LEADERSHIP AT INTERFACES:
Capitalizing on the “gaps” in science, technology and education

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March 3, 2025
Colorado School of Mines – Leadership by Design Seminar

Senior Reaction Engineer
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Mechanical and Thermal Engineering Sciences Directorate
National Renewable Energy Laboratory, Golden, CO

This presentation was produced when the laboratory operated as the National Renewable Energy Laboratory (NREL). The laboratory is now the National Laboratory of the Rockies (NLR).

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NREL at-a-Glance

4,400

Workforce, including

205 postdoctoral researchers

179 graduate students

94 undergraduate students

World-class

facilities, renowned technology experts

More than 1000

Partnerships

with industry, academia, and government

Campus

operates as a living laboratory

Introduction

- B.S. Chemical Engineering, Washington University in St. Louis, 2012
- Ph.D. Chemical Engineering, Northwestern University, 2017; *doctoral research sponsored by Dow Chemical*
  - Dissertation Title: "Understanding Silica-Supported Group 4 and 5 Metal Oxide Catalysts for Selective Oxidations with Hydrogen Peroxide and for Epoxide Activation"
- Former graduate intern at 3M, Corporate Research Materials Laboratory, 2015; *adhesive formulation R&D*
- ***Senior Reaction Engineer (and other roles) at the National Renewable Energy Laboratory, 2017–present***
- Adjunct Professor of Chemical and Biological Engineering, Colorado School of Mines, January 2024–present

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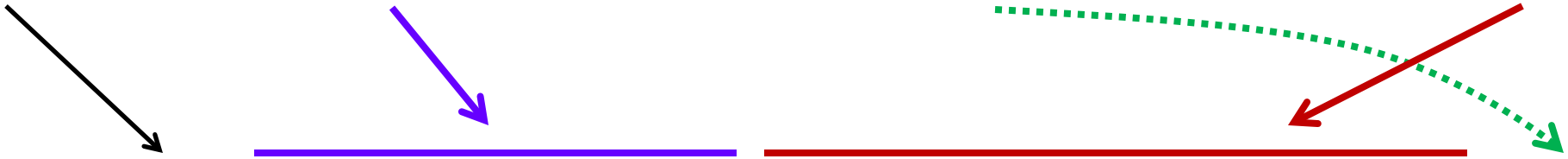
Overview of what I do for a living

I investigate **catalysts & reactors** for the **sustainable** production of **chemicals & fuels**.



"I make the stuff that makes the stuff that makes the stuff, **better**."

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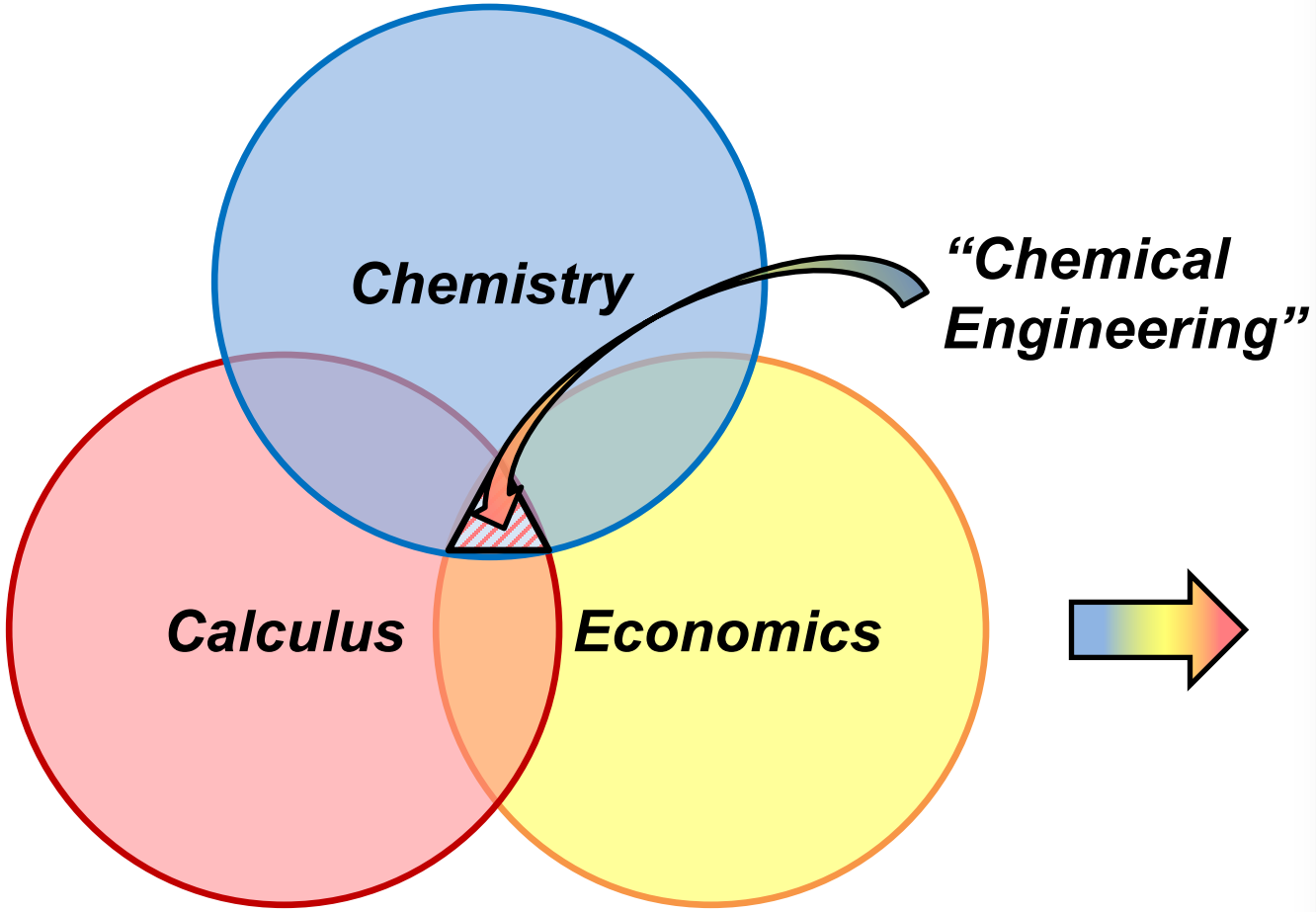
Chemical engineering – chemistry… at the largest possible scale!

6-1 Image from Google Images. Accessed 2017 April 17.

