

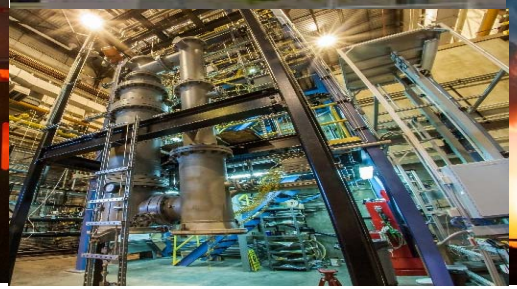


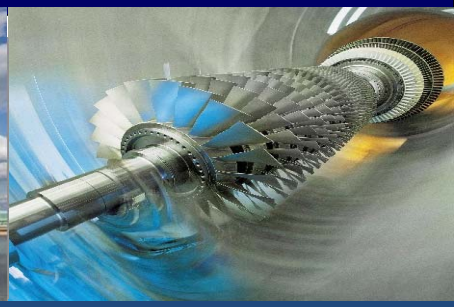

U.S. DEPARTMENT OF ENERGY | Office of Fossil Energy

U.S. Department of Energy's Efforts to Accelerate Transformational Carbon Capture R&D Through Advanced Computing and Manufacturing

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Deputy Director
Advanced Fossil Technology Systems

16 July 2019

OFFICE OF CLEAN COAL AND CARBON MANAGEMENT

The Mission of the Office of Clean Coal and Carbon Management's R&D program is to discover and develop advanced coal technologies *that ensure America's access to resilient, affordable, reliable, and near-zero emitting coal energy resources*.

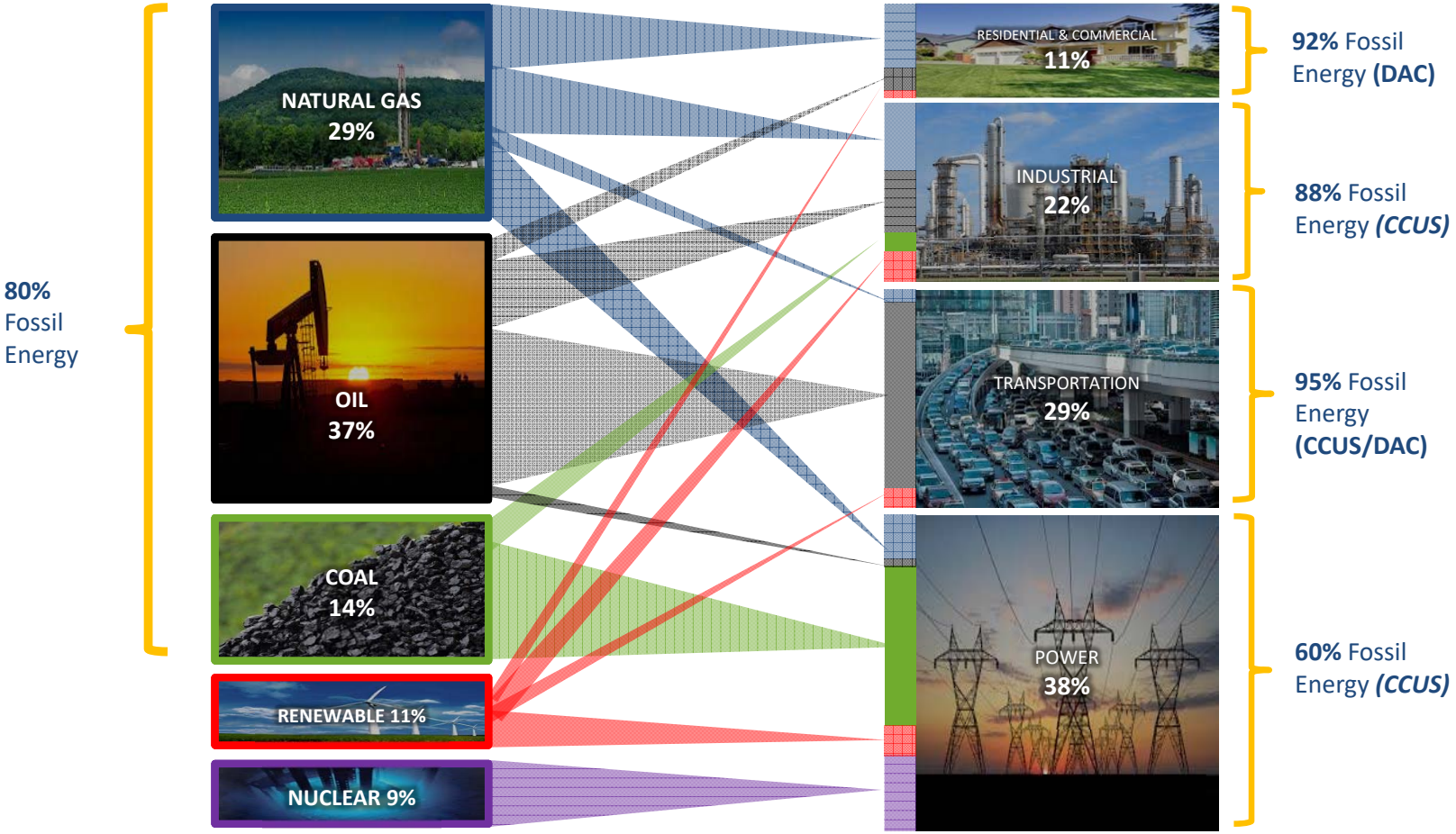
Our R&D is focused on the following priorities:

