Unique Nanotechnology Converts Carbon Dioxide to Valuable Products

(DOE Award #: DEFE0031707)

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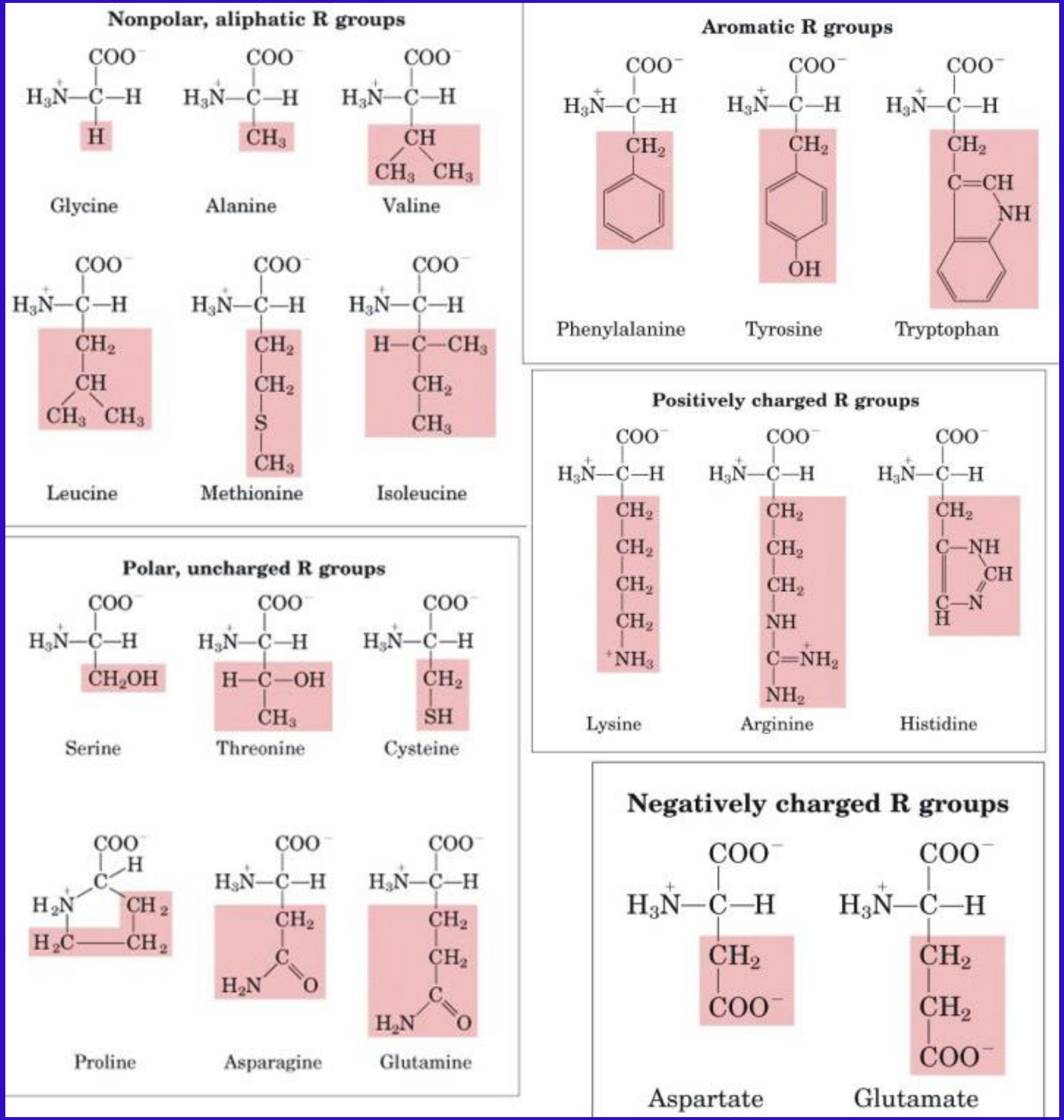
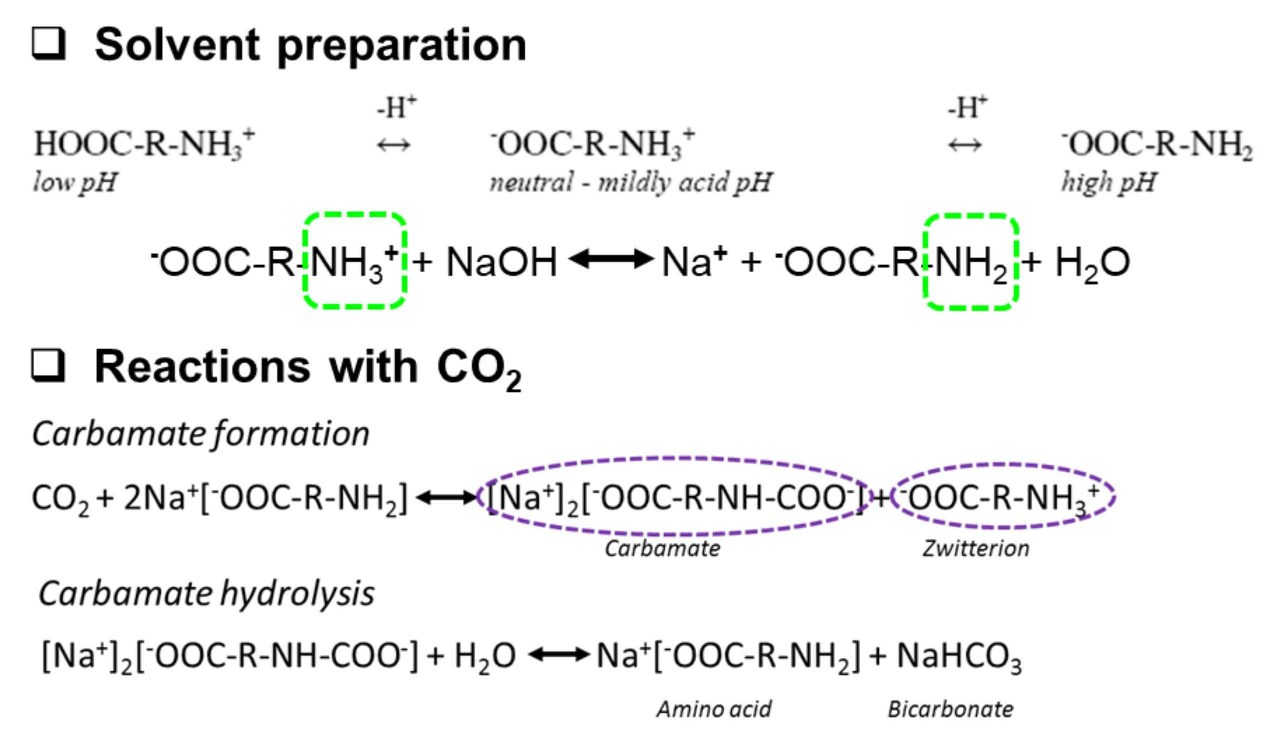
(A). Background