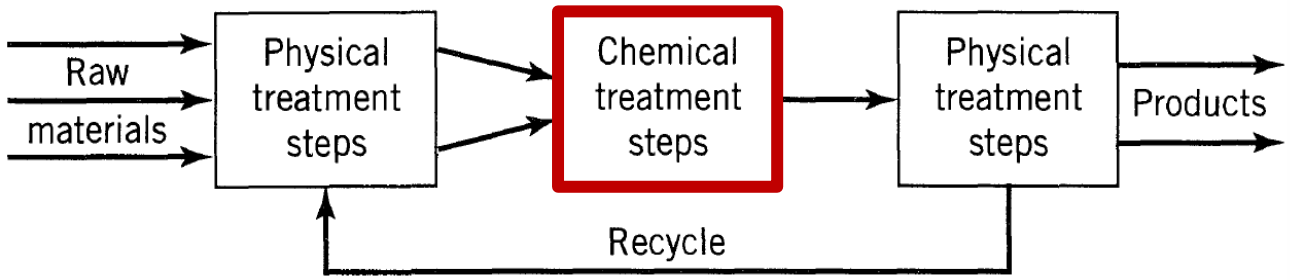
Chemical engineering – chemistry… at the largest possible scale!



7-1 Image credit: Linda Wang, Chemical & Engineering News, Vol. 94 p.18, 28 June 2016. Accessed 17 April 2017.

Chemical engineering – chemistry… at the largest possible scale!

- **Industrial chemicals** are EVERYWHERE in our homes, cars and everyday lives
  - performance plastics & fabrics
  - foams, coatings, paints & adhesives
  - cosmetics, hygiene & cleaning products
  - pharmaceutical drugs
  - nitrogen fertilizer



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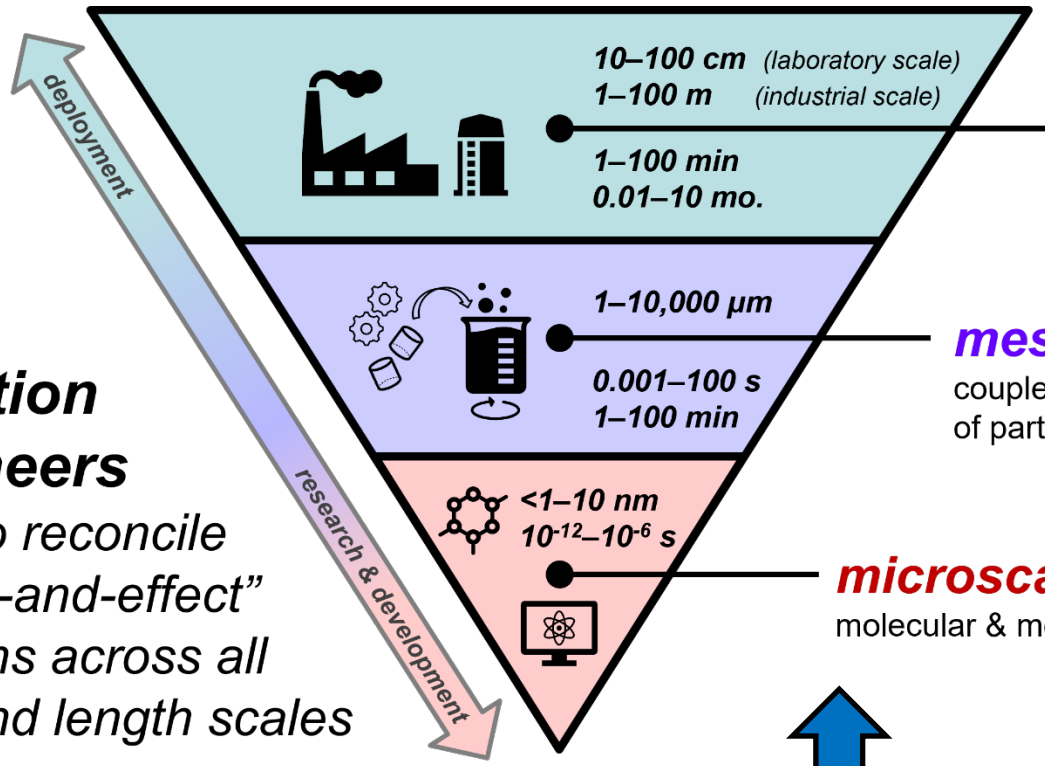
8-1 Image credit: Linda Wang, Chemical & Engineering News, Vol. 94 p.18, 28 June 2016. Accessed 17 April 2017.

8-2 Levenspiel, O. Chemical Reaction Engineering, 3rd edition, Figure 1.1, p.1 (2003).

The reaction engineering discipline encompasses many subjects and scales



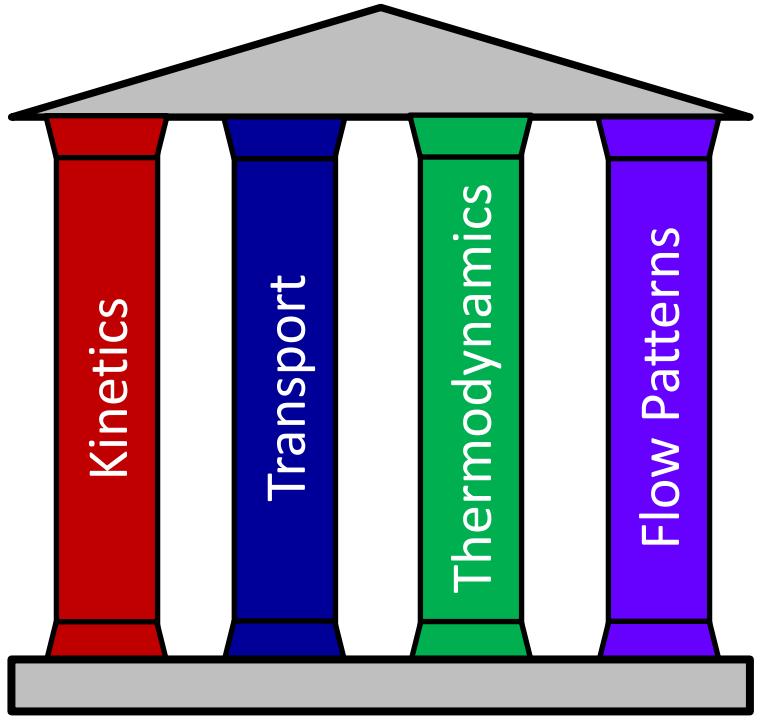
macroscale
reactor design in the context of chemical process & plant design

mesoscale
coupled chemistry and physics of particles, droplets & interfaces

microscale
molecular & mechanistic levels of scrutiny

Reaction engineers *seek to reconcile "cause-and-effect" relations across all time and length scales*

Reaction engineering exists, insists and *thrives at the interfaces* of matter, energy, science, economy & society.