1. Advancing small-scale modular coal plants of the future, which are highly efficient and flexible, with near-zero emissions
2. Improving the performance, reliability, and efficiency of the existing coal-fired fleet
3. Reducing the cost of carbon capture
4. Creating new market opportunities for coal.

HOLISTIC APPROACH TO ENERGY GENERATION FROM FOSSIL FUELS

FOSSIL ENERGY IS CRITICAL IN ALL SECTORS

CCUS OFFERS ECONOMIC PATHWAY TO LOW CARBON ECONOMY



EIA, *Annual Energy Outlook 2017*, Reference Case, https://www.eia.gov/totalenergy/data/monthly/pdf/flow/css_2017_energy.pdf

HIGH-LEVEL R&D PROGRAM GOALS AND CHALLENGES

Reduce the cost of capture by 50%

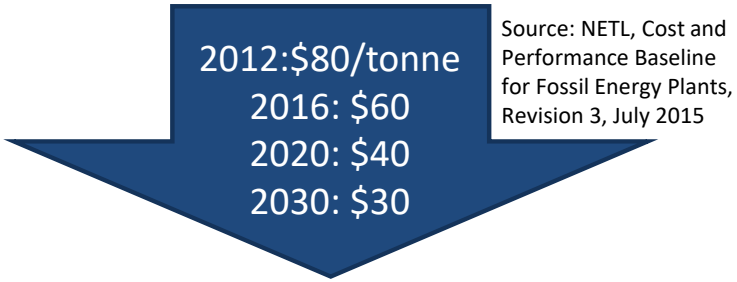
- Capital cost
- Energy penalty
- Integration or process intensification

Develop viable carbon utilization alternatives ($1T opportunity)

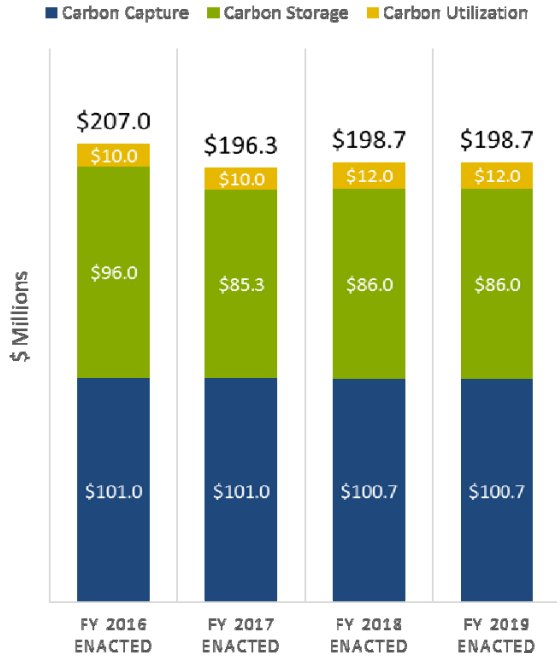
- Reduce Capital cost
- Reduce energy requirements
- Lifecycle assessment better than existing products

