of TPMS geometries



(a) Fisher Koch S (b) Gyroid (c) Neovius (d) Schwarz-D

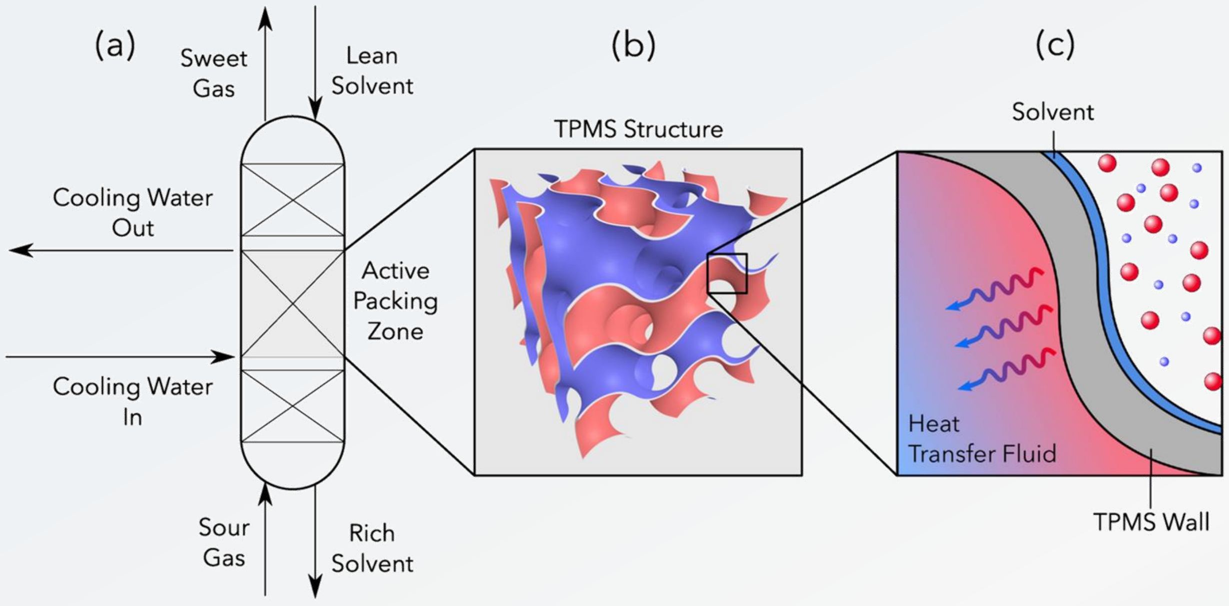
(e) Schwarz-P (f) Structure-6 (g) Structure-7 (h) Structure-8

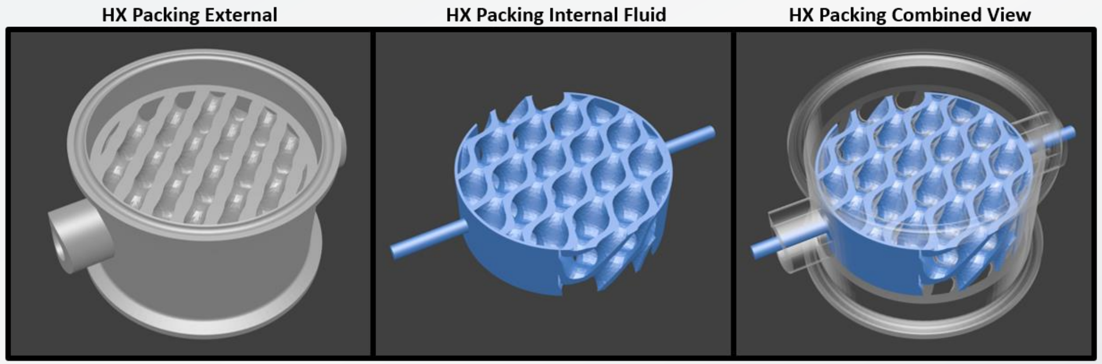


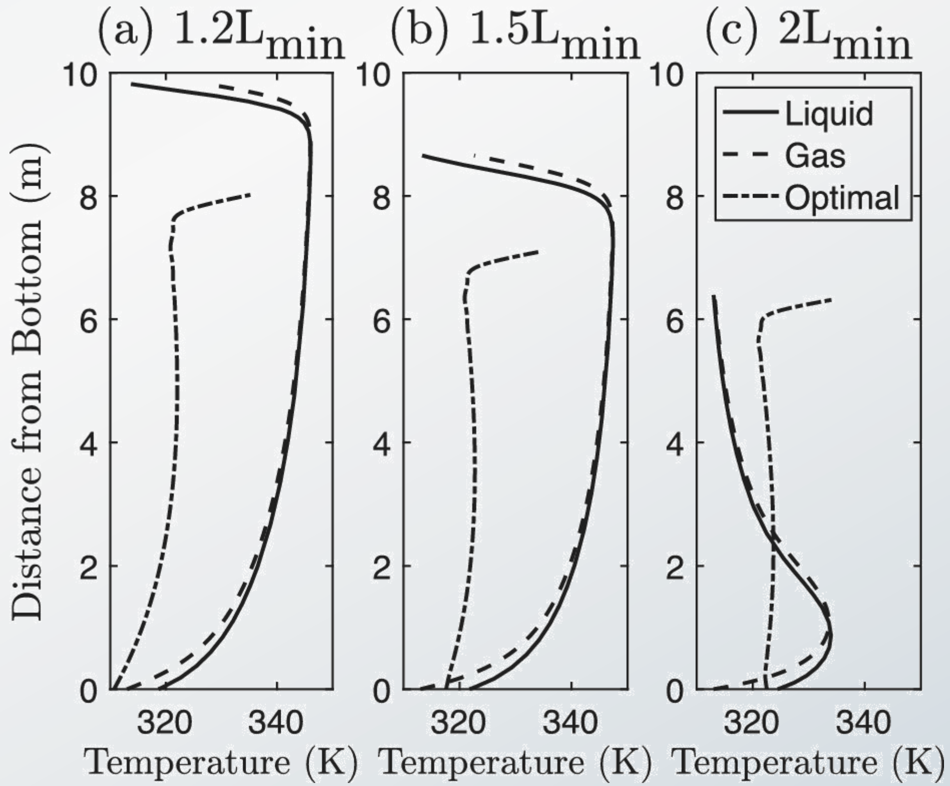


Schwarz-D has the best heat transfer performance

We have applied numerical optimization the use of absorbers with integrated heat exchange packings

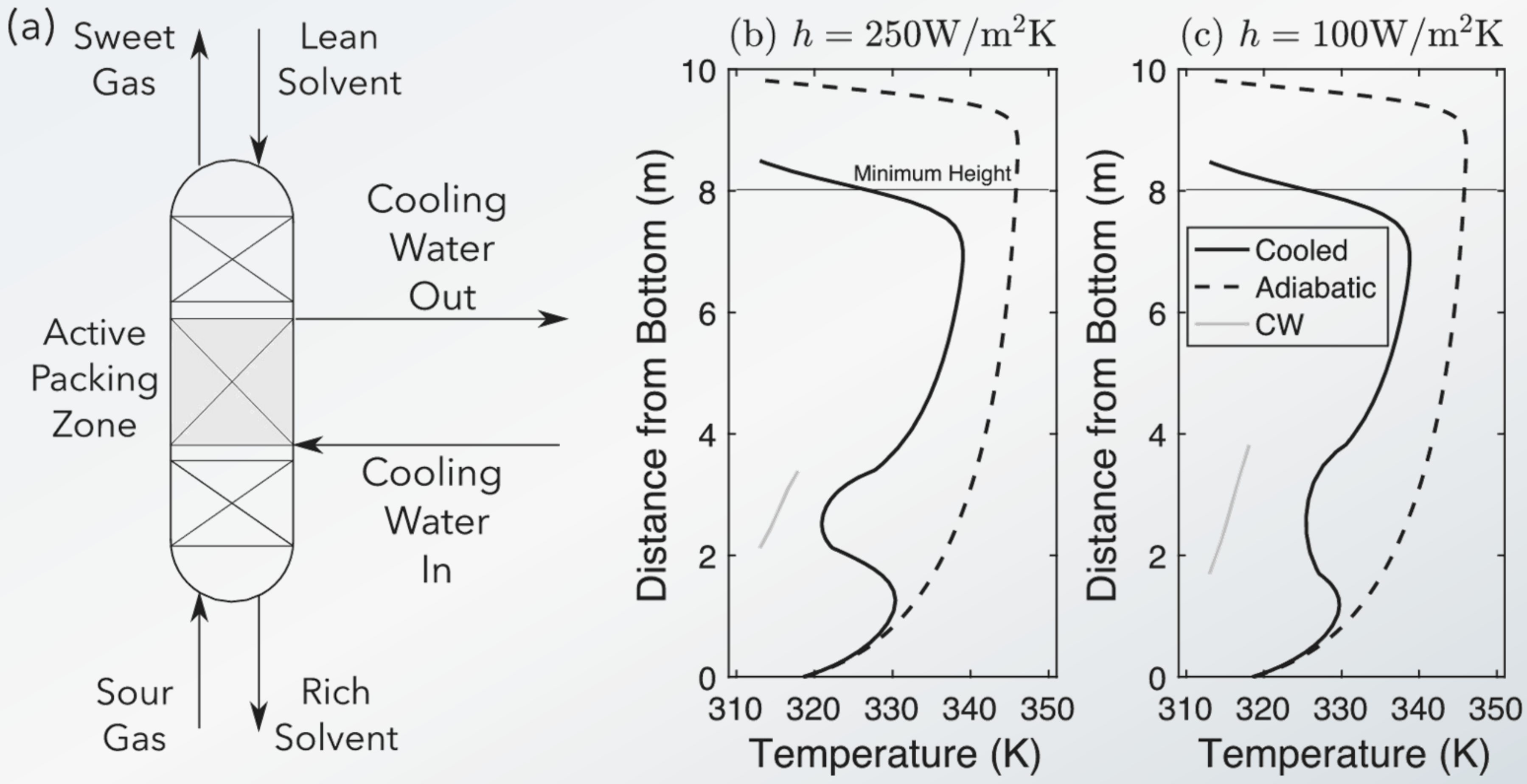






Depending on the conditions, a heat exchange packing can reduce tower height by ~80%

