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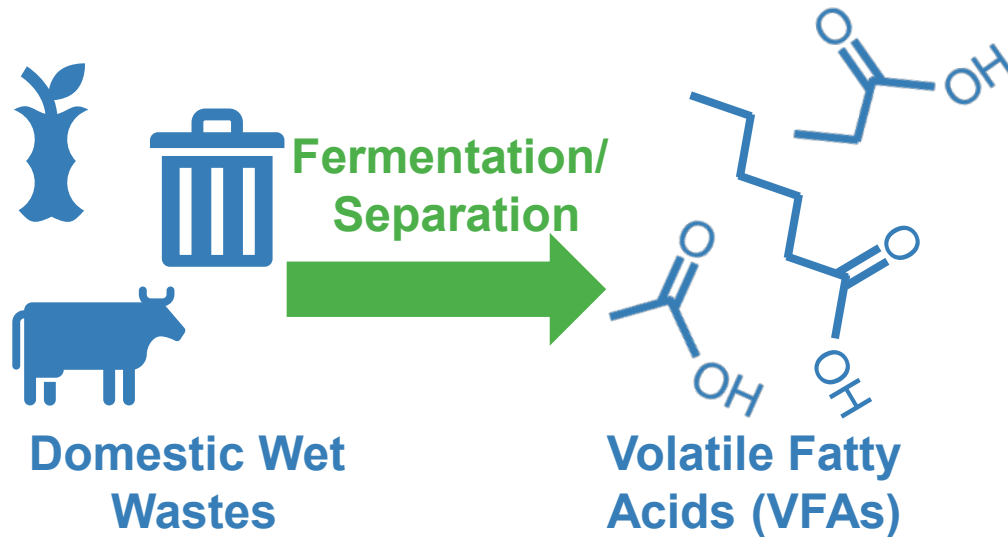
Accelerating catalyst development for wet waste to aromatic aviation fuels using active learning

Cody Wrasman (Cody.Wrasman@nlr.gov)