Reduce the risk of geologic storage – improve monitoring and simulation

- Higher resolution and quantification (e.g., accurate characterization of faults and fractures)
- Geomechanics (pressure and state of stress)
- Costs/uncertainty/enabling real-time decision making



Source: NETL, Cost and Performance Baseline for Fossil Energy Plants, Revision 3, July 2015



CARBON CAPTURE: POST-COMBUSTION, PRE-COMBUSTION, AND DIRECT AIR CAPTURE

FOCUS ON COST REDUCTION, ENERGY PENALTY, AND INTEGRATION

Summary of Carbon Capture R&D Program Advancement of 2nd Generation Technologies

Cost Reduction	Energy Penalty Reduction	Program Activity
$100+/tonne	30+%	180+ Projects
$41/tonne	14-15%	15 Technologies Tested at Pilot Scale

Pilot-scale Testing

TECHNOLOGY HIGHLIGHTS	Innovation Pathways	PRINCIPAL DEVELOPER
POST-COMBUSTION		
Imbedded Amine Sorbent*	■ ■	ADA-ES
Low-water Amine Solvent	■ ■	Fluor/MHI
Hybrid Solvent/Membrane	■ ■ ■	Gas Technology Institute
Amino-silicone Solvent*	■	General Electric Company
Amine/Imidazole Solvent Mixture* *(Large Pilot)*	■	ION Engineering
Advanced Amine Solvent Process*	■ ■	Linde/BASF
Advanced Membrane Process*	■ ■	MTR
Nozzle-based Solvent Contactor*	■	Neumann Systems Group
Mixed Salt Solvent Process*	■ ■	SRI International
Carbon-based Sorbent*	■	SRI International
Alkalized Alumina Sorbent*	■ ■	TDA Research
Optimized Amine Solvent Process	■ ■ ■	University of Kentucky
Piperazine Solvent/Flash Stripper	■ ■	URS/University of Texas
PRE-COMBUSTION		
Ammonium Carbonate/Bicarbonate Solvent*	■	SRI International
Integrated Sorbent Process	■	TDA Research