Structures of 20 typical amino acids (AAs).

Computational analysis and lab studies identifying AAs that convert CO_2 into nanomaterials



Reactions involved.

(B). Project Objective and Research Team

Overall Project Objective

- To develop and test an innovative nanotechnology that can utilize CO_2 from coal-based power systems or other industrial sources as the primary feedstock to produce commercially valuable products.

Project Tasks

- Task 1: Project management and planning (Li, Morsi, Wang)
- Task 2: Technology maturation plan (Li, Morsi, Wafle)
- Task 3: Lab-scale unit modification (Li)
- Task 4: Selection of best candidate amino acid solvent (Li)
- Task 5: Process optimization to produce high-purity nanomaterials (Li)
- Task 6: Life cycle assessment (LCA, Wang)
- Task 7: Process and techno-economic analysis (TEA, Morsi)

Project Funding, Team, and Industry Sponsor

Funding: DOE-NETL: $800,000; Cost-share: $218,205

- Bingyun Li, PhD (PI, WVU)
- Badie Morsi, PhD (Co-PI, Univ. of Pitt)
- Jingxin Wang, PhD (Co-PI, WVU)
- Ron Rosinski (Longview Power, LLC)
- Trina Wafle (Coordinator, WVU)

- Naomi R. O’Neil (Project manger, NETL)
- (Andy Aurelio, Steven A. Mascaro; NETL)

(C). Accomplishments (Task by Task)

Task 1: Project management and planning

Task 2: Technology maturation plan (10/21/2019)

A. TARGET COMMERCIAL APPLICATION

The proposed carbon capture and conversion technology encompasses addresses two market segments:

- Those who want to capture carbon
- Those who want to use the byproduct

B. CURRENT TECHNOLOGY READINESS LEVEL - BEGINNING OF PROJECT TRL

- AA salt solvent: TRL 2-3
- Process engineering system: TRL 1

C. PROPOSED WORK – END OF PROJECT TRL

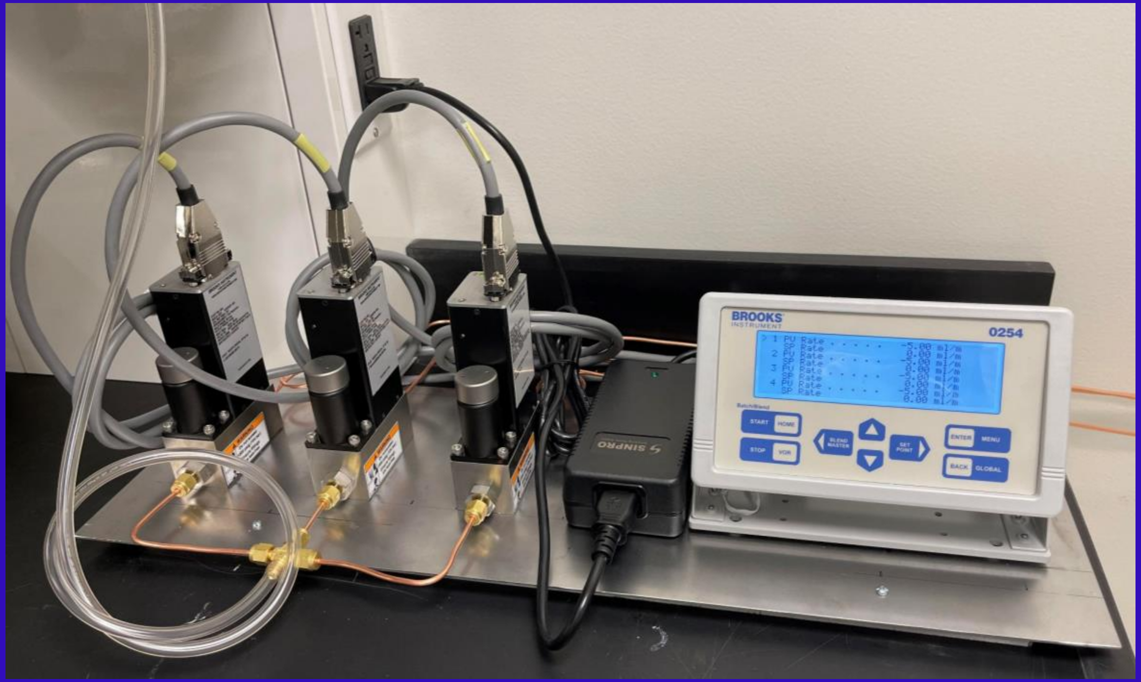
- AA salt solvent: TRL 4
- Process engineering system: TRL 4

TRL	Definition	Description
1	Basic principles observed and reported	Core Technology Identified. Scientific research and/or principles ex and have been assessed. Translation into a new idea, concept, and application has begun.
2	Technology concept and/or application formulated	Invention Initiated. Analysis has been conducted on the core technology for practical use. Detailed analysis to support the assumptions has been initiated. Initial performance attributes have been established.
3	Analytical and experimental critical function and/or characteristic proof-of-concept validated	Proof-of-Concept Validated. Performance requirements that can be tested in the laboratory environment have been analytically and physically validated. The core technology should not fundamentally change beyond this point. Performance attributes have been upda and initial performance requirements have been established.
4	Basic technology components integrated and validated in a laboratory environment	Technology Validated in a Laboratory Environment. The basic technology components have been integrated to the extent practic (a relatively low-fidelity integration) to establish that key pieces wi work together, and validated in a laboratory environment. Performance attributes and requirements have been updated.
5	Basic technology components integrated and validated in a relevant environment	Technology Validated in a Relevant Environment. Basic technology component configurations have been validated in a relevant environment. Component integration is similar to the final application in many respects. Data sufficient to support planning ar design of the next TRL test phase have been obtained. Performanc attributes and requirements have been updated.

D. POST-PROJECT PLANS

To seek funding to build a laboratory scale system based on the engineering design, to demonstrate the feasibility in lab columns (e.g., 10 kWe), to determine phase equilibria data, *etc.*

Task 3: Lab-scale unit modification



- Three mass flow meters have been purchased and assembled.

Task 4: Selection of best candidate amino acid solvent

- **Reproducibility check:**

  Nanomaterials were produced by three individuals at different times.