Intercooled sections can reach close to the numerically optimized results in a variety of configurations



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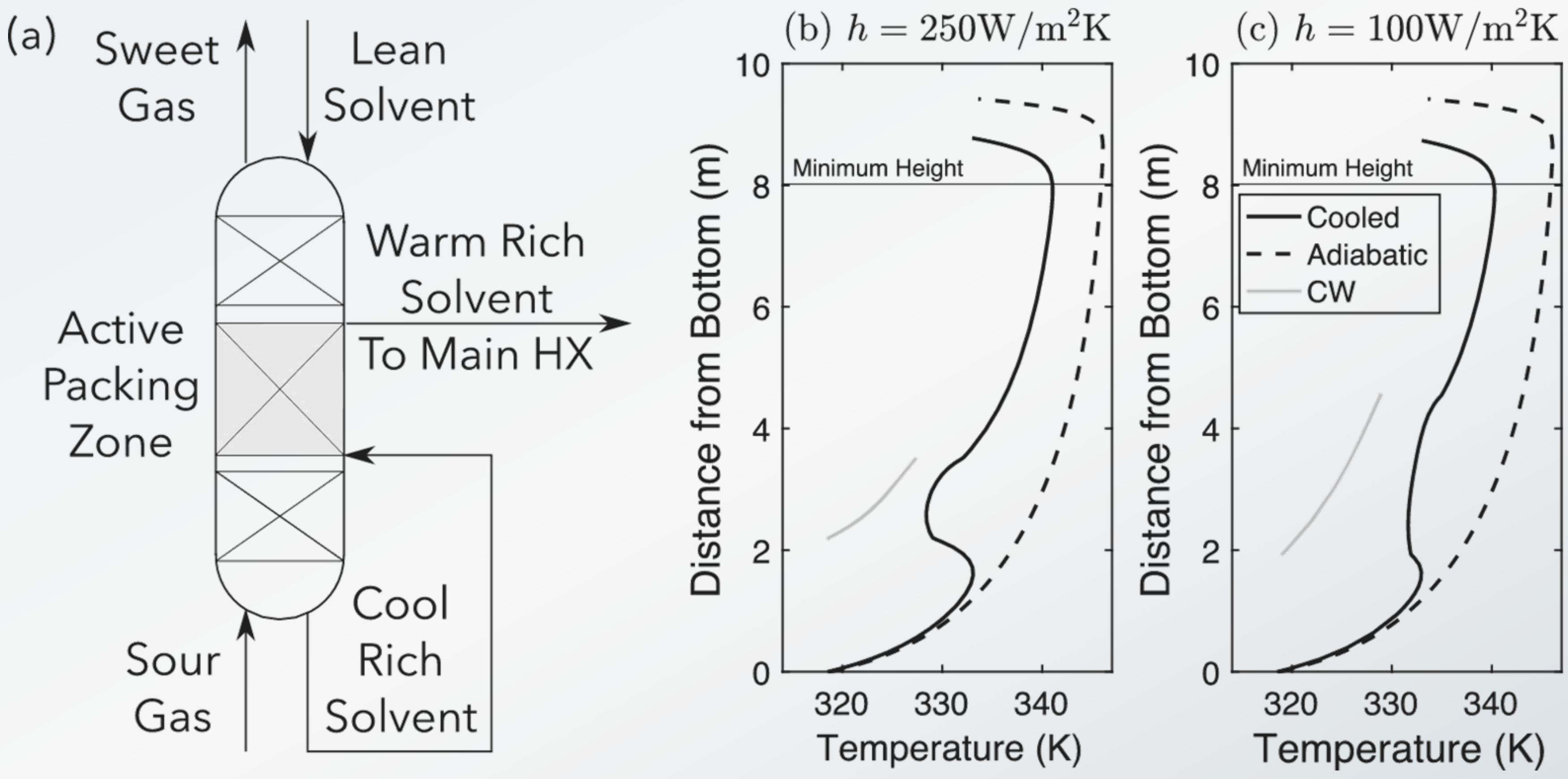

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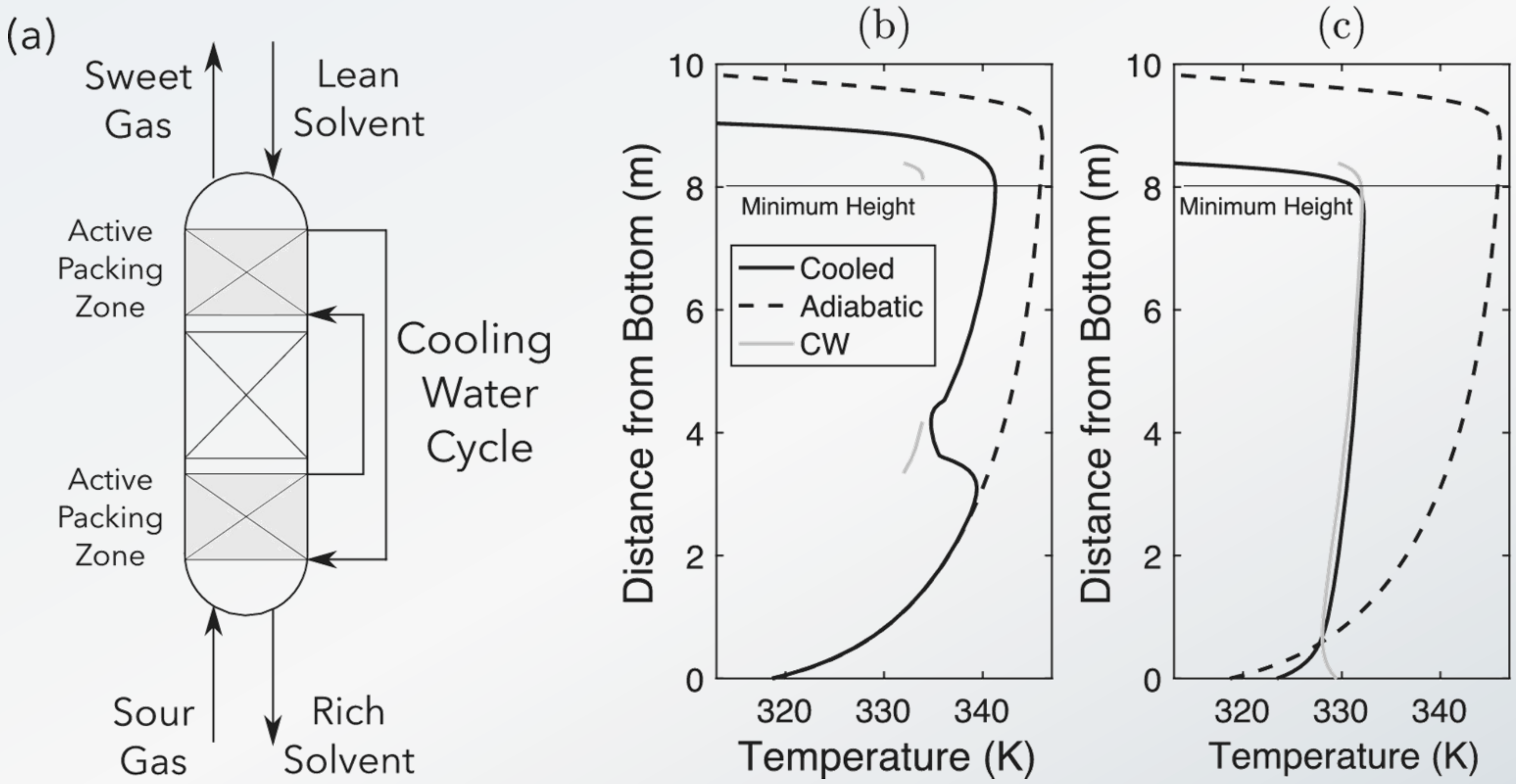
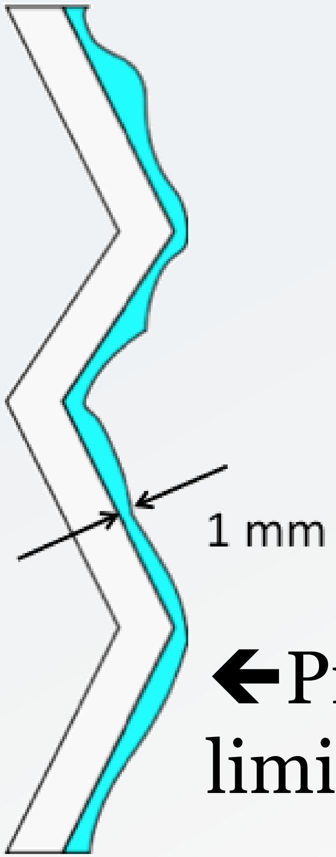


Can packed towers be improved?