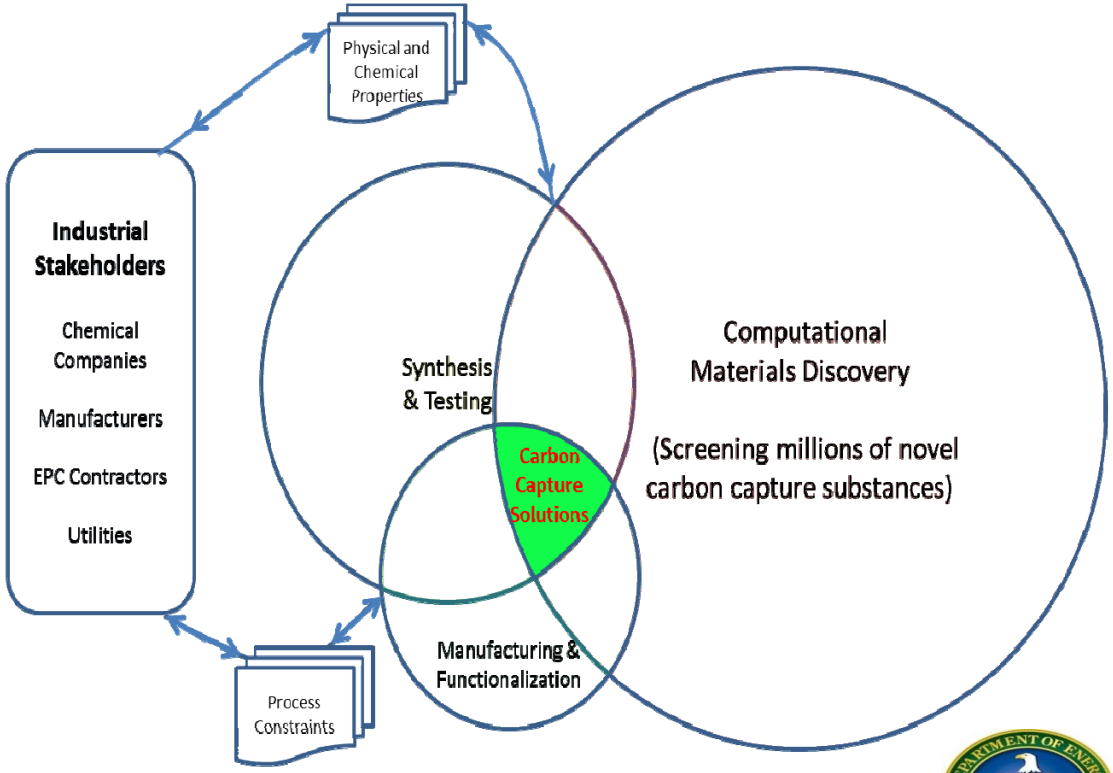
Materials / Processes / Equipment

* Project Completed

Requires improvements in multiple areas

DOCCSS - DISCOVERY OF CARBON CAPTURE SUBSTANCES SYSTEMS

- **Challenge – Accelerate development by 50%**
- Integrates technical expertise of national laboratories, market perspectives of industrial partners, and the computational insight of CCSI^2
- Improves data generation methods to target materials performance characteristics, and rigorous materials/ devices/systems optimization
- Lab Selection 2017
  - PNNL
  - LBNL
  - LLNL
- Adopting model in other areas of program



Carbon Capture Simulation for Industry Impact

Work with industry partners on pilot & early TRL projects

Ensure success & maximize learning at this scale

- Data collection & experimental design
- Develop & validate models
- Uncertainty quantification to identify critical data
- Develop demonstration plant design
- Utilize optimization tools (optimization under uncertainty, heat integration)
- Quantitative confidence on predicted performance
- Predict dynamic performance

CCSI² Carbon Capture Simulation for Industry Impact

Accomplishments

- Framework for non-aqueous solvents developed
- Use of rigorous models to inform accurate and predicative feed forward control resulting in rapidly achieving optimal operations
- NG interest

NETL National Energy Technology Laboratory · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · Carnegie Mellon · West Virginia University · Princeton University · Boston University · The University of Texas at Austin