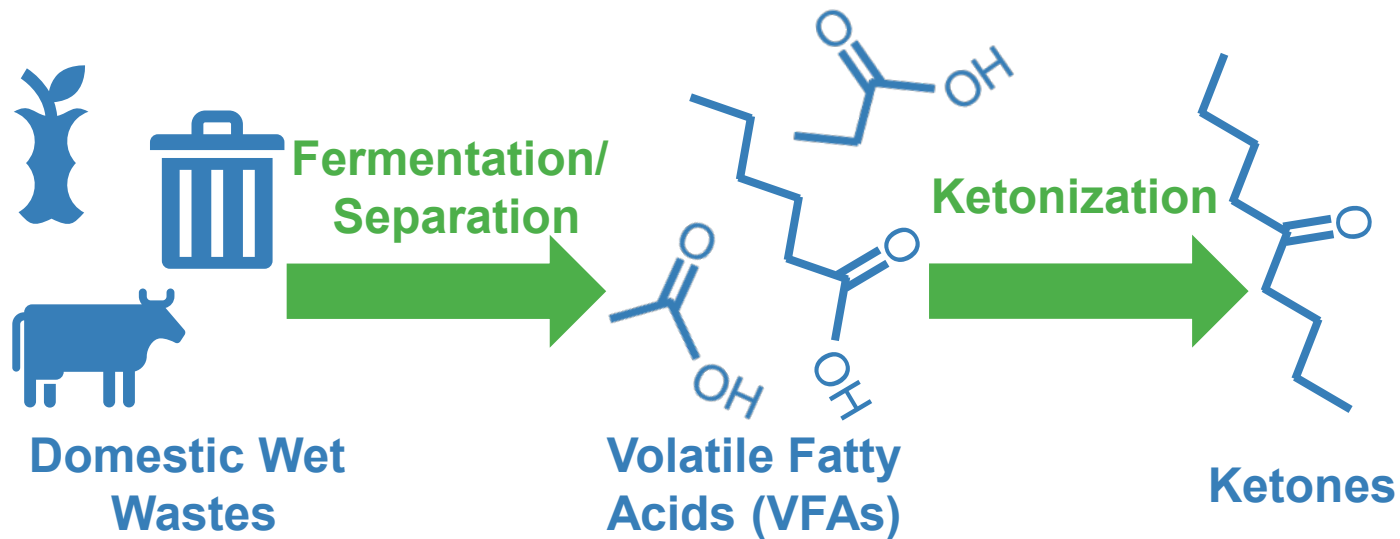
TCBiomass 2026

8/27/2026

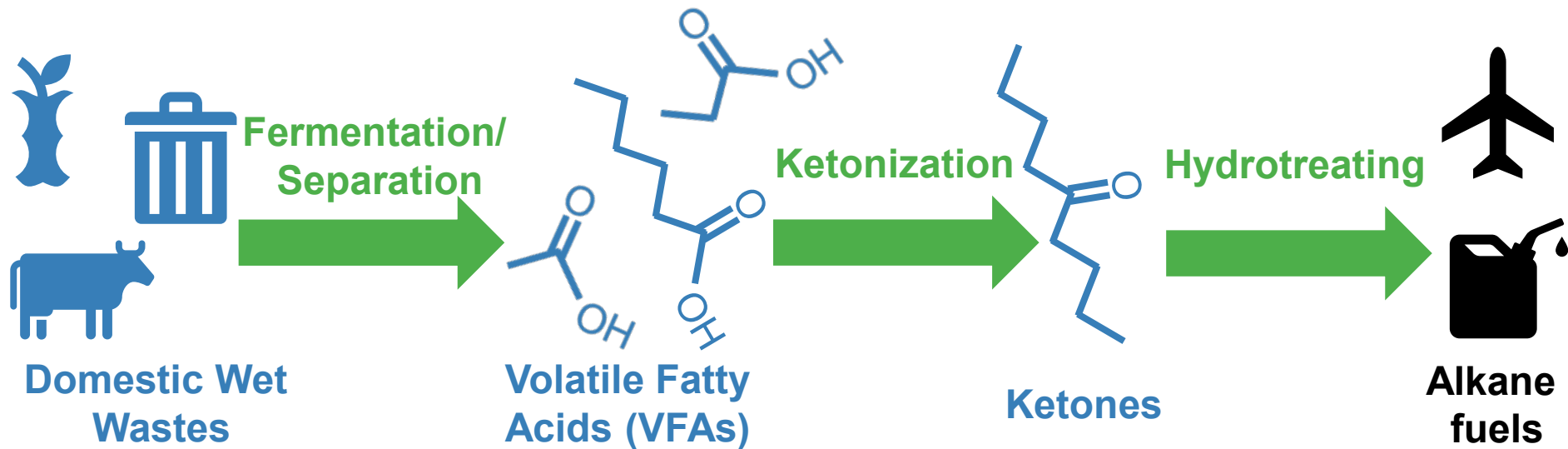
Volatile fatty acids can be transformed into transportation fuels