Raschig rings:
"Since 1894"

Structured packing:
"A little better"

🡐Process intensification limited by film thickness

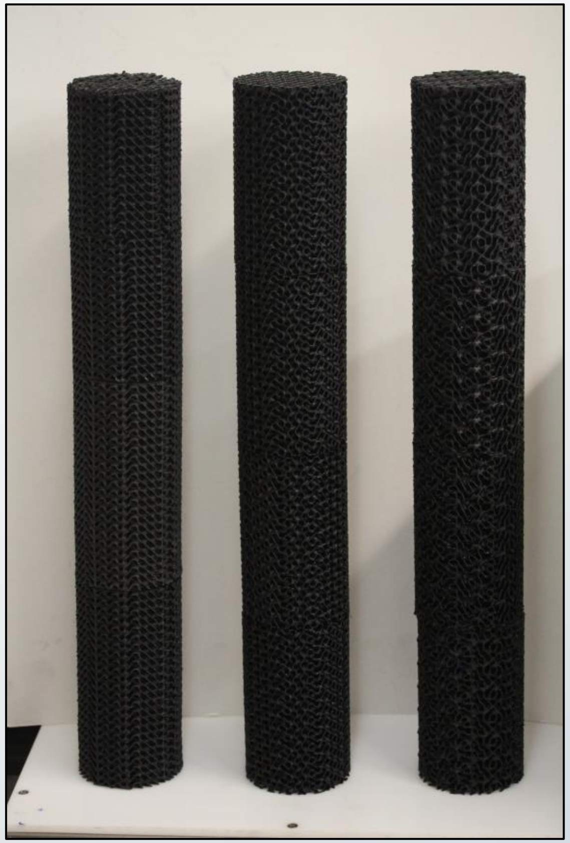
… and fabrication technology?

3D-printed packings can improve on conventional packings in four ways:

1. Improved flow distribution
2. Integrated heat exchange
3. Enhanced mixing

Several TPMS geometries were successfully 3D-printed for use as structured packings

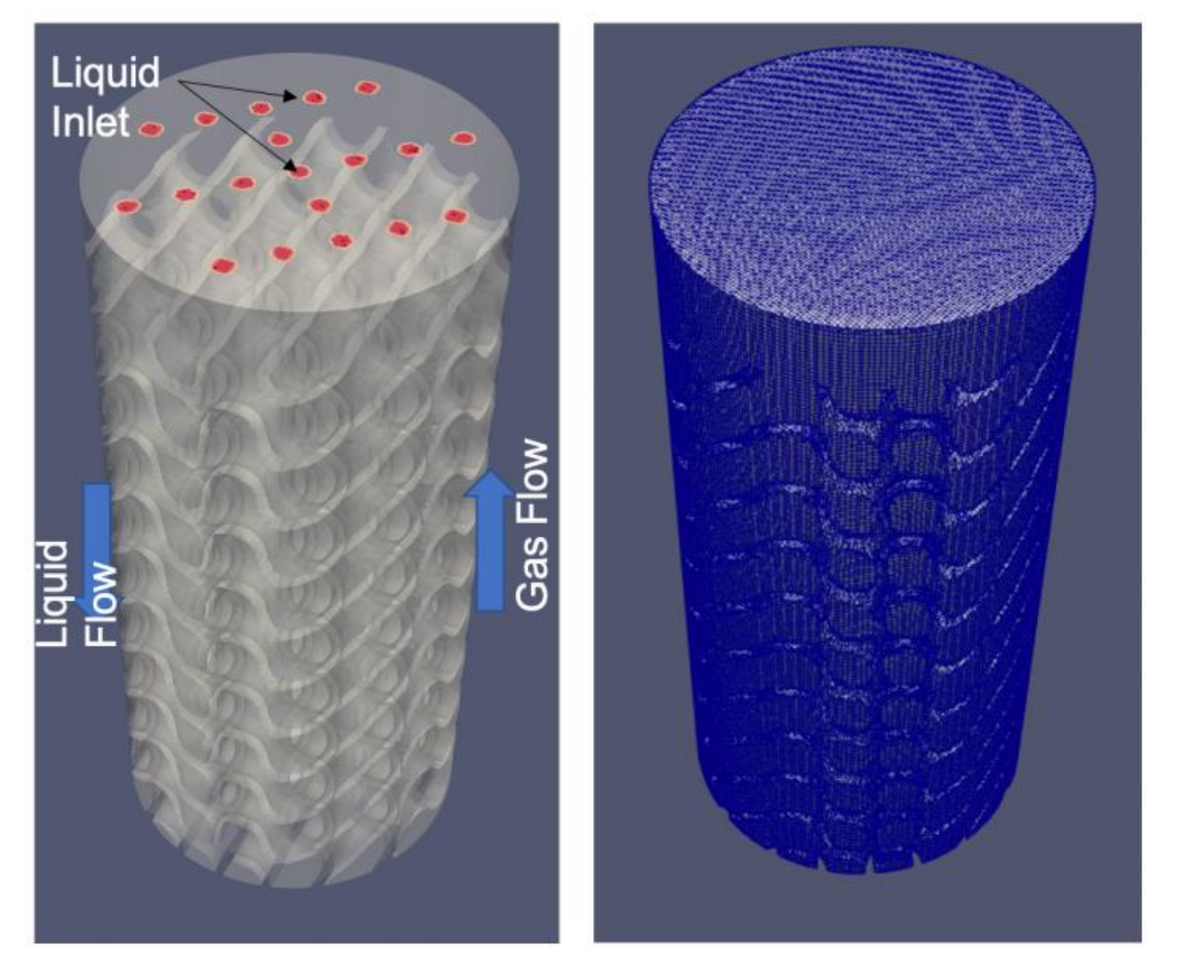
Stereolithography



Fused Deposition Modeling

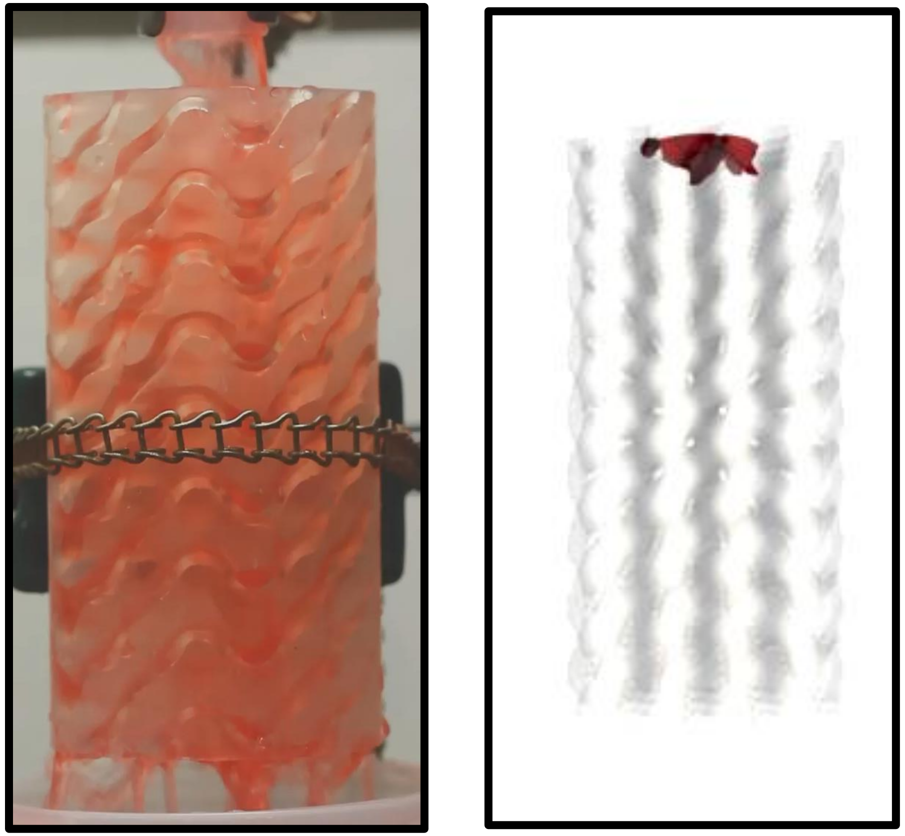
CFD was used to model the performance of the TPMS structured packings

Boundary	Velocity BC	Concentration BC
Liquid inlet	Uniform velocity	Uniform concentration
Liquid outlet	Pressure outlet	Zero gradient
Gas inlet	Fixed pressure	Uniform concentration
Walls	No slip with contact angle	Zero gradient