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An aside: Original course creation: *CBEN 428/528 – Advanced Reactor Design*

Traditional Reactors

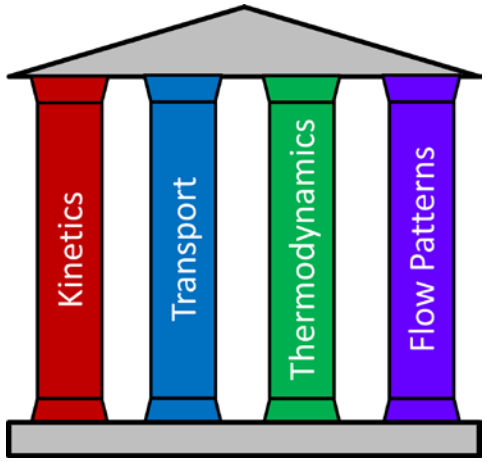
- Idealized reactor archetypes (*review*)
- Catalyst transport limitations (*review*)
- Fixed beds
- Trickle bed reactors
- Stirred tank and slurry reactors
- Tubular reactors and static mixers
- Bubble columns
- Fluidized bed reactors
- Rotating packed beds
- Moving bed reactors

Non-traditional Reactors

- Continuous oscillatory baffled reactors
- Microreactors
- Electrified reactors
- Electrochemical reactors
- Photochemical reactors
- Plasma reactors

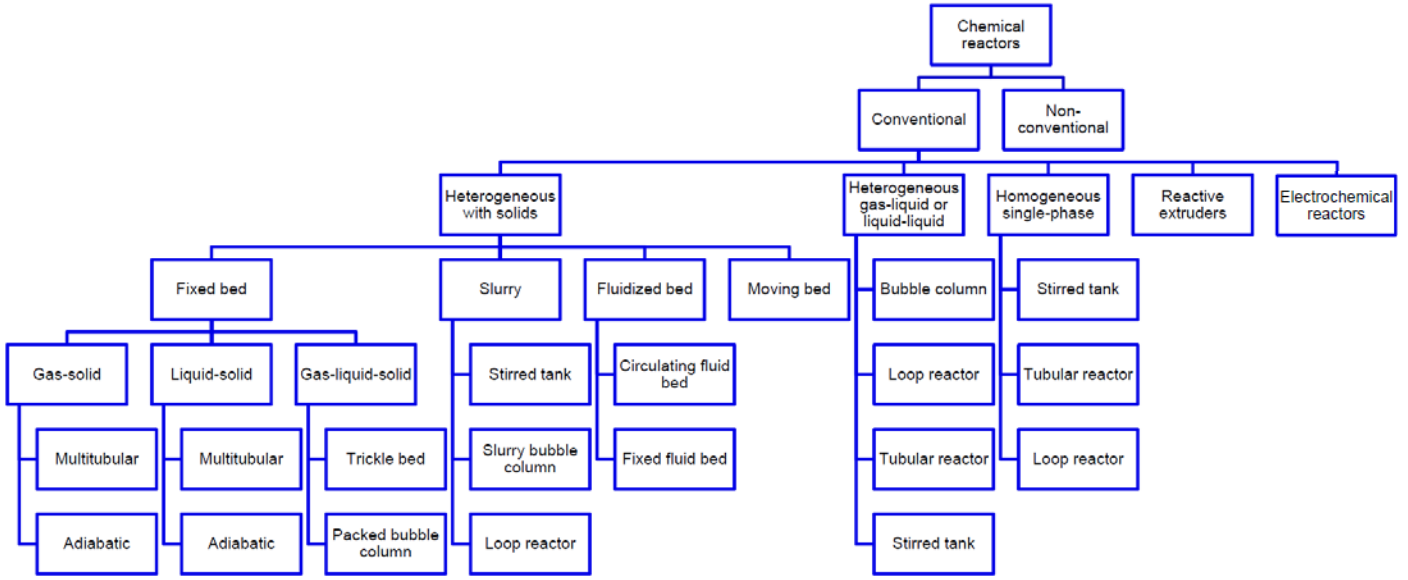
Cross-department enrollment by seniors, masters and Ph.D. students.

I encourage audits for those unsure.



For each reactor type, we assess five key design aspects:

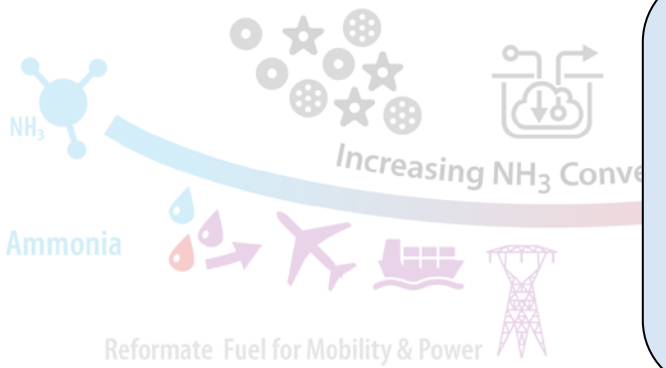
1. Vessel geometry
2. Transport limitations
3. Contacting patterns
4. Heat management options
5. Scale-up strategies



10-1 Reactor taxonomy tree adapted from Dow Industrial Reaction Engineering Course, CISTAR Exclusive Professional Development, The Dow Chemical Company. Accessed 2021 April 16.

I study reaction engineering across a multitude of energy technologies

Catalyst discovery for ammonia autothermal reforming



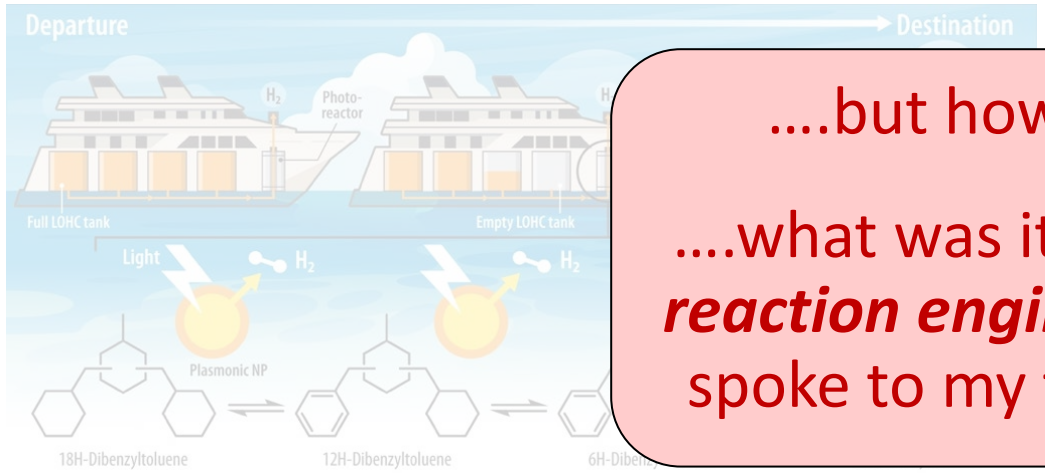
Electrochemical reactor scale-up for CO_x reduction

➢ (The only) common theme:

All my projects involve a chemical reactor and a chemical reaction.

I am agnostic to application.

Photoreaction engineering for liquid organic H_2 carriers



Aviation turbine-relevant soot generation and

….but how did I get here?

….what was it about becoming a ***reaction engineering leader*** that spoke to my true way of being?