Volatile fatty acids can be transformed into transportation fuels

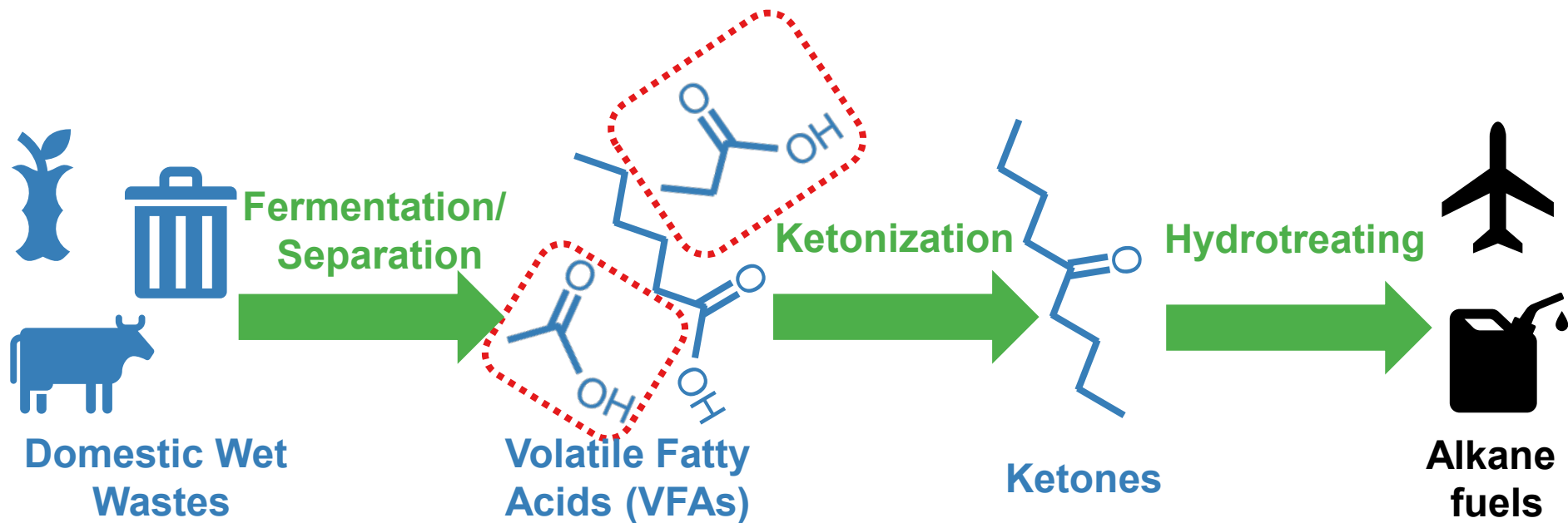


Volatile fatty acids can be transformed into transportation fuels



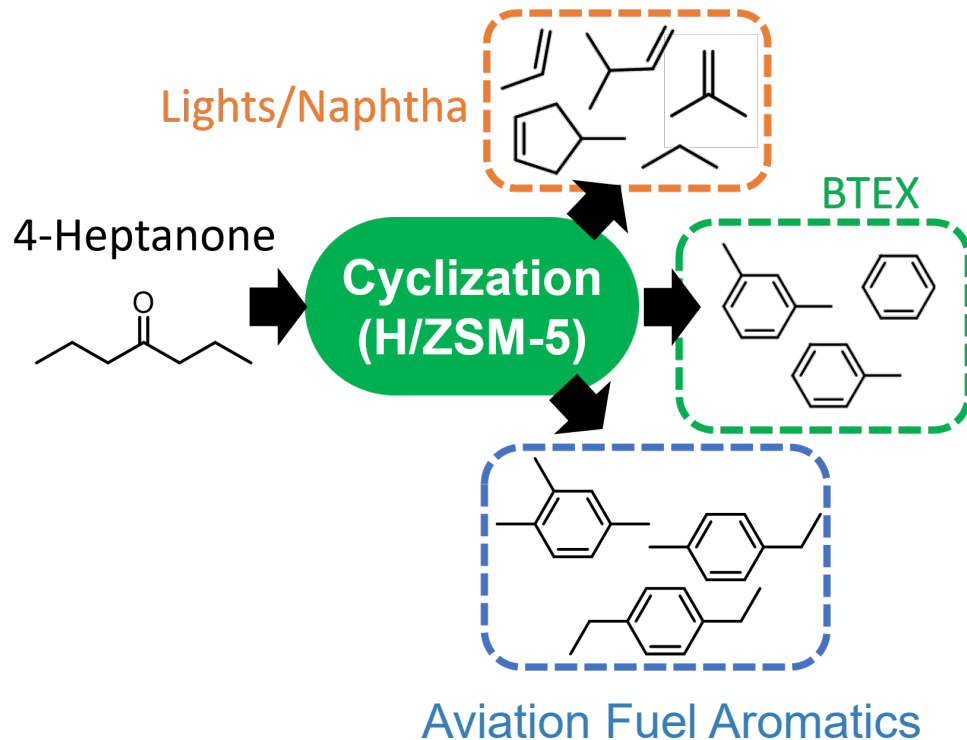
+Pathway utilizes negative cost feedstock and can achieve negative GHG emissions

Volatile fatty acids can be transformed into transportation fuels



Short chain acids produce ketones too short for fuels (can exceed 50 wt. % depending on fermentation)