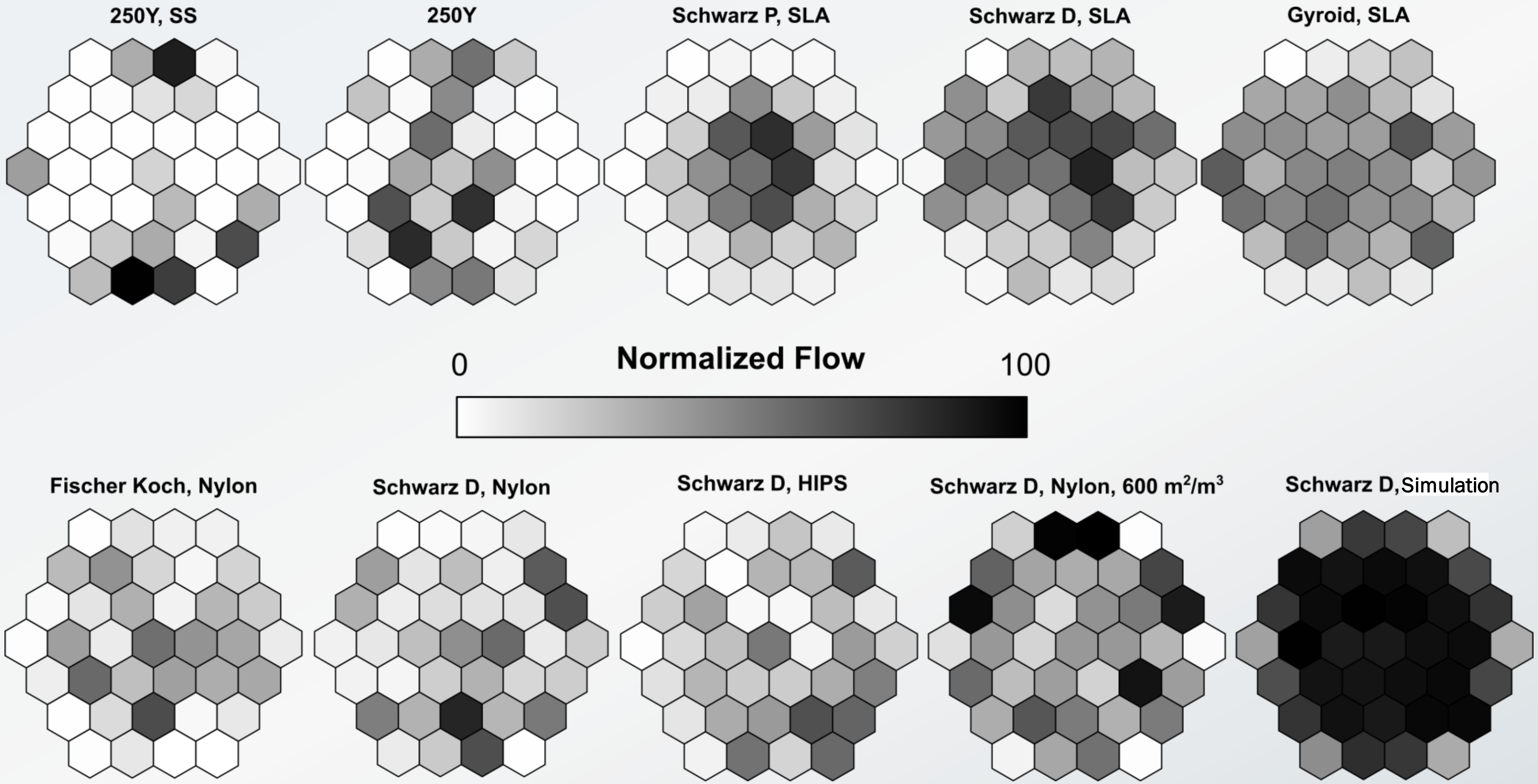
TPMS packings improve liquid distributions and have been computationally simulated

250Y



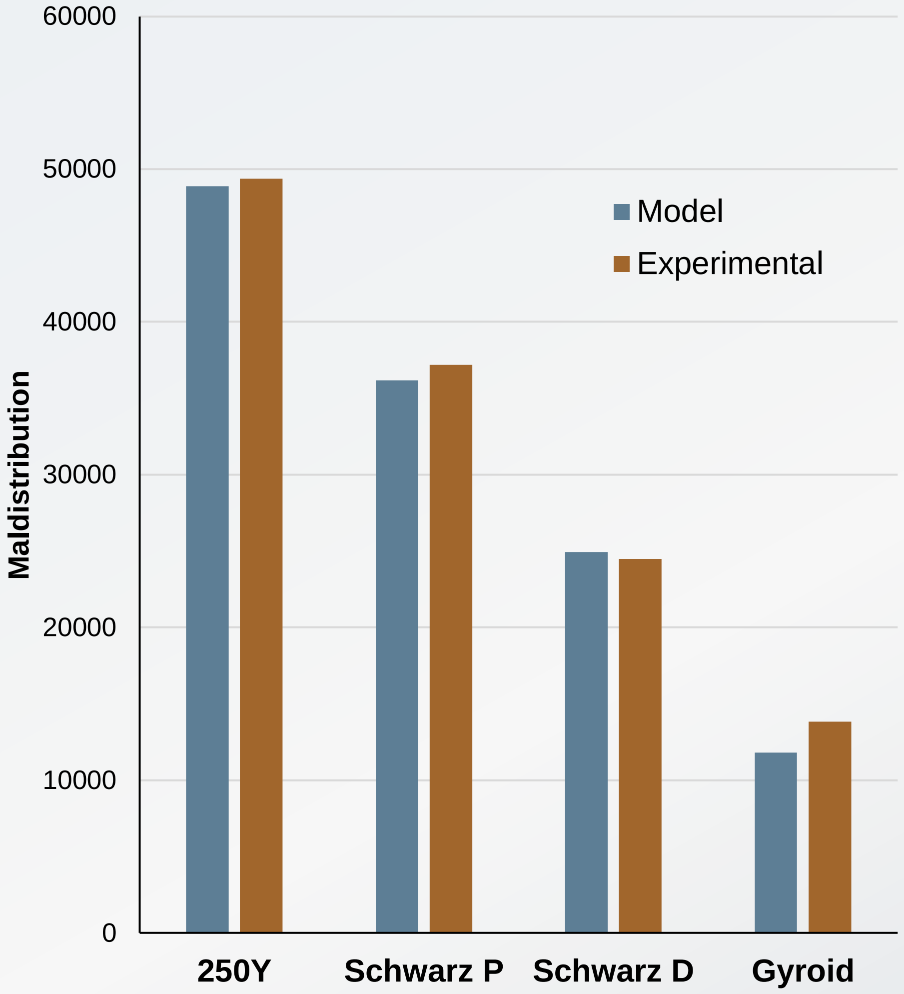
Schwarz D

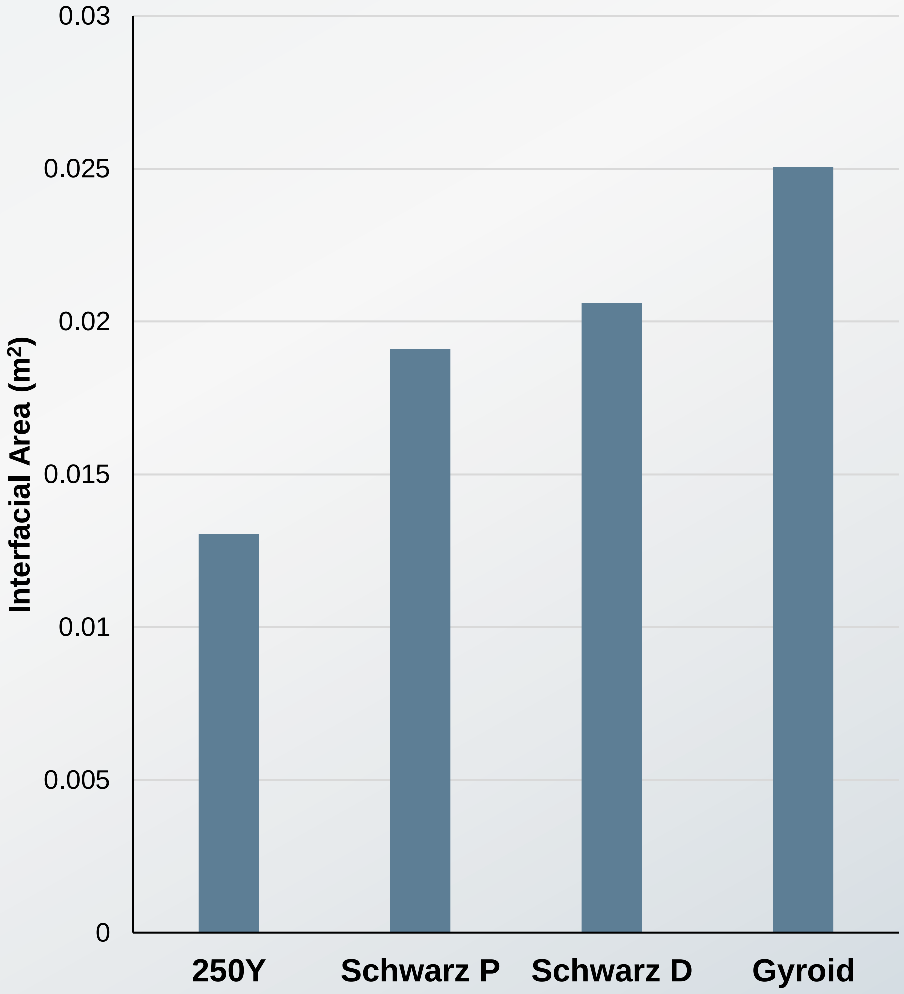
TPMS packings improve liquid distributions