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I’m instinctively drawn to the interfaces—and powered by purpose

- I like to color, **but not inside the lines**
- I like to compete **by <u>not</u> competing**
- Reaction engineering is the **ultimate puzzle**
  - I solve crucial problems in technological, generational, economic, political, social, financial and ethical dimensions
- Reaction engineering has become **a lost (and found) art**
  - I found purpose in preserving its practice, discipline, legacy and educational training
  - ➢ **A metaphor for my leadership identity:** *achieving understanding, being understood, creating intrinsic value & connecting others*

12-1 “Indiana Jones and the Raiders of the Lost Ark” photographs adapted from Google Images. Accessed 12 February 2025.

VIGNETTE #1: grand challenges in biofuels—ghosts of past and present

Elegant concept, but several technical and economic shortcomings at commercial scale.

- HUGE challenges with the biomass itself!
  - Challenges at the commercial scale with ***feedstock variability*** and ***handling***
  - Plants are very complex at a molecular level… and ***certain things (acetate, lignin) get in the way*** of making cellulosic fuels

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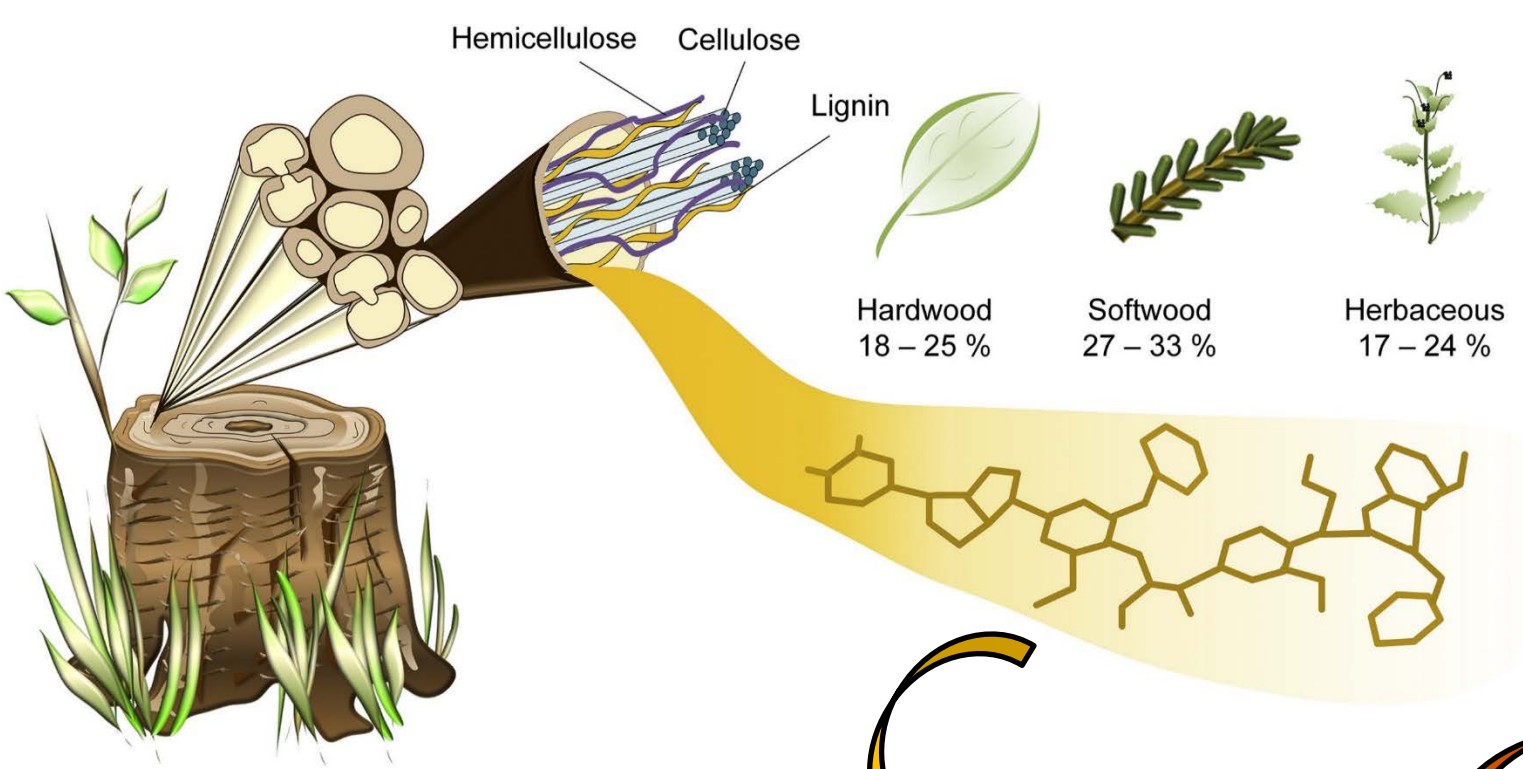
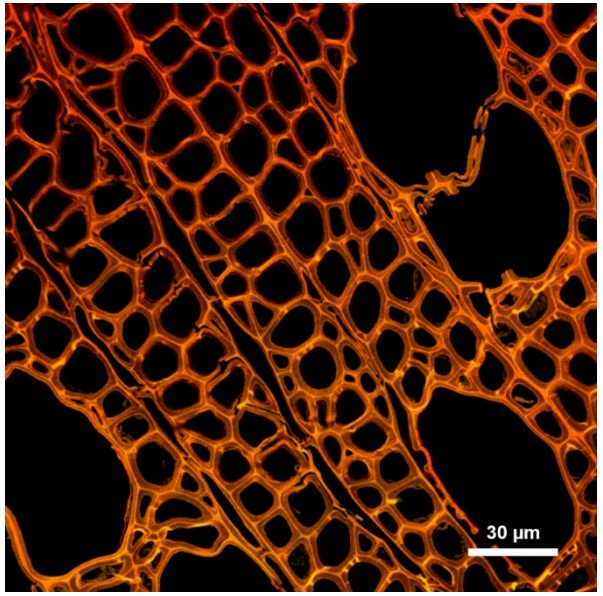
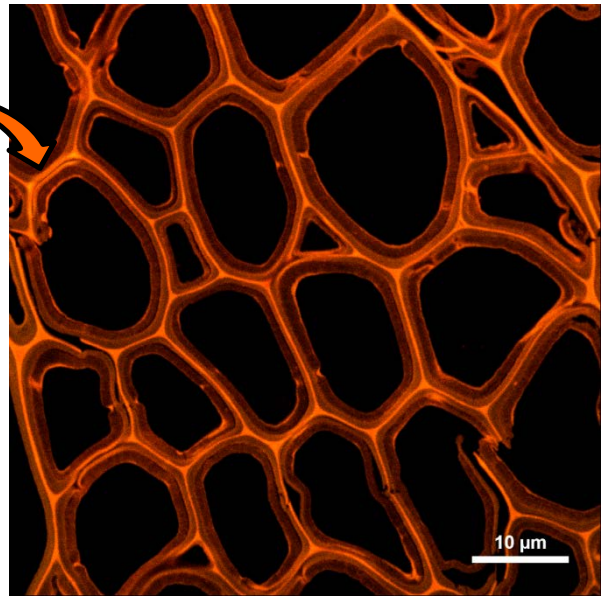
13-1 Images from Google Images. Accessed 16 April 2019.