Previous work has demonstrated several potential products for short ketones

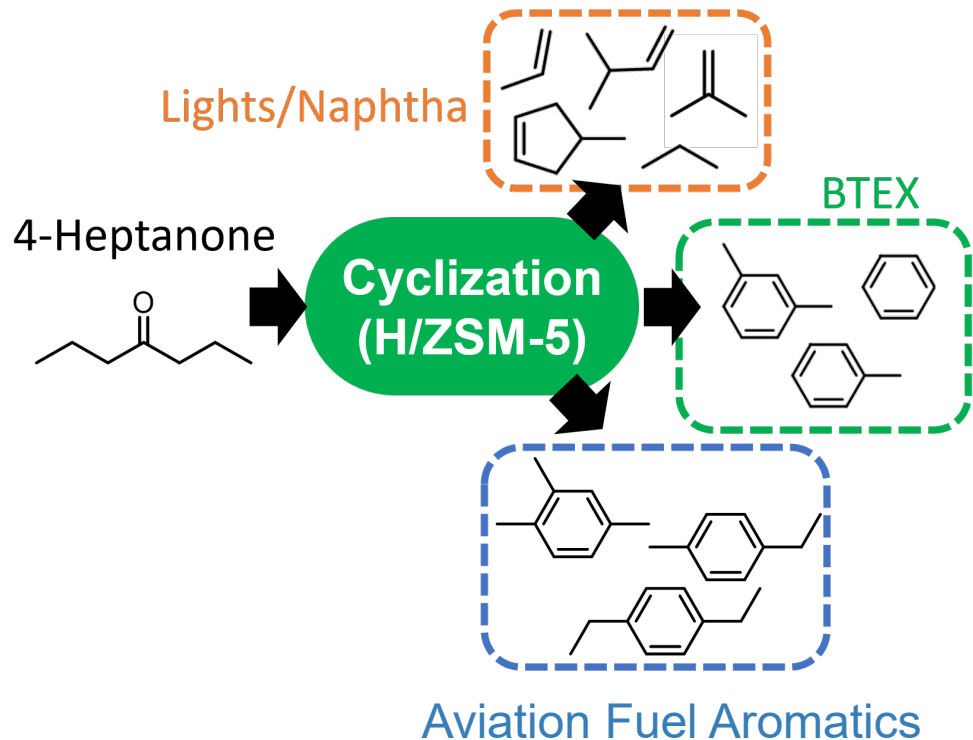


Use ZSM-5 catalyst to carry out cyclization of model short ketone

- Incomplete (>95%) conversion favors olefins
- Complete conversion maximizes aromatic products



Previous work has demonstrated several potential products for short ketones



Project objectives:

1. Identify most favorable product to pursue from short ketones
2. Optimize ZSM-5 catalyst to maximize yields of the desired product

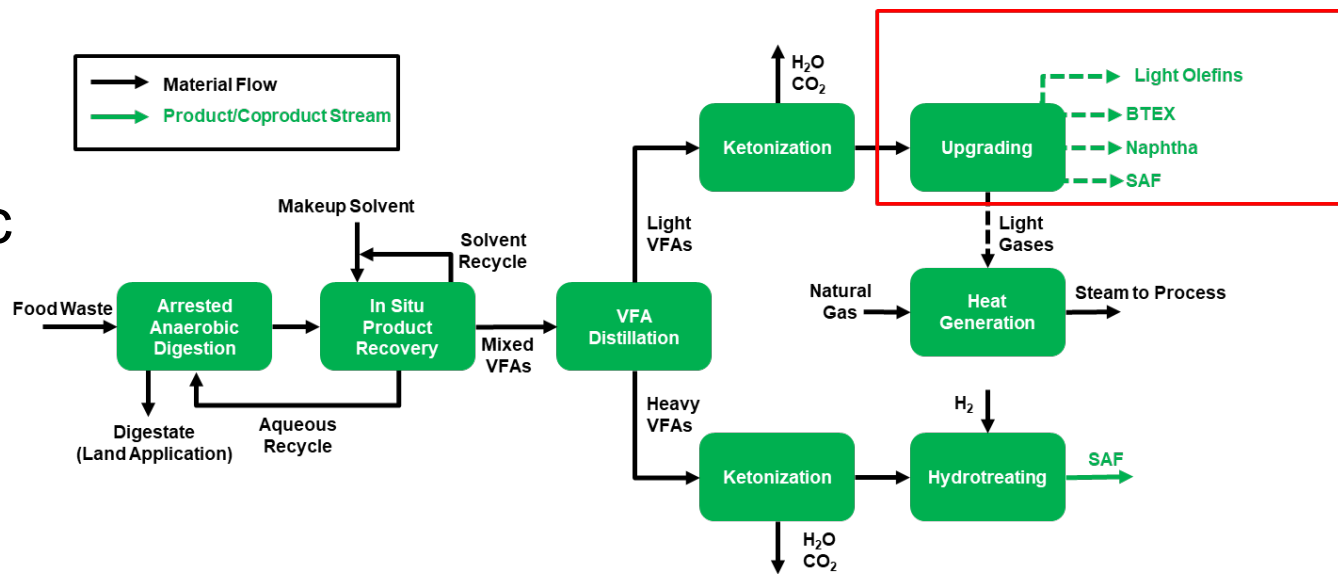


Develop a Technoeconomic model to identify the most attractive short ketone products

Wiatrowski, M. et al. *Renew. Energ.* 2024

Consider hypothetical yields directed to olefins, BTEX, and aromatic aviation fuel (SAF)