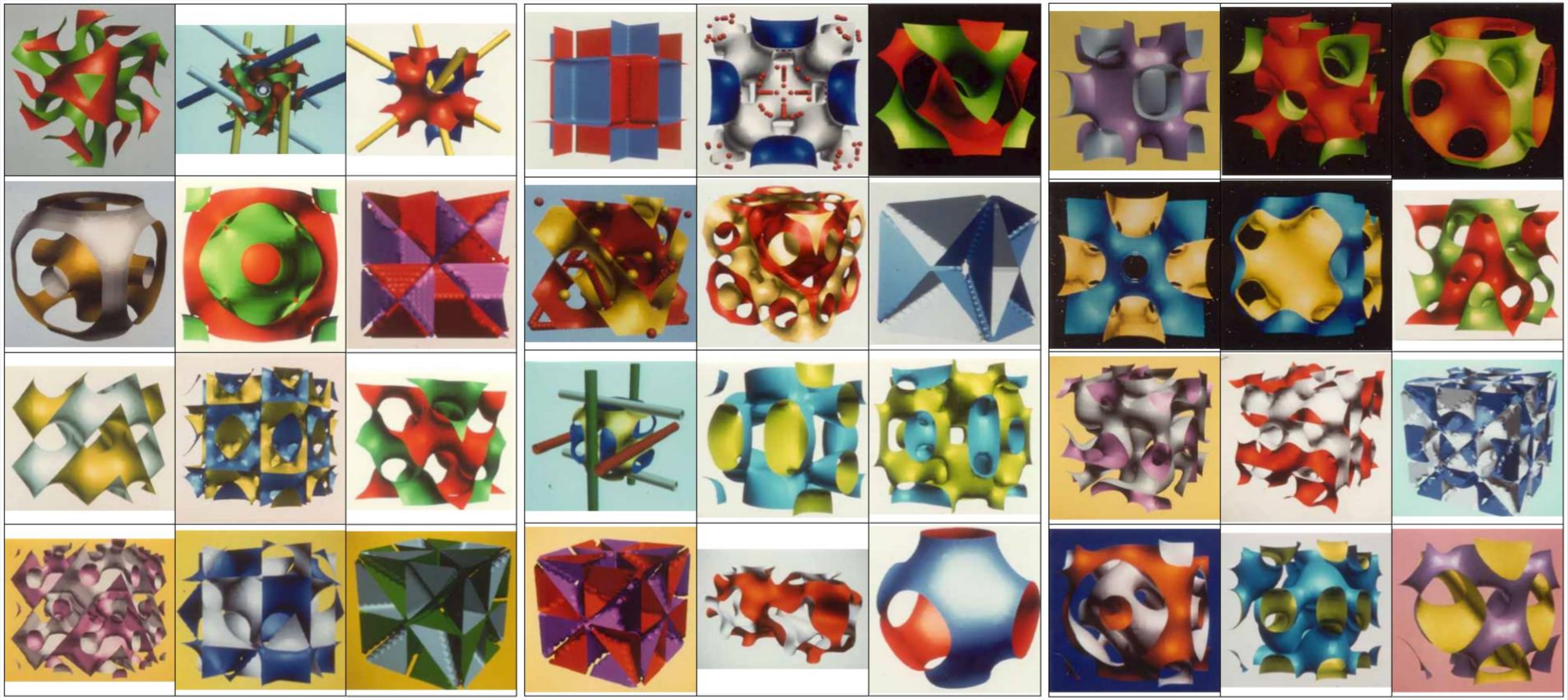
All TPMS geometries show improvements, but some are better than others

TPMS packings are predicted to have better liquid distributions and liquid-gas interfacial area

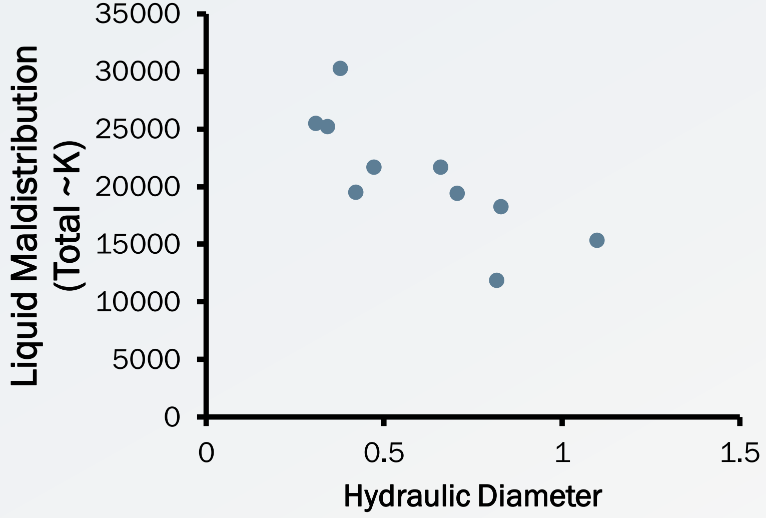


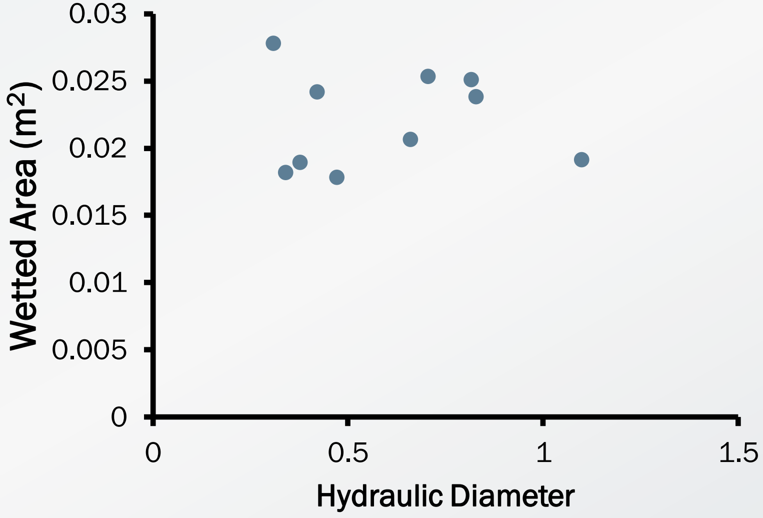


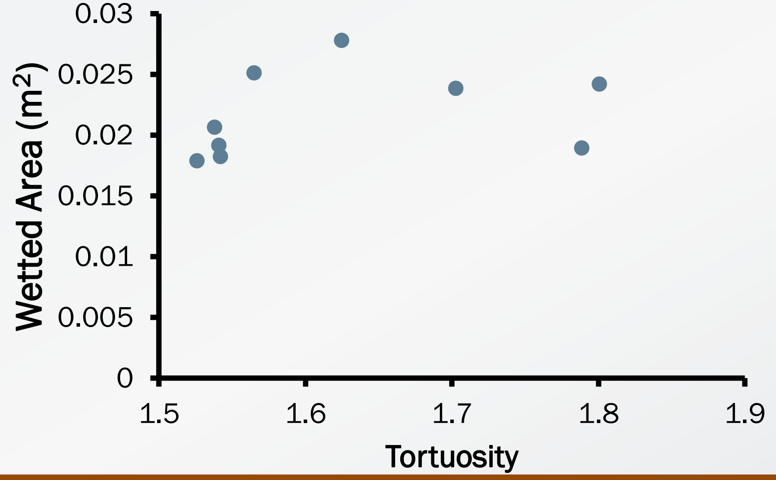
Amgad, M.; Itoh, A.; Tsui, M. M. K. Extending Ripley's K-Function to Quantify Aggregation in 2-D Grayscale Images. *PLoS ONE* **2015**, *10* (12), e0144404. https://doi.org/10.1371/journal.pone.0144404.

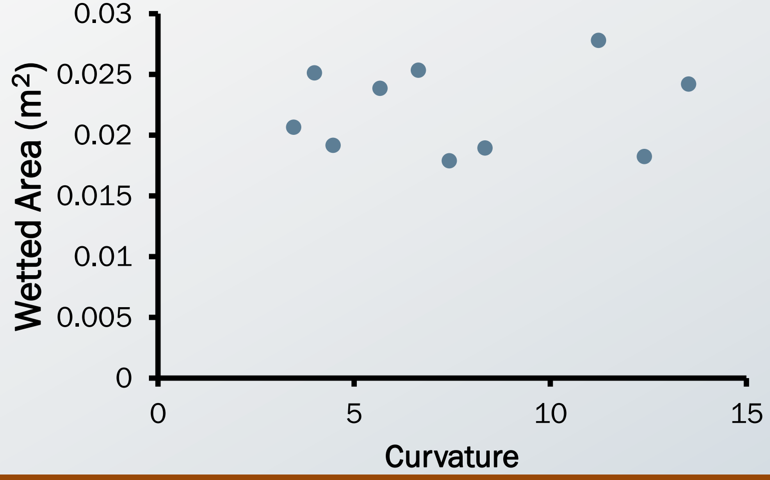


Correlations between performance and geometric parameters are difficult to identify