Ironically, lignin sits at the interfaces of plant cell walls (and it is *annoying*)





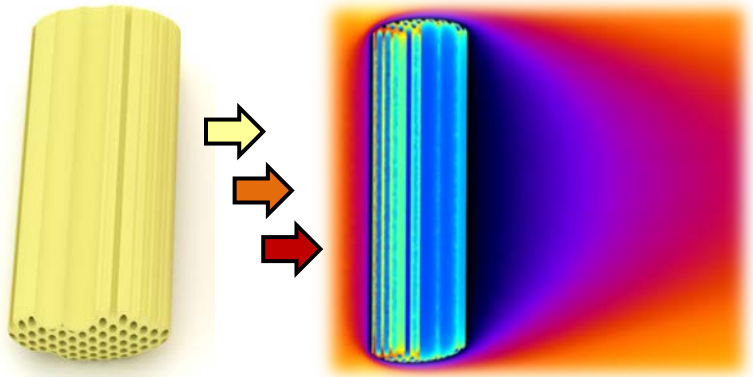


LIGNIN is the "glue" that holds plant cell walls and their components together.

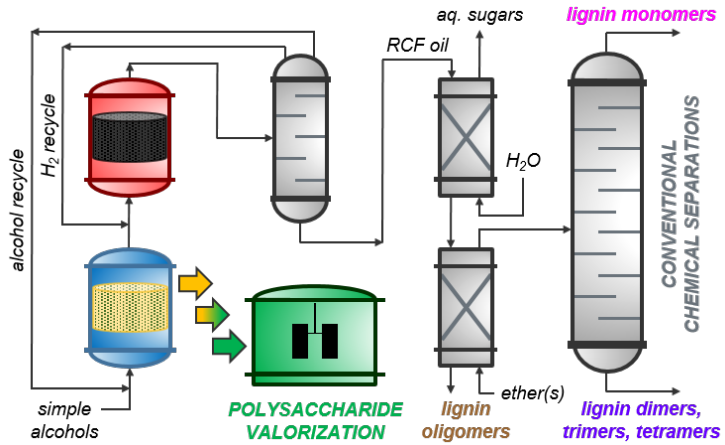
14-1 Cartoon adapted from J. Becker, C. Wittmann, *Biotechnology Advances* (2019).

Reaction engineering uncovered governing phenomena of biomass conversion

Studying ***model lignin molecules*** to identify sound approaches



Deconstructing real lignin at the ***laboratory process scale***



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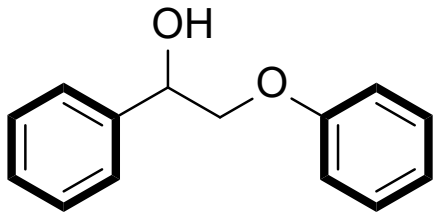

Engineering the chemistry & physics inside of ***single sawdust particles***

INCREASING TIME & LENGTH SCALES

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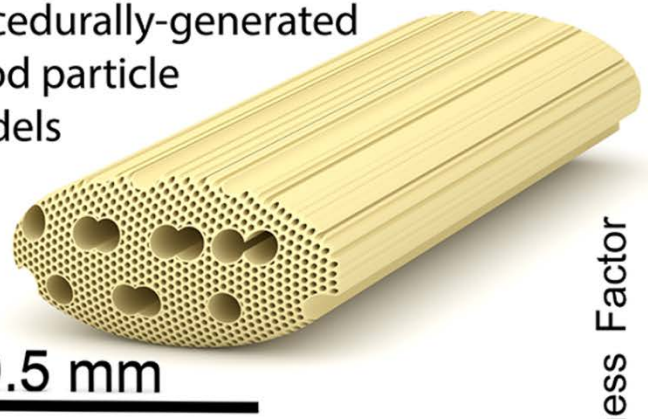
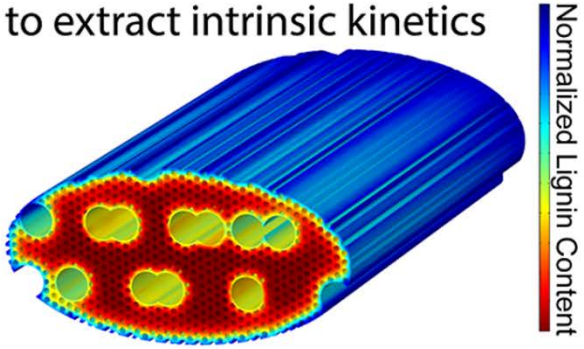
15-1 N. E. Thornburg, M. B. Pecha, D. G. Brandner, M. L. Reed, J. V. Vermaas, W. E. Michener, R. Katahira, T. B. Vinzant, T. D. Foust, B. S. Donohoe, Y. Román-Leshkov, P. N. Ciesielski, G. T. Beckham, *ChemSusChem* 13 4495–4509 (2020)

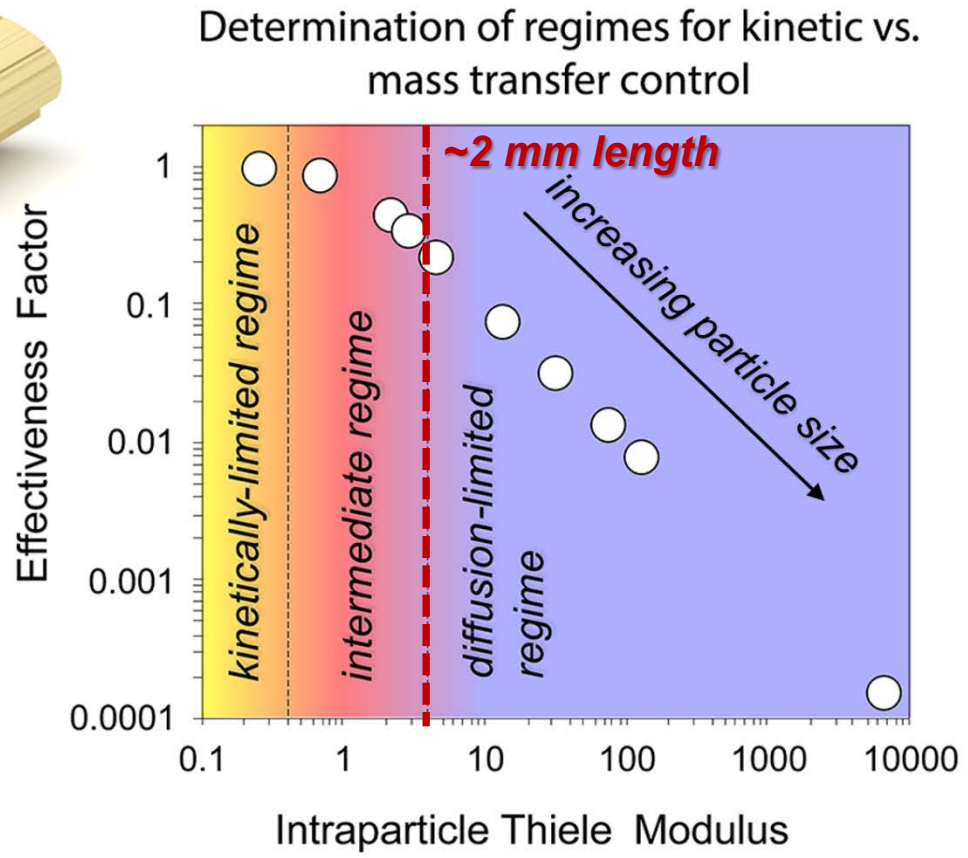
Reaction engineering uncovered governing phenomena of biomass conversion