- **Optimization:**

  The CO_2 absorption in 100% CO_2 at different AA/NaOH ratio and time was optimized.

  The CO_2 absorption in a simulated flue gas (e.g., 10% CO_2) at different AA/NaOH ratio and time was further optimized. Formation of nanomaterials was presented.

Task 5: Process optimization to produce high-purity nanomaterials

This task will be conducted next year. The potential approaches that may improve the purity were discussed.

Task 6: Life cycle assessment (LCA)

1. Completed LCA Phase I: Goal and Scope Definition

Study goal definition

The goal of this LCA study is to:

- Quantify the life-cycle environmental burdens, especially Global Warming Potential (GWP) impact, of the proposed ***nanotechnology System.***
- Compare the environmental burdens of the proposed technology to comparison product system (i.e., the MEA technology system and the power plant without CCUS).

Study boundary identification

In terms of LCA, study scope includes five unit processes: flue gas washing, reverse osmosis, CO_2 absorbing, ultrafiltration, NaOH solvent makeup.

All the resources, materials, and energy input into the system, and emission to water, emission to air, and emission to soil will be included.

LCA approach path definition

Integrated ***consequential*** and ***attributional cradle-to-gate*** LCA with TRACI 2.1

Functional Unit

Conversion of 1 ton of CO_2 from the flue gas stream of an existing power plant in the U.S.

2. Completed LCI Phase for Comparison System - MEA Technology

Developed specific life cycle inventory procedures and datasheets to guarantee the data quality and consistency

- **LCI for MEA technology (Operation Phase and Construction Phase) based on literature review:**

Completed life cycle inventory for MEA technology

3. Completed LCIA Phase for Comparison System - MEA Technology

Global warming potential (GWP) impact for the functional –unit base was determined for both operation phase and construction phase.

The contribution analysis was conducted to identify the major contributing unit processes for GWP.

- **Other Environmental Impacts:**

Other environmental impacts including ozone depletion, smog, acidification, eutrophication carcinogenics, non carcinogenics , respiratory effects, ecotoxicity, fossil fuel depletion, were also assessed with TRACI.

Task 7: Process and techno-economic analysis (TEA)

Objective: To carry out TEA of the CO_2 capture process using Gly to produce high-value sodium bicarbonate nanoparticles from a conceptual 10 MW pre-combustion power plant using Aspen Plus v.10.

WCCS Flue Gas [1]

Temperature, °C	80	
Pressure, atm	1	
Components	mol %	wt %
CO_2	13.33	20.18
H_2O	12.31	7.63
N_2	70.36	67.79
O_2	4.000	4.40
SO_2	2.346E-03	0.0052

Flue gas flow rate	Wolverine Power Plant	Power Plant used
	600 MW	10 MW
Volume flow rate, m^3/s	742.80	12.38
Mass flow rate, kg/s	745.80	12.43

[1] Hoffman, H., Wu, S., Pardini, R., Tripp, E., & Barnes, D. (2010). *Expansion of Michigan EOR Operations Using Advanced Amine Technology at a 600 MW Project Wolverine Carbon Capture and Storage Project*. Wolverine Power Supply Cooperative.

Proposed CO_2 capture process

Process main units:

- Washing unit (WU)
- CO_2 capture unit (Absorber)
- Reserve Osmosis Unit (ROU)
- Ultrafiltration and $NaHCO_3$ production Unit (UFU)
- NaOH makeup chamber

Process constraints:

- CO_2 absorption efficiency = 90%
- Absorber L/D ≥ 6
- No flooding in the Washing Unit and CO_2 absorber

Washing Unit (WU)

Reactions in the washing unit	ΔH_r at 298.15 K (kJ/mol)
$SO_3 + H_2O \rightleftharpoons H_2SO_4(aq)$	- 227.72
$2SO_2 + O_2 \rightleftharpoons 2SO_3$	- 197.76

Column diameter, m	2.12
Column height, m	15.23
Packing height, m	12.72
Packing type	Mellapak 250Y
ROU membrane type	BW30-400 membrane [1,2]
# Membrane module	60
Pump for ROU	42.2 kW centrifugal pump

Performance	Inlet flue gas	Inlet water	Desulfurized flue gas	Outlet water	Reject stream
Temperature, °C	80	40	41.78	52.94	52.94
Pressure, atm	1.003	1	1	1	15.3
Mass flow rate, kg/s	12.43	23.75	12.10	24.08	0.33

[1] Dow Water & Process Solution. "Filmtec™ Reverse Osmosis Membranes." *Technical Manual, Form* 609-00071 (2010): 1-180.
[2] Lu, Yan-Yue, et al. "Optimum design of reverse osmosis system under different feed concentration and product specification." Journal of membrane science 287.2 (2007): 219-229.