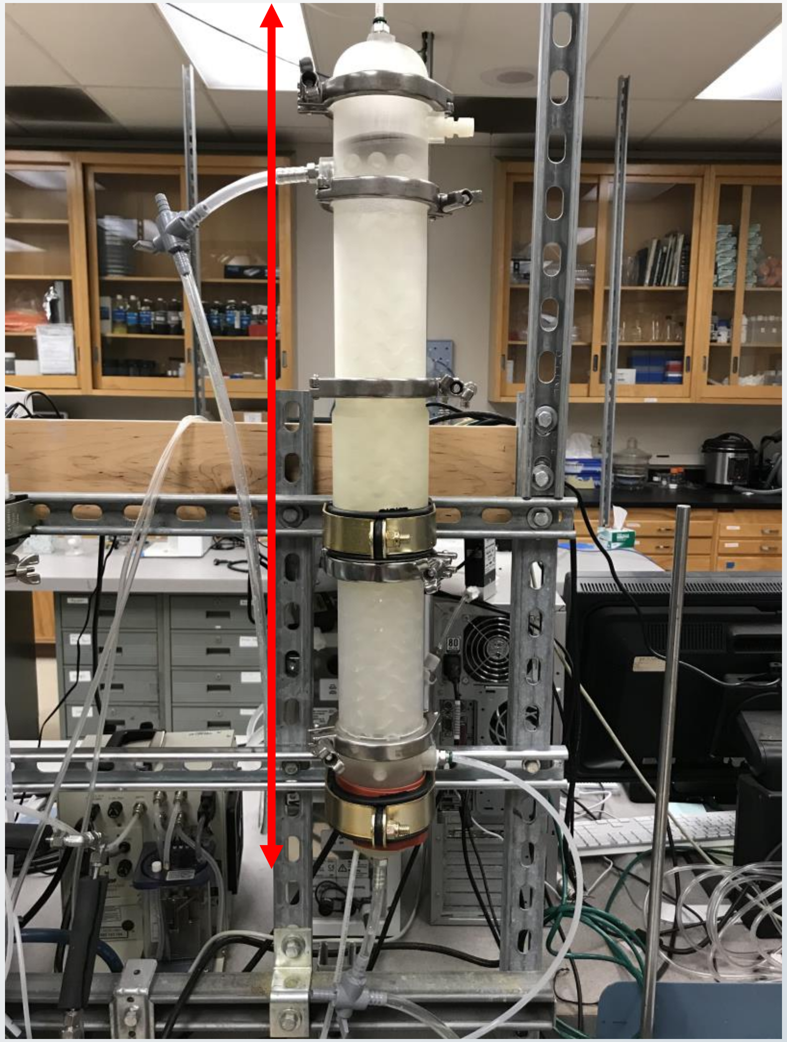




TPMS geometries with larger unit-cell hydraulic diameters have better liquid distributions

Kg-scale testing and kg-scale production now solved

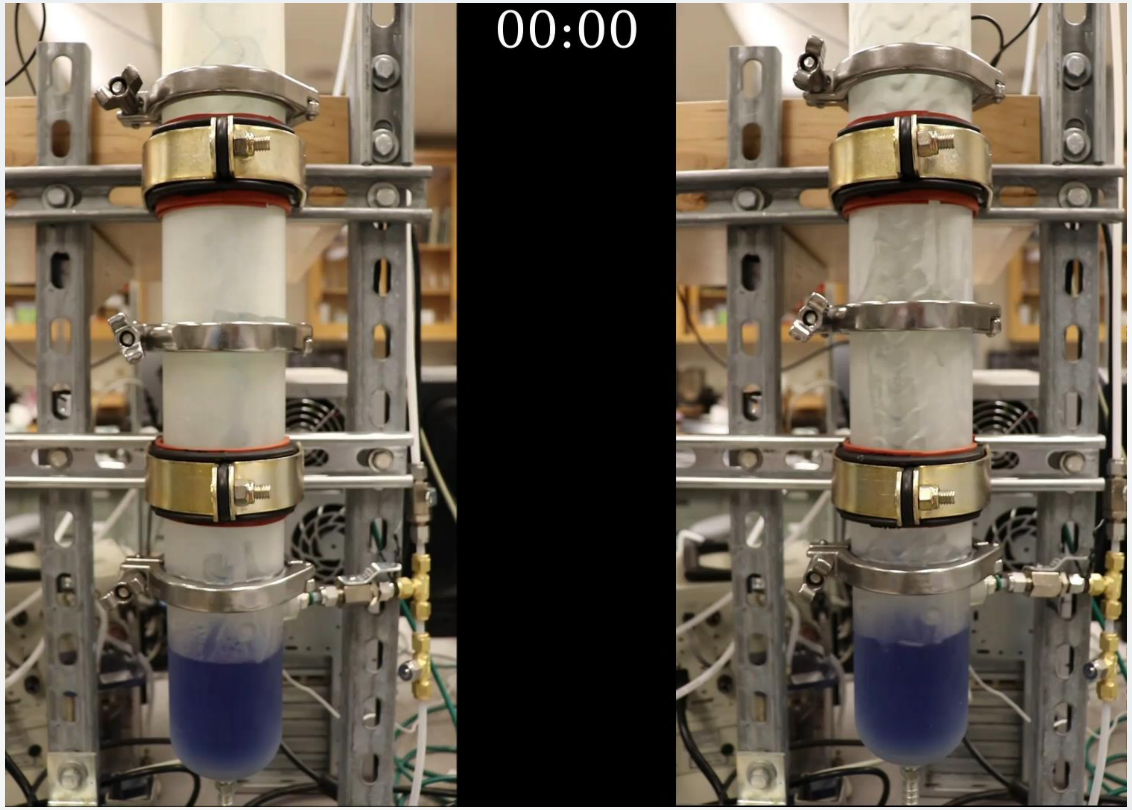
Gemini apparatus for sorbent testing

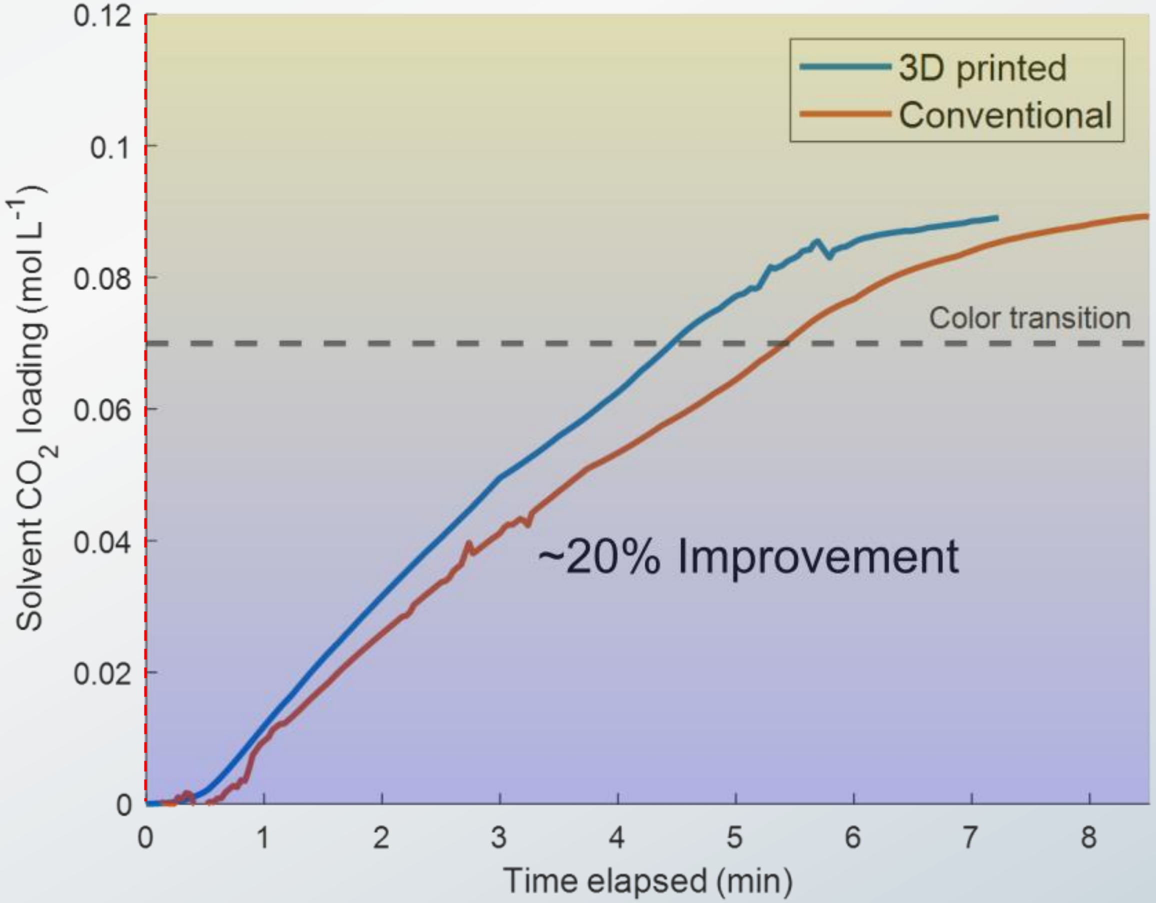


Proteus apparatus for solvent systems

3D printed structured packings enable performance enhancements over conventional packings for CO_2 capture