Procedurally-generated wood particle models



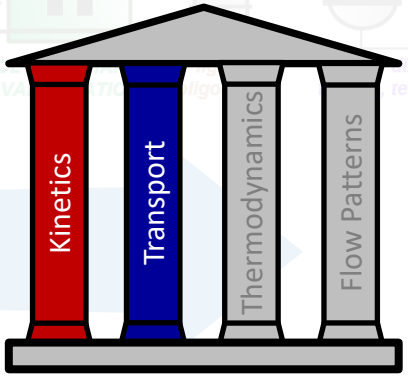
Reaction-diffusion simulations to extract intrinsic kinetics





Mass transfer completely controls the productivity of lignin removal from hardwoods.

The biomass field wasn't aware of its influence on their performance data!



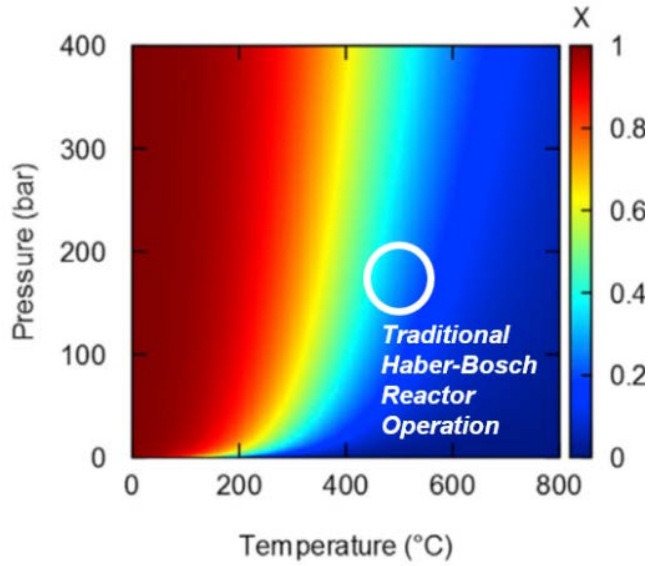
16-1 N. E. Thornburg, M. B. Pecha, D. G. Brandner, M. L. Reed, J. V. Vermaas, W. E. Michener, R. Katahira, T. B. Vinzant, T. D. Foust, B. S. Donohoe, Y. Román-Leshkov, P. N. Ciesielski, G. T. Beckham, *ChemSusChem* 13 4495–4509 (2020)

VIGNETTE #2: Liquid sorption-enhanced Haber-Bosch process discovery

- Ammonia synthesis is **extraordinarily energy-intensive**
  - Consumes 1–2% of global energy supply, and 5% of all natural gas
- **High *T* (>400°C) & high *P* (>100 bar)** required for fast catalyst kinetics and favorable equilibria, followed by **condensation** of NH_3 liquid **(<3 bar)**

➢ ***NH_3 separation costs are staggering!***
Massive decompression–recompression cycles require severely inefficient *P dV* mechanical work—a major energy sink

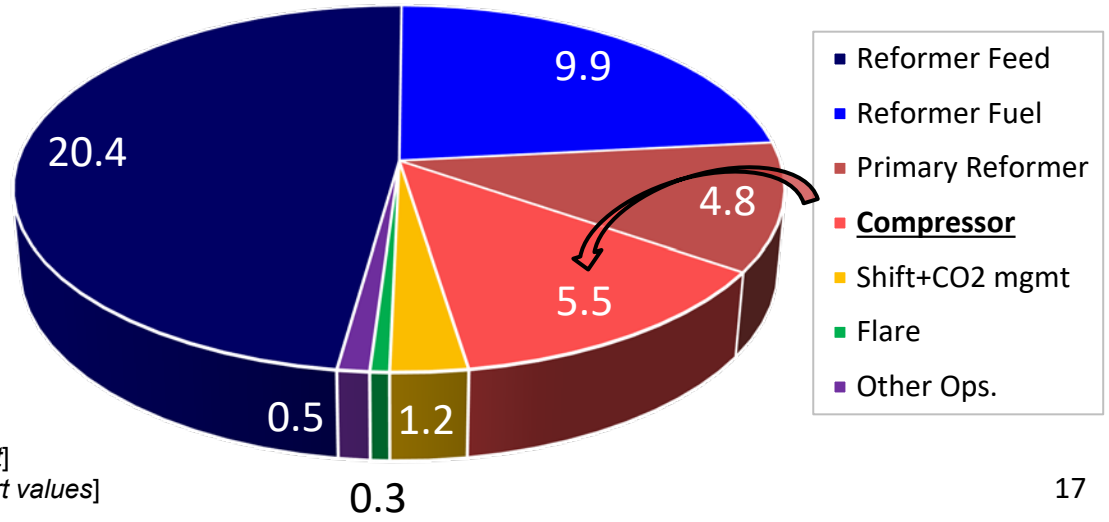
➢ ***Alternative: use an incompressible liquid sorbent for NH_3 to minimize P dV work and recover up to 60% of energy losses***