- Predict implications on aviation fuel selling price



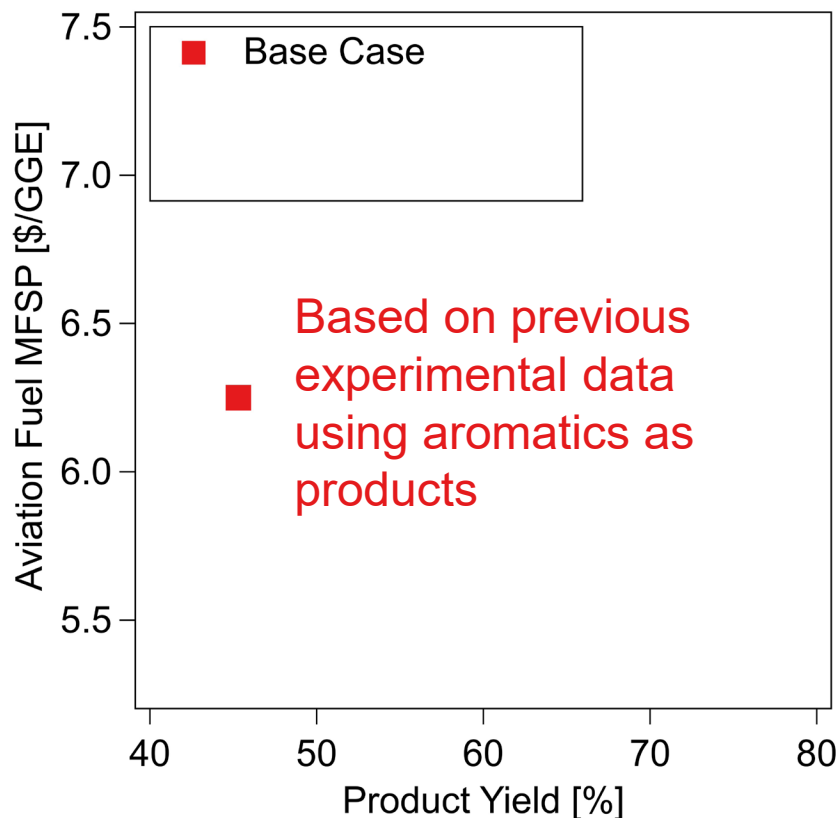
Model scale: 1000 wet tons/day food waste

Feedstock cost: 0 \$/ton

Develop a Technoeconomic model to identify the most attractive short ketone products

Consider hypothetical yields directed to olefins, BTEX, and aromatic aviation fuel (SAF)

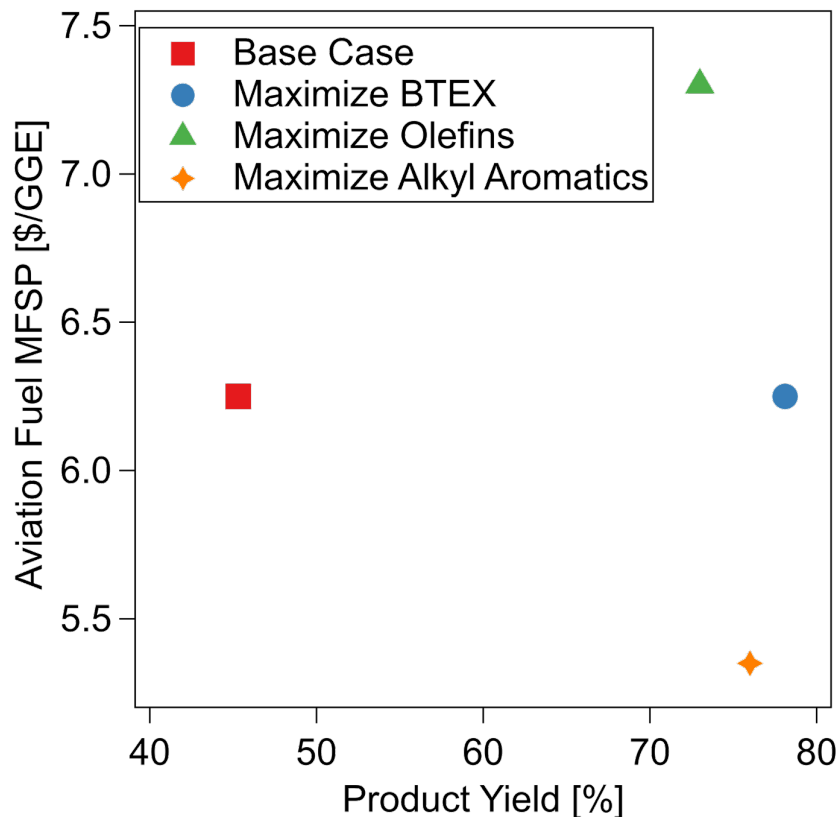
- Predict implications on aviation fuel selling price



Develop a Technoeconomic model to identify the most attractive short ketone products

TEA reveals 2 \$/GGE difference between possible target products

- Olefin separation is too costly at this relatively small scale
- BTEX value is fixed at 614 \$/ton in MFSP calculation
 - less valuable than calculated MFSP and typical aviation fuel at 750 \$/ton
- Model recommends pursuing alkyl aromatics



