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

NETL Carbon Management and Oil and Gas Research Project Review Meeting
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Carbon capture, utilization, and storage technologies are driven by a need to improve efficiency.
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

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<th>Theoretical Assessment</th>
<th>Year 1</th>
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<th>Fabrication Assessment</th>
<th>Year 1</th>
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<td>▲ Proof of concept reactor</td>
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<th>Generation 1 Reactor</th>
<th>Year 1</th>
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<td>Design→</td>
<td>▲ 1st-gen design</td>
<td>Prototype demo→</td>
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<td>Design→</td>
<td>Bench-scale test</td>
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- 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**

- Active projects

**Membrane Contactor**

- Liquid Solvent
- Permeable Membrane
- Feed Gas
- Active projects

**Gas Separation Membrane**

- Selective Coating
- Feed Gas
- Permeate Gas
- Permeable Printed Support
- Unclear advantage

**Gas Absorption Monolith w/ Heat Exchange**

- Feed Gas
- Heat Transfer Fluid
- Printed Composite Sorbent
- Unclear advantage

**Conventional packing**

- Impermeable Conductive Support
- Solvent
- Heat exchange packing
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
- Outlet pressure

Mass transfer simulation
- Constant wall concentration

Periodic boundary conditions in all other directions
Silicone-based membrane reactors explored for intensified CO$_2$ absorption

![Image of membrane reactor](image1.png)

![Graph showing volumetric mass transfer coefficient vs flow rate](image2.png)

- Volumetric Mass Transfer Coefficient (1/s)
- Flow Rate (mL/min)
- 1% Na$_2$CO$_3$
- 1% MEA
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. 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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Can packed towers be improved?

Raschig rings: “Since 1894”

Process intensification limited by film thickness... and fabrication technology?

Structured packing: “A little better”
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.
CFD was used to model the performance of the TPMS structured packings.
TPMS packings improve liquid distributions and have been computationally simulated.
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.
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.
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, Jₜₚₓₓ, Jₓ₂, IP₂, IZ, and P₂YSVP₂Y 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
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


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Prints in multiple materials have been demonstrated.

- ABS
- High-Density Polyethylene
- Polycarbonate
Temperature in Cold Fluid in Countercurrent Heat Exchanger

TPMS geometries enhance fluid mixing

Gyroid

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