CO_2 capture unit (Absorber)

Reactions in the CO_2 absorber [1]	ΔH_r at 298.15 K (kJ/mol)
$NH_2CH_2COOH + OH^- \rightleftharpoons NH_2CH_2COO^- + H_2O$	- 11.636
$NH_2CH_2COO^- + H_2O + CO_2 \rightleftharpoons NH_2CH_2COOH + HCO_3^-$	- 56.85

Column diameter, m	5
Column height, m	33.24
Packing height, m	30
Packing type	Mellapak 250Y

Performance	Inlet Desulfurized gas	Inlet GLY/NaOH solution	Cleaned vented gas	Outlet Rich solution
Temperature, °C	41.78	20	44.61	45.58
Pressure, atm	1.003	1	1	1
Mass flow rate, kg/s	12.10	34.19	9.84	36.45

1. Ziemer, S. P., T. L. Niederhauser, E. D. Merkley, J. L. Price, E. C. Sorenson, B. R. McRae, B. A. Patterson, M. L. Origlia-Luster, and E. M. Woolley. "Thermodynamics of proton dissociations from aqueous glycine at temperatures from 278.15 to 393.15 K, molalities from 0 to 1.0 mol· kg− 1, and at the pressure 0.35 MPa: Apparent molar heat capacities and apparent molar volumes of glycine, glycinium chloride, and sodium glycinate." The Journal of Chemical Thermodynamics 38, no. 4 (2006): 467-483.

UFU for $NaHCO_3$ production and NaOH makeup Chamber

UFU membrane type	SFP-2660
# of Membrane module	52
Pump for UFU	8.5 kW centrifugal pump
NaOH makeup chamber	0.252 m^3 CSTR
Agitator/motor	Pitched blade turbine
Pump for NaOH makeup	0.82 kW centrifugal pump
Pump for solvent recycle	12 kW centrifugal pump

Reaction in the NaOH makeup chamber[1]	ΔH_r at 298.15 K (kJ/mol)
$NH_2CH_2COOH + OH^- \rightleftharpoons NH_2CH_2COO^- + H_2O$	- 11.636

Performance	Rich solution	$NaHCO_3$ phase	Glycine solution	NaOH makeup	Water vapor	Inlet GLY/NaOH solution
Temperature, °C	45.58	45.58	45.58	20	103.2	20
Pressure, atm	14.31	1	14.31	14.31	1	1
Mass flow rate, kg/s	36.45	4.32	32.13	2.45	0.39	34.19

1. Ziemer, S. P., T. L. Niederhauser, E. D. Merkley, J. L. Price, E. C. Sorenson, B. R. McRae, B. A. Patterson, M. L. Origlia-Luster, and E. M. Woolley. "Thermodynamics of proton dissociations from aqueous glycine at temperatures from 278.15 to 393.15 K, molalities from 0 to 1.0 mol· kg− 1, and at the pressure 0.35 MPa: Apparent molar heat capacities and apparent molar volumes of glycine, glycinium chloride, and sodium glycinate." The Journal of Chemical Thermodynamics 38, no. 4 (2006): 467-483.

Calculations

$$\mathbf{OPEX_{2020}} = (60 \sum \mathrm{W}) + \mathrm{C_{NaOH}}\dot{m}_{NaOH} - \mathrm{C_{NaHCO3}}\dot{m}_{NaHCO3} + 0.04(\mathrm{CAPEX_{2020}})$$

$$\mathbf{LCOC} = \left(\frac{f_{CR}}{f_c}\right) \sum (CAPEX_{2020})/\dot{m}_{CO2} + OPEX_{2020}/\dot{m}_{CO2}$$

$$f_{CR} = \frac{i(1+i)^N}{(1+i)^N - 1}$$

Electricity cost = 60 $/MWh
C_{NaOH} = NaOH makeup cost, 450 $/ton
C_{NaHCO3} = $NaHCO_3$ produced prices, 203 $/ton
O & M cost = 4% of the total CAPEX in $/year
N = project lifetime, year