Modify baseline ZSM-5 catalyst to push selectivity towards aromatic products

Ketone cyclization is catalyzed by acid sites within ZSM-5

Consider modifying

1. Catalyst acidity – balance cyclization and cracking to lights
2. Addition of Ga or Zn – facilitate H-transfer to make aromatics
3. Metal loading – modify acid/metal site ratio
4. Reaction temperature – alter rates in reaction network

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Factorial Design of Experiments
with midpoints
would require 81 experiments

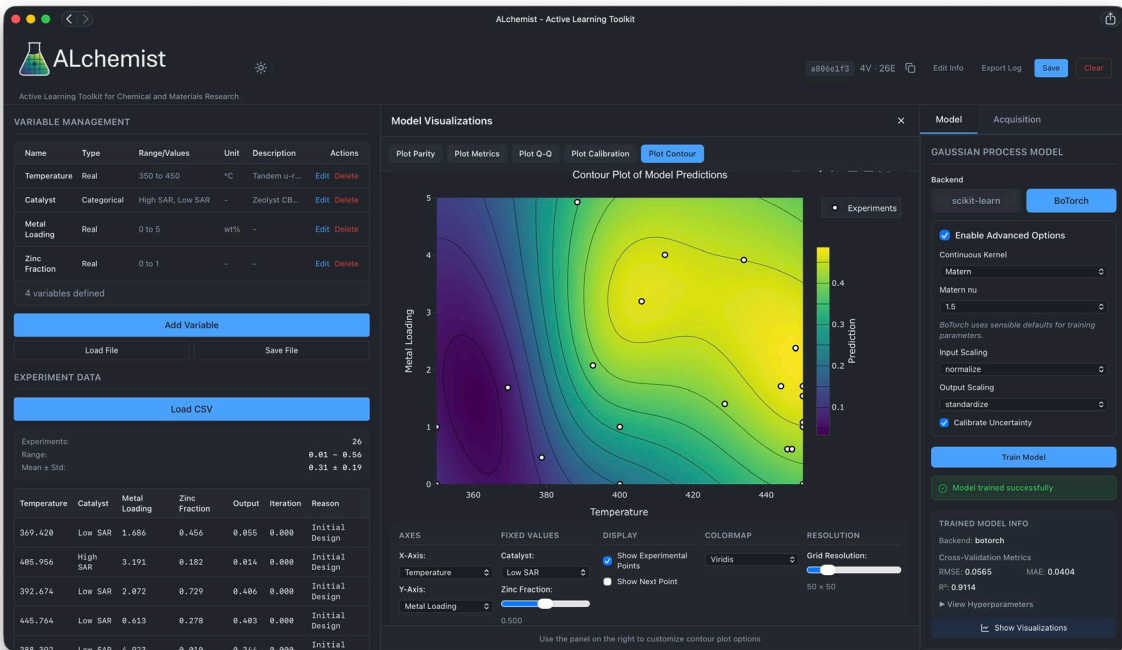


Leverage active learning
to accelerate
optimization

NLR developed the ALchemist active learning toolkit to accelerate process optimization

ALchemist allows non-experts to leverage active learning to iteratively optimize their system

- No coding required
- Creates experimental designs with all variable types
- Open source
- Advanced data visualization options



NLR developed the ALchemist active learning toolkit to accelerate process optimization

1. Define
parameter space



2. Identify initial
experiments



3. Train
initial model

Model Initiation

NLR developed the ALchemist active learning toolkit to accelerate process optimization

1. Define parameter space



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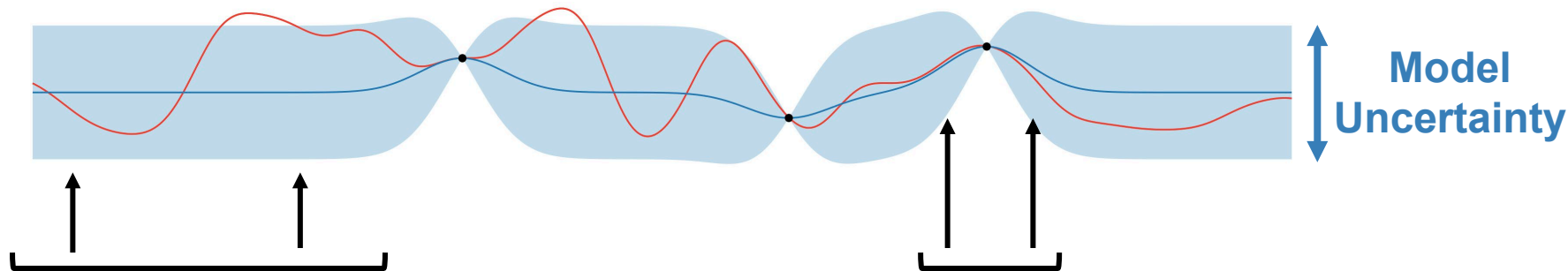
Model Initiation