NETL-RIC: AN INTEGRATED MODELING AND EXPERIMENTAL APPROACH TO CARBON CAPTURE

Objective

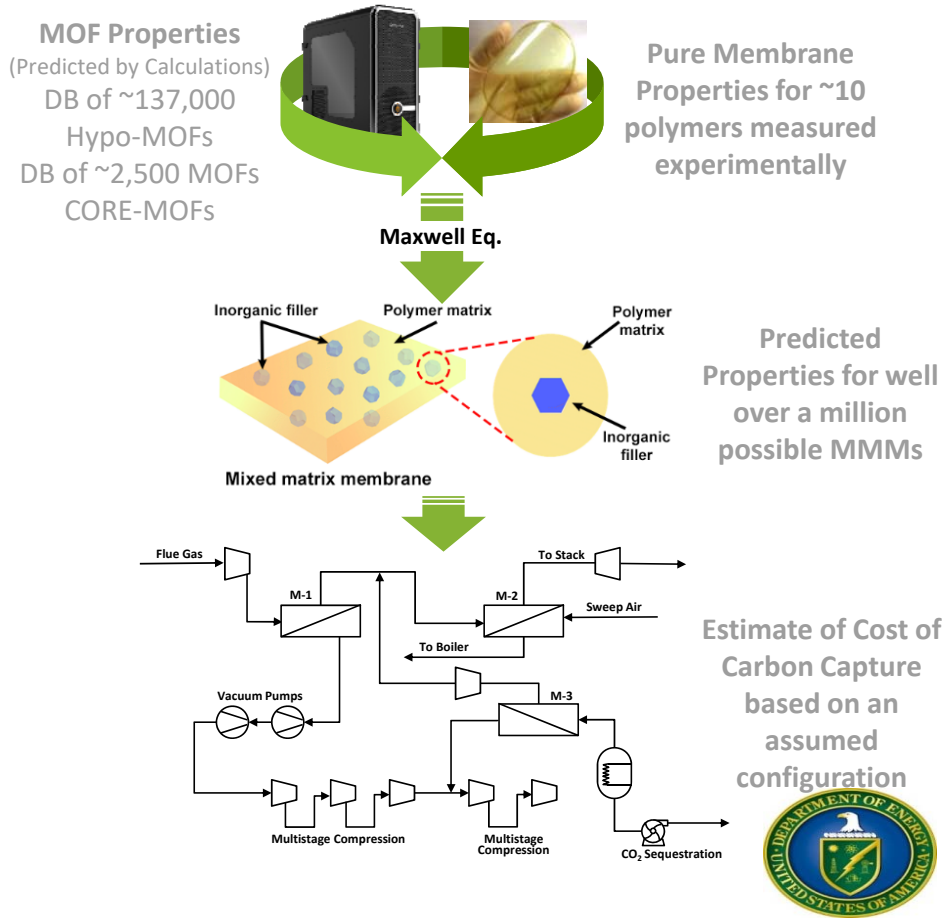
- Examine novel classes of materials
- Explore innovative process configurations
- Develop advanced screening approaches

Approach

- Develop material types with unique properties
- Integrated computational and experimental approach for high throughput materials screening
- Develop novel process configurations

Research Focus

- Solvents for Pre-combustion: Hybrid PEG-Siloxane; Silicon oil-MOF suspensions; Commercial solvents identified by data mining
- Sorbents: Polybenzimidazole porous polymer sorbent
- Membranes: Mixed matrix membranes, high performance polymer blends; ion gel membranes; facilitated transport membranes



AMINE-APPENDED METAL-ORGANIC FRAMEWORKS AS SWITCH-LIKE ADSORBENTS FOR ENERGY EFFICIENT CARBON CAPTURE

Lawrence Berkeley National Laboratory

Approach – Computational design & synthesis of solid sorbents based upon diamine-appended metal-organic frameworks (MOFs) for post-combustion CO_2 capture, followed by comprehensive characterization using simulated flue gas to identify most promising adsorbents for scale-up

Advantages

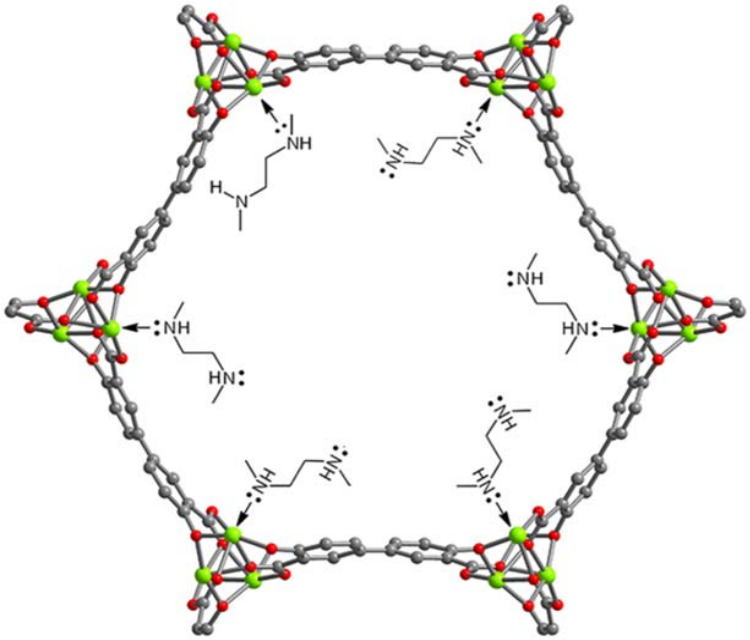
- No loss of CO_2 capacity under humid flue gas conditions
- Rapid CO_2 diffusion
- Large working capacity with moderate temperature swings
- High CO_2 selectivity