$$N_{2\,(g)} + 3\,H_{2\,(g)} \rightleftharpoons 2\,NH_{3\,(g)}$$

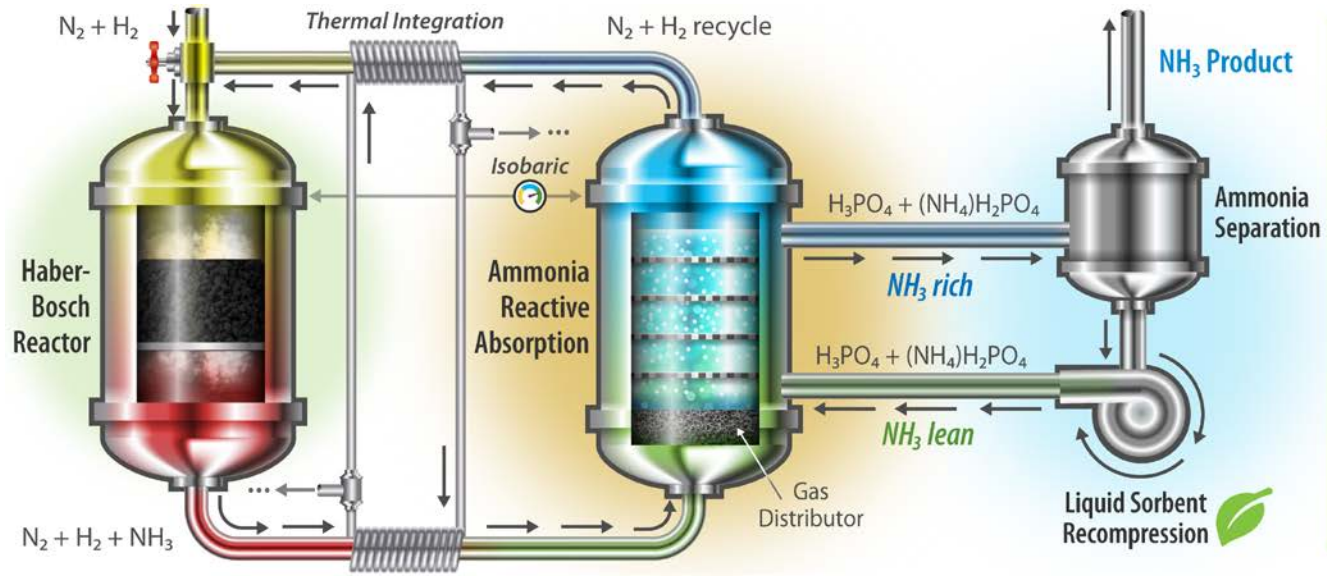
$$\Delta H_{rxn} = -45.9\ \text{kJ mol}^{-1}$$

Estimated energy inputs in GJ (LHV) t^{-1} NH_3 for U.S. Ammonia Plants (*1996*)



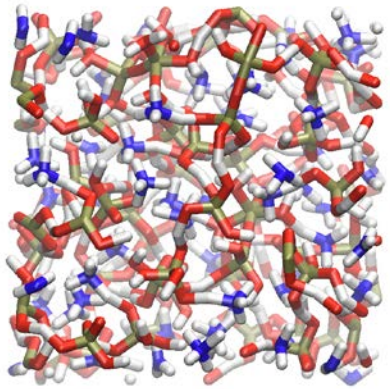
17-1 Z. J. Schiffer, K. Manthiram, *Joule* 1 10–14 (2017) [*rainbow plot*]
17-2 I. Rafiqul, A. Voss et al., *Energy* 30 2487–2504 (2005) [*pie chart values*]

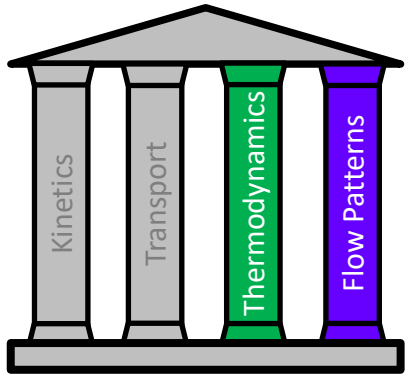
Reaction engineering enabled “new” separation routes for an “old” chemical

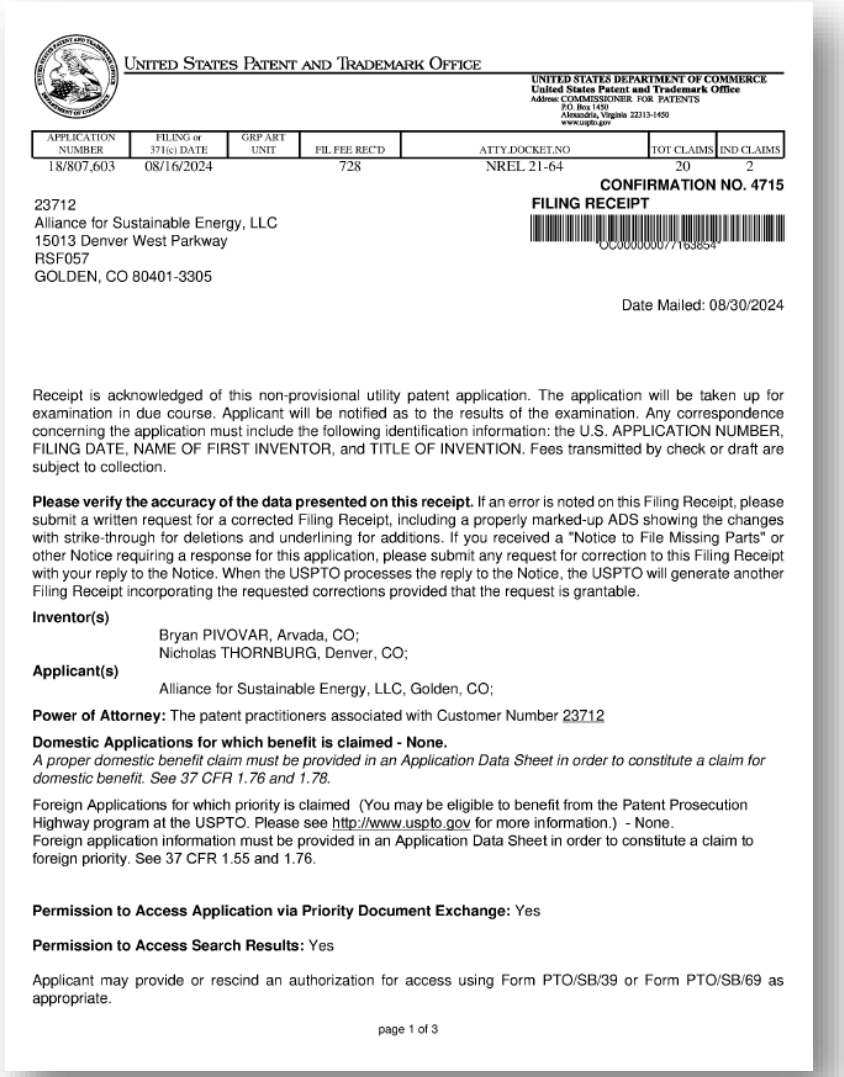


CRITICAL ADVANTAGES:

1. Minimal energy losses to compression and mechanical work
2. New opportunities for thermal integration
3. Options for direct process intensification combining ammonia synthesis & liquid absorptive capture







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APPLICATION NUMBER	FILING or 371(c) DATE	GRP ART UNIT	FIL FEE REC'D	ATTY.DOCKET.NO	TOT CLAIMS	IND CLAIMS
18/807,603	08/16/2024		728	NREL 21-64	20	2

CONFIRMATION NO. 4715

23712
Alliance for Sustainable Energy, LLC
15013 Denver West Parkway
RSF057
GOLDEN, CO 80401-3305

FILING RECEIPT

Date Mailed: 08/30/2024

Receipt is acknowledged of this non-provisional utility patent application. The application will be taken up for examination in due course. Applicant will be notified as to the results of the examination. Any correspondence concerning the application must include the following identification information: the U.S. APPLICATION NUMBER, FILING DATE, NAME OF FIRST INVENTOR, and TITLE OF INVENTION. Fees transmitted by check or draft are subject to collection.