4a. Evaluate acquisition function

Experimental Iteration

• Observations — Predictions — Actual Function



Explore – Most unknown area

Exploit – predicted maximum

NLR developed the ALchemist active learning toolkit to accelerate process optimization

1. Define parameter space



2. Identify initial experiments



3. Train initial model

Model Initiation



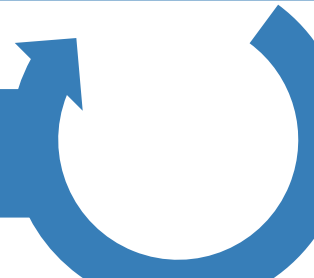
4a. Evaluate acquisition function

Experimental Iteration

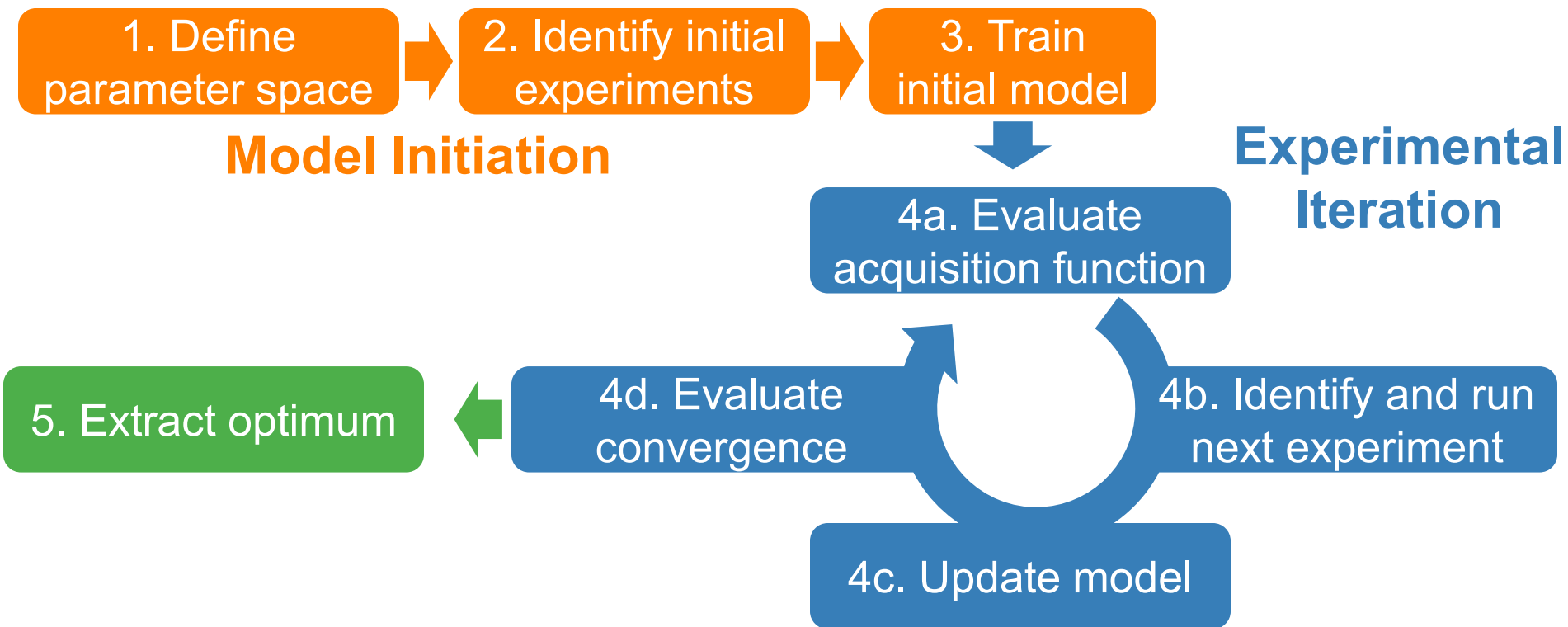
4d. Evaluate convergence

4b. Identify and run next experiment

4c. Update model



NLR developed the ALchemist active learning toolkit to accelerate process optimization



Utilize ALchemist to evaluate cyclization of 4-heptanone



Model Initiation

1. Define boundaries for parameters of interest
 1. Catalyst acidity – ZSM-5 SAR 40 and 80
 2. Addition of Ga or Zn – Zn fraction from 0 to 1
 3. Metal loading – metal loading between 0 and 5 wt. %
 4. Reaction temperature – 350 – 450 °C (system defined)