Challenges

- Sorbent scale up
- Rendering materials into a structured form

Benefits

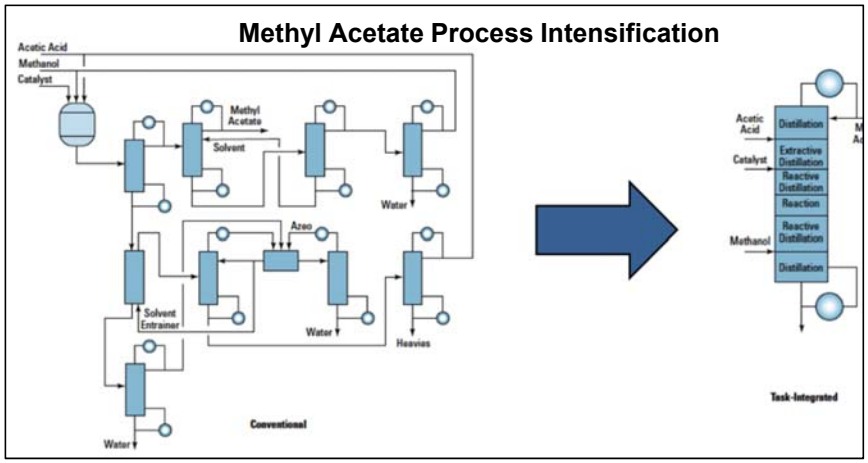
- MOF framework is inexpensive, reducing CAPEX
- Increased working capacity & reduced temperature swing of the sorbent allows for increased energy efficiency & decreased OPEX

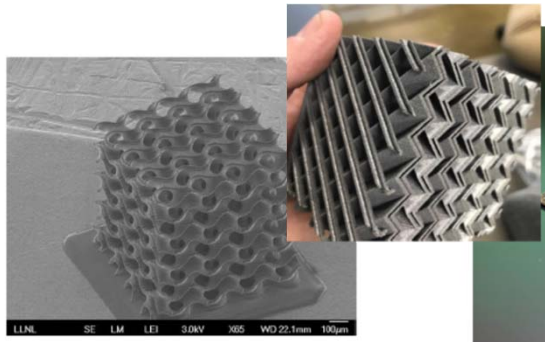


MOF with appended amines

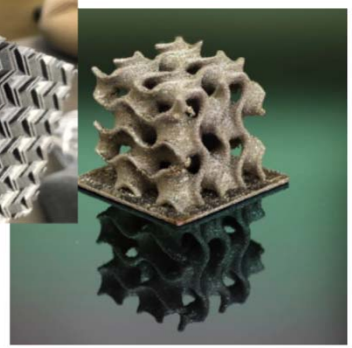
PROCESS INTENSIFICATION BASICS

- Sequential unit operations drive up cost
- Multi-functional equipment designs reduce total equipment required, *potentially* cost…
- However, intensified processes are often more complex and may offset savings some
- We rely on *advanced manufacturing* to enable these designs at reasonable prices
- Highly-specific designs can perform better, may be less expensive, but…





Printed at LLNL with Projection Microstereolithography (PμSL)



Stainless steel gyroid printed at LLNL

Figure Source: NETL

ADDITIVE MANUFACTURING PROJECTS

OAK RIDGE National Laboratory

- Baselines conventional packing
- Baselines manufacturability
- Prototypes Packing improvements
- CFD → Fundamental ROM understanding