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Inventor(s)
Bryan PIVOVAR, Arvada, CO;
Nicholas THORNBURG, Denver, CO;

Applicant(s)
Alliance for Sustainable Energy, LLC, Golden, CO;

Power of Attorney: The patent practitioners associated with Customer Number 23712

Domestic Applications for which benefit is claimed - None.
A proper domestic benefit claim must be provided in an Application Data Sheet in order to constitute a claim for domestic benefit. See 37 CFR 1.76 and 1.78.

Foreign Applications for which priority is claimed (You may be eligible to benefit from the Patent Prosecution Highway program at the USPTO. Please see http://www.uspto.gov for more information.) - None.
Foreign application information must be provided in an Application Data Sheet in order to constitute a claim to foreign priority. See 37 CFR 1.55 and 1.76.

Permission to Access Application via Priority Document Exchange: Yes

Permission to Access Search Results: Yes

Applicant may provide or rescind an authorization for access using Form PTO/SB/39 or Form PTO/SB/69 as appropriate.

page 1 of 3

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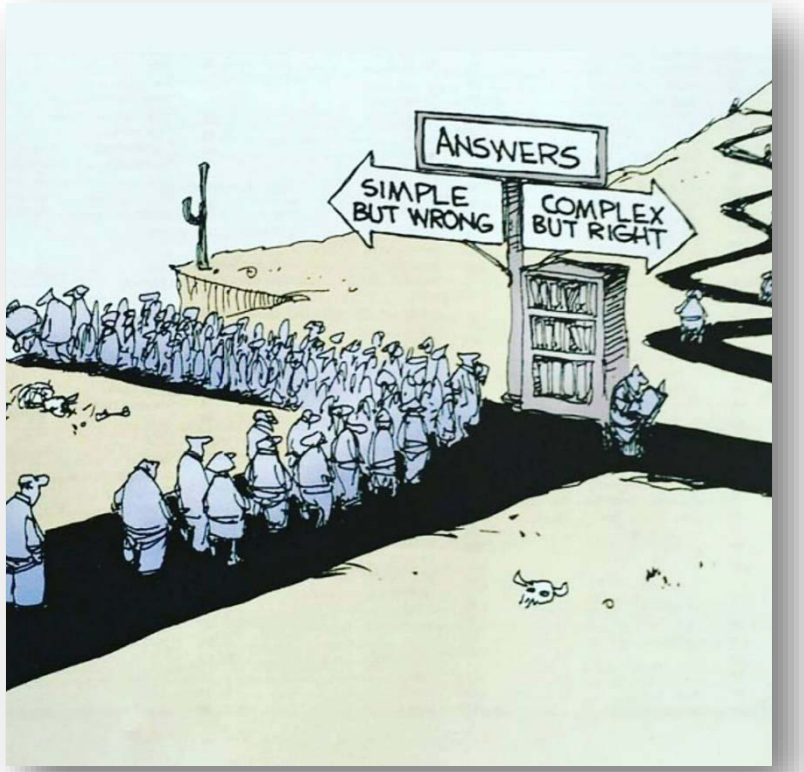
18-1 B. S. Pivovar, N. E. Thornburg, “LIQUID SORBENT-ENHANCED AMMONIA PRODUCTION,” U.S. Patent Application No. 18/807,603. Filed 16 August 2024.

Parting advice and inspiration from interfacial philosophies

- **Critical thinking matters now more than ever**
- Be 10% more skeptical of people you agree with—and 10% more charitable to people you disagree with
  - Thoughtful disagreement doesn't start with "You're wrong!" It begins with "I'd love to understand your thinking better"
  - ➢ ***Let ideas flow like music:*** remember, harmony is the pleasing arrangement of different tones, voices, or instruments—not the combination of identical sounds
- Make a list of your values, and revisit it every year
- **Stay present, notice more, focus on being (vs. doing)**
  - Insights flow naturally and effortlessly when you are present, well-rested and leaning into your inner craft
  - Give ourselves and others the privilege of our own process



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19-1 Cartoon adapted from Adam Grant social media. Accessed 12 February 2025.

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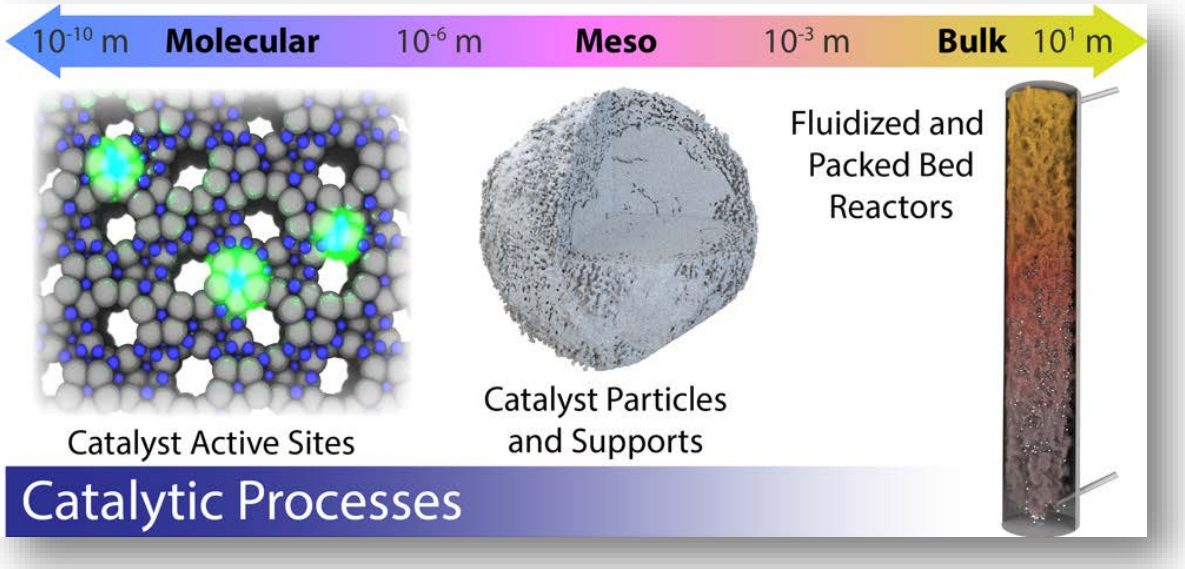

Thank you!

Terrified of mass balances?
Do reactor equations keep you up at night?
Did your horoscope mention transport limitations?

Let's create together!

Nicholas.Thornburg@nrel.gov

21-1 P. N. Ciesielski, M. B. Pecha, N. E. Thornburg, M. F. Crowley, X. Gao, O. Oyedeji, H. Sitaraman, N. Brunhart-Lupo, *Energy & Fuels* 35 14282-14400 (2021)

NREL