W = total power required, MW
$\dot{m}_{NaOH}$ = NaOH makeup, ton/h
$\dot{m}_{NaHCO3}$ = $NaHCO_3$ produced, ton/h
$\dot{m}_{CO2}$ = CO_2 captured, ton/h
i = discount rate = 10%/year

TEA of the CO_2 capture process

CAPEX	Heat Exchangers
	Packing Cost
	Absorber
	Ultrafiltration unit
	Reaction chamber
	Flash drum
	Washing unit capital
	Initial solvent
	Rotating equipment
	Total CAPEX = 4,456,975 USD
OPEX	Heat exchanger, MW
	Rotating equipment, MW
	Ultrafiltration power, MW
	NaOH makeup, MW
	Washing unit power, MW
	Total electricity Cost, US$ 2020/h
	O&M, US$ 2020/h
	(NaOH makeup – $NaHCO_3$ production), US$/h
	Total OPEX = 223 USD/h

Capacity factor, f_C	0.8	-
Discount rate, i	10%	1/year
Lifetime, N	30	year
Capital recovery factor, f_{CR}	0.106079	1/year
$\dot{m}_{CO2}$	8.144	ton CO_2/h

CAPEX contribution to LCOC USD/ton CO_2	8.28
OPEX contribution to LCOC USD/ton CO_2	27.35
LCOC USD/ton CO_2	33.63

Summary

- AA candidates for phase-change CO_2 conversion have been identified and optimized.
- Life cycle assessment has been used to assess potential environmental impacts.
- Preliminary TEA has shown that the innovative phase-change nanotechnology could achieve a LCOC of \$33.63/ton CO_2.

Relevant Products

Publications, abstracts, presentations, inventions, grants, honors, *etc.*

- Wickramasinghe S, Wang J, Morsi B, Li B*. (2021). Carbon dioxide conversion to nanomaterials: Methods, applications, and challenges. ***ACS Energy & Fuels*** https://doi.org/10.1021/acs.energyfuels.1c01533.
- Wang R, Ashkanani HE, Li B, and Morsi B*. (2021) Development of an innovative process for post-combustion CO2 capture to produce high-value NaHCO3 nanoparticles. ***Int J Greenhouse Gas Control*** (submitted).
- Li B, et al. Amino acids react with carbon dioxide (CO_2) and form nanofibers and nanoflowers. ***US patent US10,583,388***. Date of patent granted: March 10, 2020.
- Training: one PhD student at Pitt, one PhD student at WVU, one postdoc at WVU, and two short term rotation students at WVU.
- Dr. Wang was awarded a USDA grant and Dr. Li is a Co-PI of the grant [NIFA 2019-08303, Mid-Atlantic Sustainable Biomass for Value-added Products Consortium (MASBio), $10,000,000, 9/1/20-8/31/25].

Relevant Products (cont.)

- Dr. Li received the *Vice President's Outstanding Achievement in Research and Scholarly Activities Award*, WVU Health Sciences Center, 2020.
- Wang R, Li B, Morsi B. ***Poster presentation***. Nanotechnology converts CO_2 from power plants flue gas to valuable products. U.S. DOE 2020 Virtual Integrated Project Review Meeting, Carbon Utilization sessions, October 21-22, 2020.
- Wang R, Ashkanani HE, Li B, Morsi BI. ***Poster presentation***. Development of a continuous nanotechnology process for converting carbon dioxide to valuable products. 37th Annual International Pittsburgh Coal Conference (Virtual Conference), Pittsburgh, Sept. 8-11, 2020.
- Wang R, Ashkanani H, Li B, Morsi B. ***Poster presentation***. Modeling of CO_2 absorption from gas mixtures using chemical absorbents in adiabatic packed-beds. 36th Annual International Pittsburgh Coal Conference, September 3-6, 2019, Pittsburgh, PA.
- Wang R, Ashkanani H, Li B, Morsi B. Modeling of CO_2 absorption from gas mixtures using chemical absorbents in adiabatic packed-beds. Paper to appear in the Proceedings of the 36th Annual International Pittsburgh Coal Conference, September 3-6, 2019, Pittsburgh, PA.

Acknowledgement

Funding: DoE/NETL

Trainees: Ross Fladeland, James Mersch, Rui Wang, Sameera Wickramasinghe, Xufeng Zhang

Collaborators:

(Current) Badie Morsi, Jingxin Wang,

Trina Waffle, Ron Rosinski

NETL project manager: Naomi R. O'Neil (Andy Aurelio, Steven A. Mascaro)