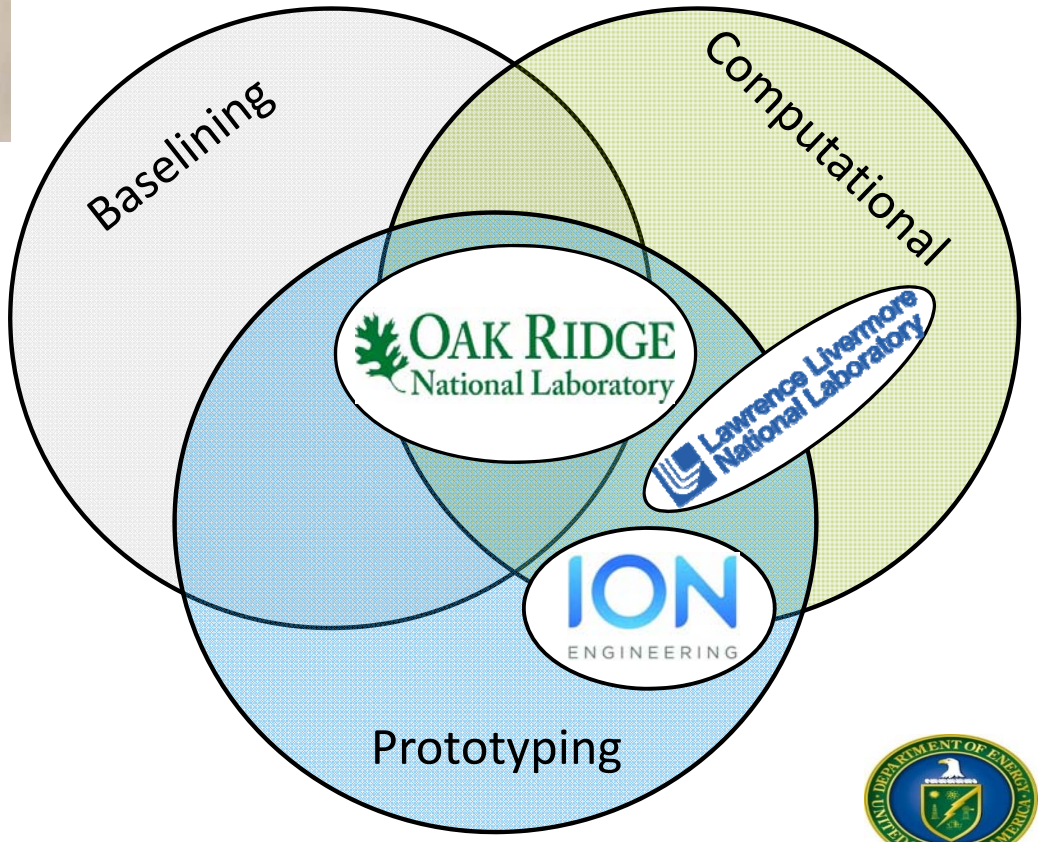
Courtesy of ORNL

ION ENGINEERING

- Intercooled packing
- Packing screening – test rig
- Design modeling tools

Lawrence Livermore National Laboratory

- Whitespace exploration of optimal geometry
- 3D printing of TPMS Structures
- Optimal design prototyping
- Geometry optimization framework



ADDITIVELY MANUFACTURED INTENSIFIED DEVICE FOR ENHANCED CARBON CAPTURE

Oak Ridge National Laboratory

Approach – Use additive manufacturing (AM), a device-scale prototype reactor that combines multiple thermodynamic operations into one unit (intensified device) for enhanced solvent-based CO_2 capture, & test using simulated flue gas

Advantages

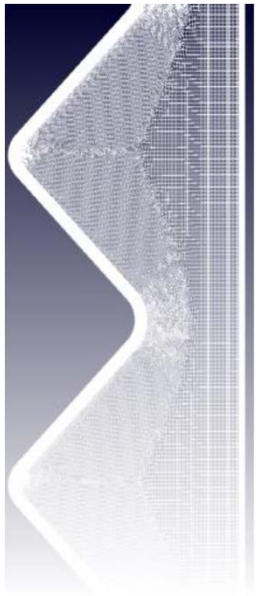
- Enhanced absorption kinetics due to increased reactive surface area
- Enhanced heat exchange efficiency
- Smaller equipment size