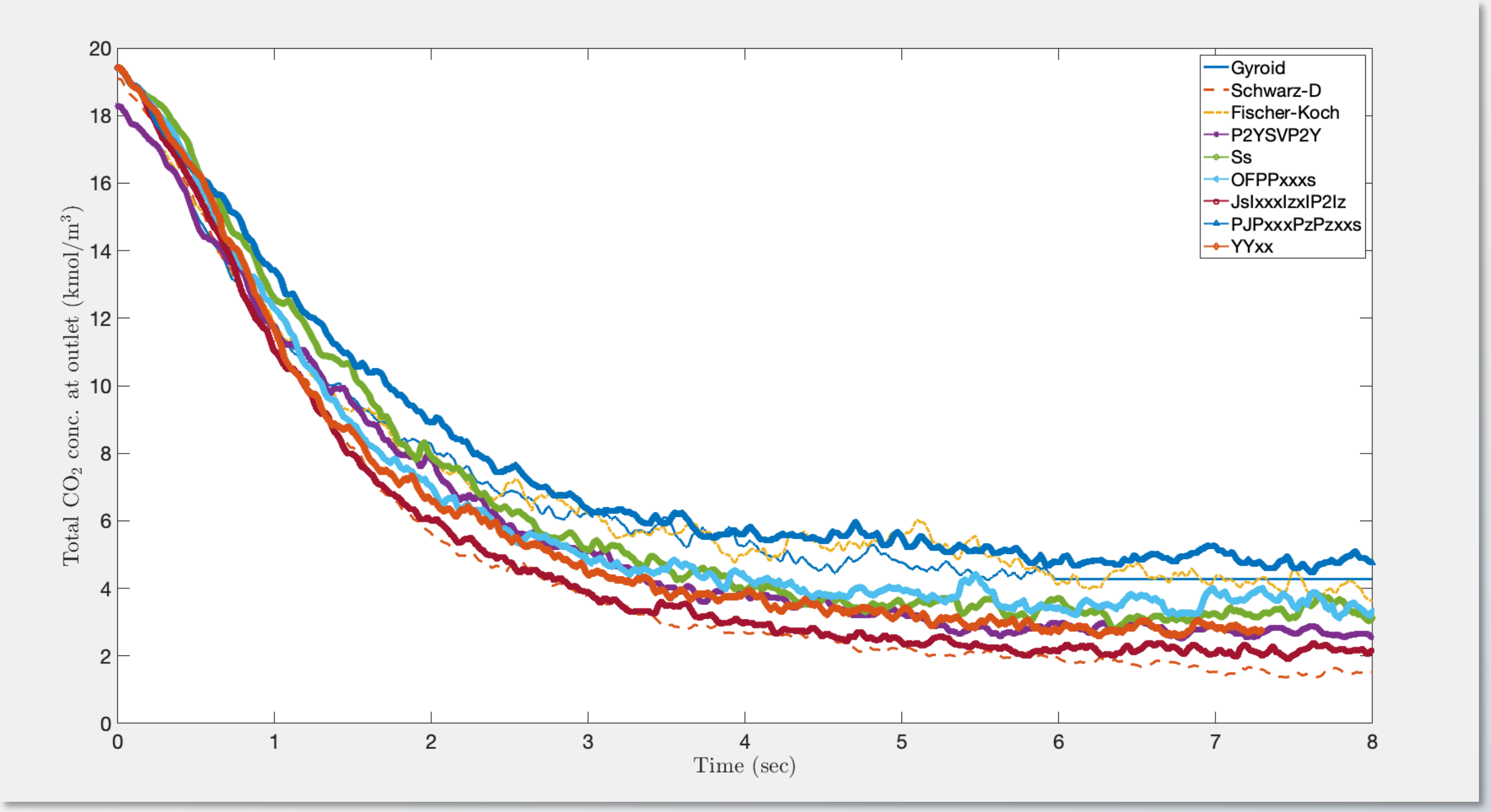
Conventional Packing **3D Printed Packing**





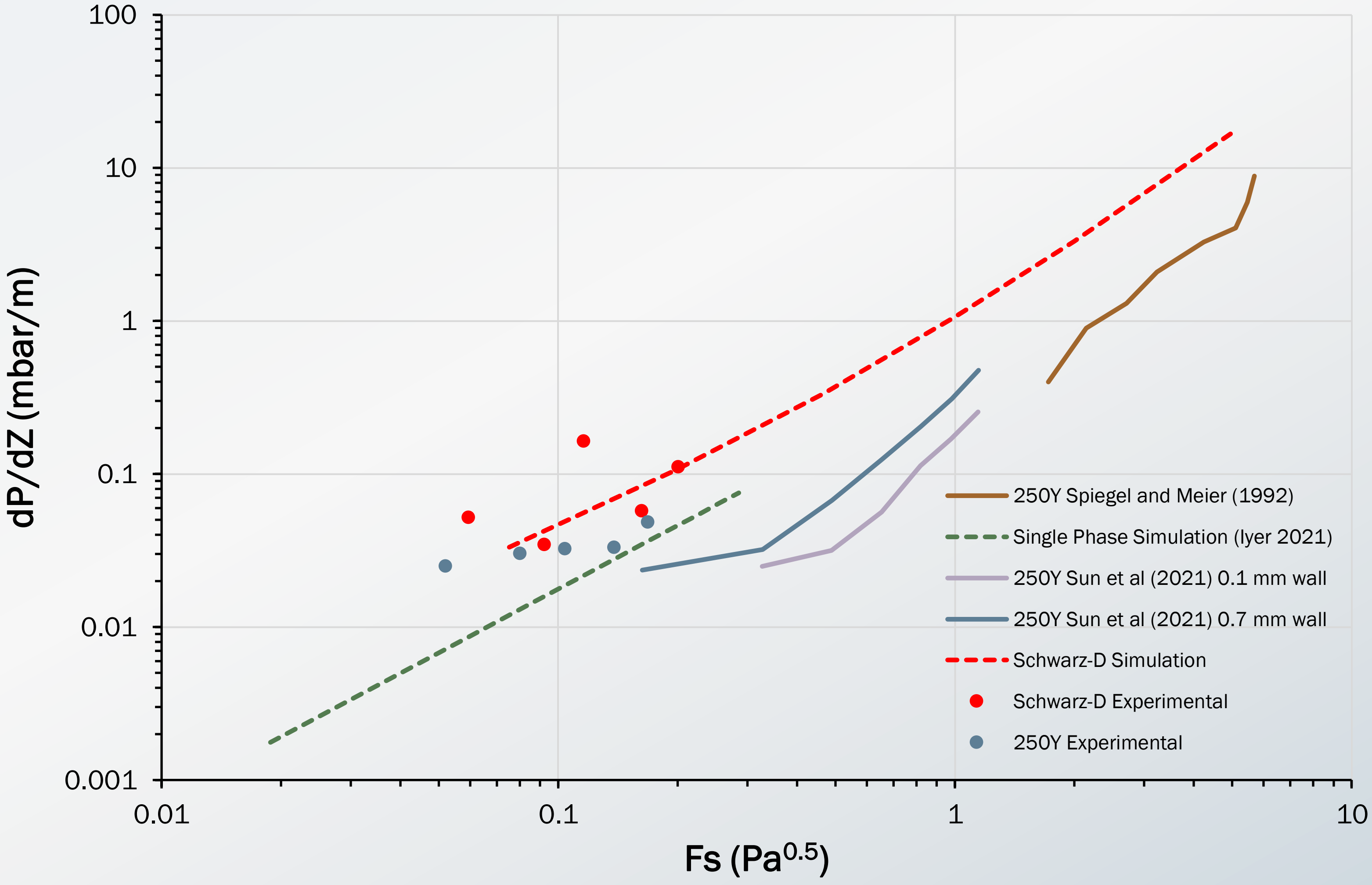
Simulation results predict the Schwarz D geometry to have the best mass transfer rates

- Framework for two-phase mass transport simulations was achieved
  - Capable of both first- and second-order reactions
- Schwarz D, $J_sI_{xxx}I_{zx}IP_2IZ$, and P_2YSVP_2Y structures are the best performing TPMS geometries
- Relative performance matches with experimental results for Schwarz D, Gyroid, and 250Y



Pressure drops are expected to be higher with TPMS geometries

- Schwarz-D structure have higher predicted pressure drops than 250Y
  - Current wall thicknesses are 1 mm, which may also result in increased
- Current experiments match with modeled results



Conclusions

- TPMS membrane reactors showed promise, but the fabrication process was limited by scalability
- TPMS geometries exhibit high thermal transport properties
  - Within a wide range of geometries, the Schwarz-D structure demonstrated the best performance
- An optimization framework was made for structured packings with integrated heat exchange
- TPMS structured packings exhibited improved liquid distributions and improved performance

Project Team

Lawrence Livermore National Laboratory

Du Nguyen, Nathan Ellebracht, Pratanu Roy, Jaisree Iyer, Julie Mancini, Simon Pang, Thomas Moore, Siwei Liang, Samantha Ruelas, Matthew Worthington, William Smith, Joshuah K. Stolaroff