Challenges

- Printing devices with intricate geometric features using AM
- Ensuring the prototype is structurally sound with increasing height

Benefits

- Combining multiple thermodynamic operations into one intensified device increases energy efficiency
- Reduced equipment size lowers CAPEX & OPEX



Model of absorption in corrugated structured packing sheet

https://www.netl.doe.gov/research/coal/project-information/proj?k=FWP-FEAA130

RAPID DESIGN AND TESTING OF NOVEL GAS-LIQUID CONTACTING DEVICES FOR POST-COMBUSTION CO_2 CAPTURE VIA 3D PRINTING: MODULAR ADAPTIVE PACKING

ION Engineering LLC

Approach – Design & characterize 3D-printed modular adaptive packings with internal heating or cooling capabilities for gas-liquid contacting

ION's 0.01 MWe CO_2 capture lab pilot unit

Advantages

- Modular and adaptable to both small- & large-scale applications
- Dual functionality of heat & mass transfer in single packing medium
- Improved mass transfer & pressure drop across packing

Challenges

- Module leakage
- Structure of 3D-printed modules
- Blockage of intercooling tubes in 3D-printed modules

Benefits

- 3D-printing minimizes manufacturing costs (reduced CAPEX), accelerates design, & expedites deployment timeline in the field
- Maximized contactor surface area/volume ratio is smaller footprint (lower CAPEX) & higher mass transfer rate
- Lower solvent make-up rates (reduced OPEX) & reduced emissions, allows for lower CAPEX on the water wash section

HIGH-EFFICIENCY INTEGRATED REACTORS FOR SORBENTS, SOLVENTS, AND MEMBRANES USING ADDITIVE MANUFACTURING

Lawrence Livermore National Laboratory

Approach – Design novel geometries (triply periodic minimal surface [TPMS] & hierarchical structures) that support an advanced sorbent, solvent, or membrane to achieve transformational CO_2 capture

Advantages

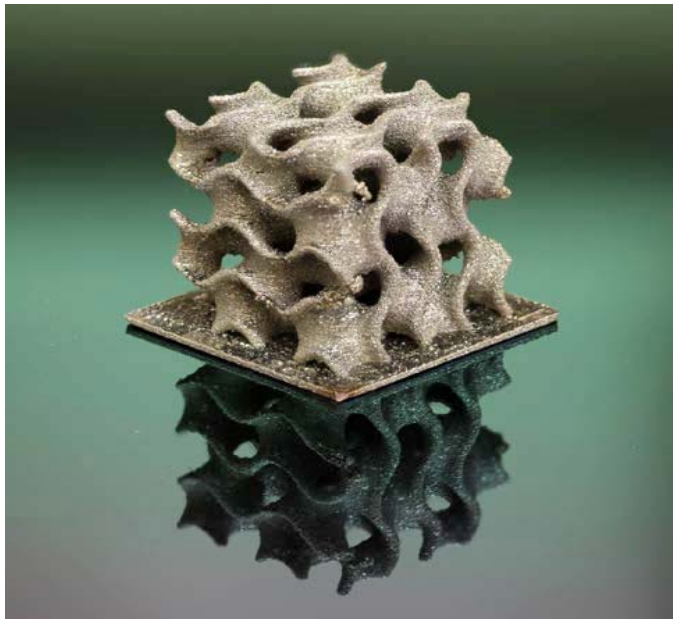
- Reduced reactor volume & improved material utilization
- Enhanced mass & heat transfer

Challenges

- Optimization of reactor structure for enhanced efficiency
- Practicality of materials used to print 3D modules

Benefits

- AM of novel designs with advanced capture materials improves energy efficiency and reduces CAPEX & OPEX
- Increased interfacial area reduces footprint & lowers CAPEX



TPMS structure printed using additive manufacturing at LLNL

https://www.netl.doe.gov/research/coal/project-information/proj?k=fwp-few0225

Questions