Acknowledgements

CCSI2 Carbon Capture Simulation for Industry Impact

Grigorios Panagakos
Mike Matuszewski

NETL National Energy Technology Laboratory

Andy Aurelio
Mariah Richardson
Lynn Brickett

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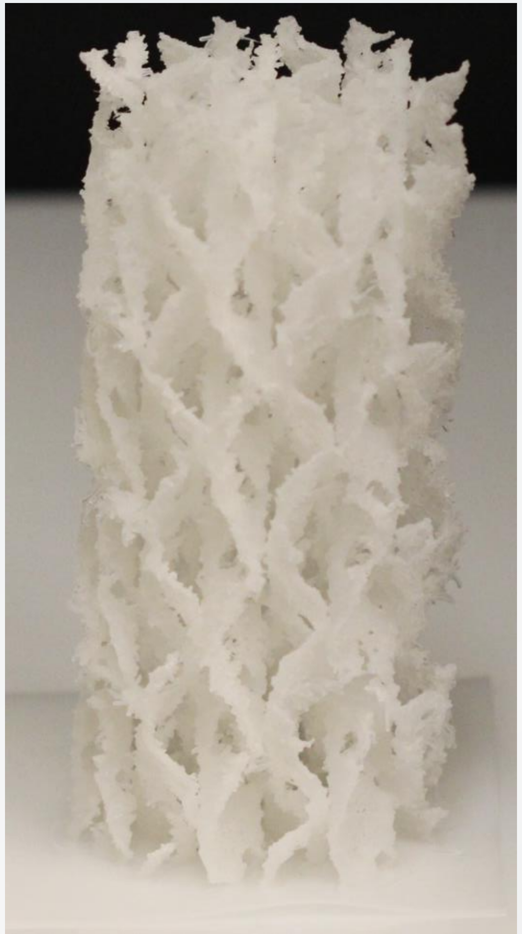
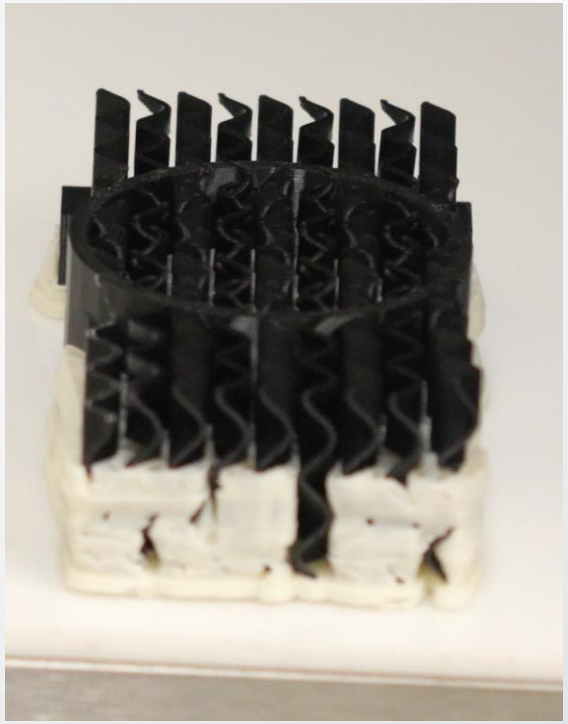
Prints in multiple materials have been demonstrated

ABS



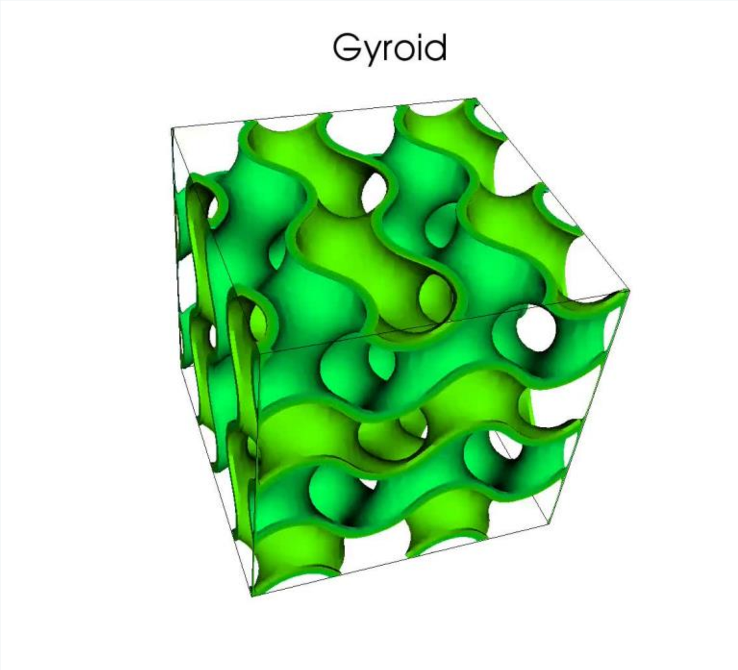
High-Density
Polyethylene

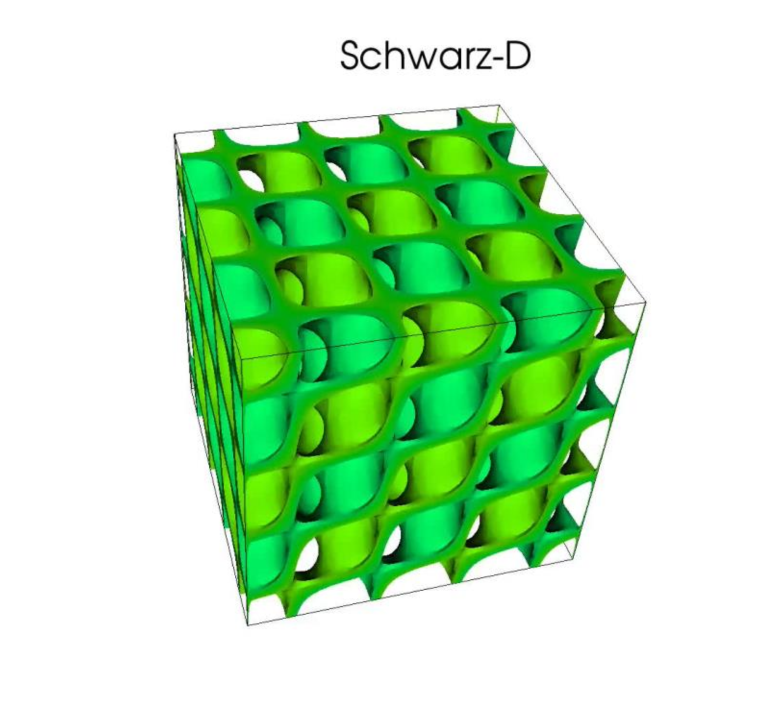
Polycarbonate



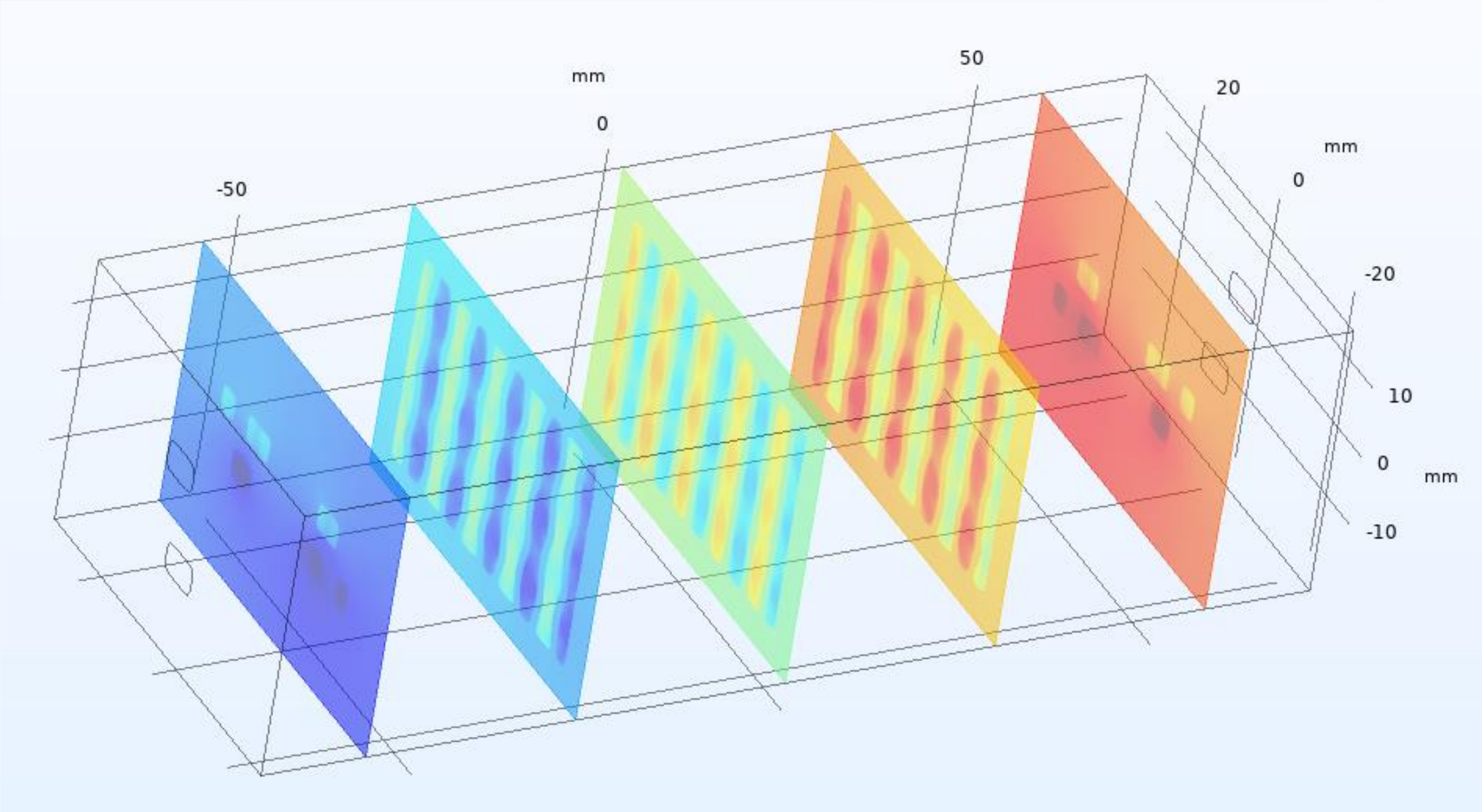
ABS

TPMS geometries enhance fluid mixing





Temperature in Cold Fluid in Countercurrent Heat Exchanger



Other design motifs can be added to a TPMS structured packing for improved performance or alternative applications