Utilize ALchemist to evaluate cyclization of 4-heptanone

1. Define
parameter space



2. Identify initial
experiments



3. Train
initial model

Model Initiation

1. Define boundaries for parameters of interest
2. Use ALchemist to generate initial experiments to fill parameter space

Utilize ALchemist to evaluate cyclization of 4-heptanone

1. Define
parameter space



2. Identify initial
experiments



3. Train
initial model

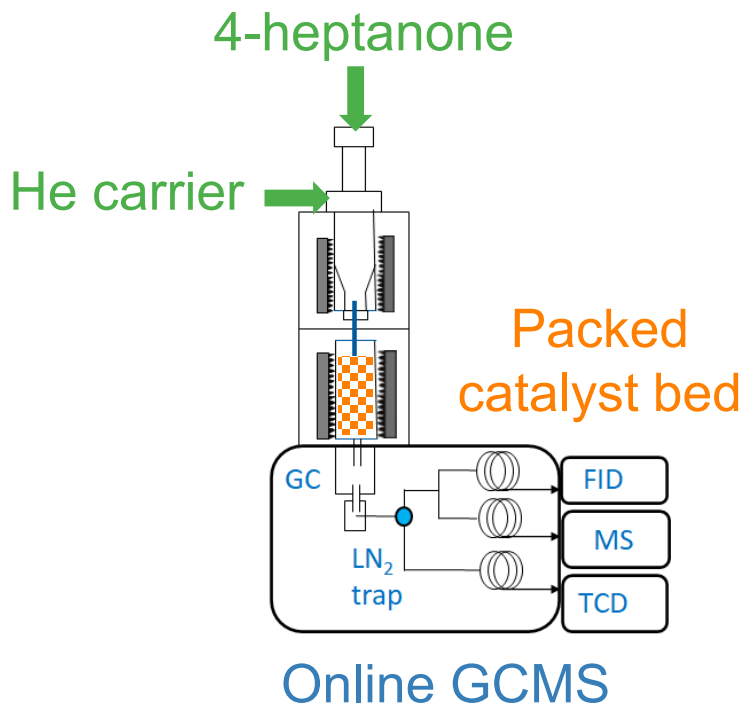
Model Initiation

1. Define boundaries for parameters of interest
2. Use ALchemist to generate initial experiments to fill parameter space
3. Fit Gaussian Process model from initial data

Collect data in a Frontier tandem micro-reactor

Inject 1 μL 4-heptanone over 25 mg catalyst

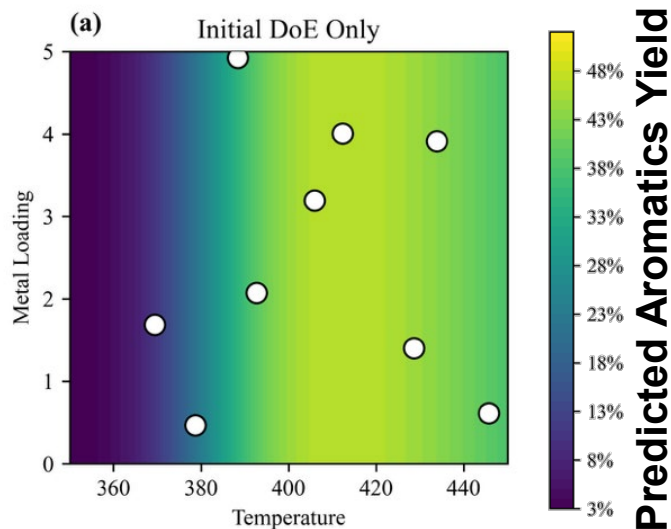
- Collect 10 initial points identified by ALchemist to cover parameter space
- Add 9 experiments from previous work



Collect data in a Frontier tandem micro-reactor

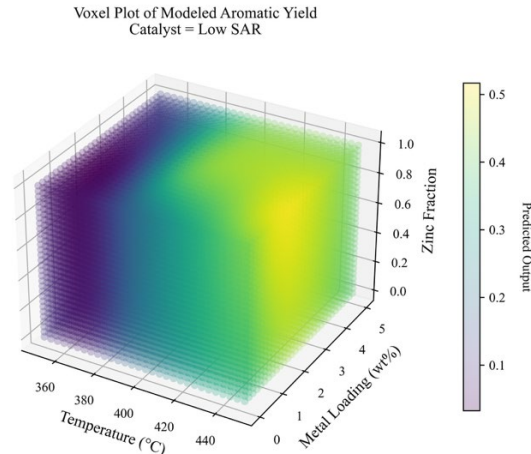
ALchemist recommended initialization points

Slice for 100% Zn, High acidity



Inject 1 μL 4-heptanone over 25 mg catalyst

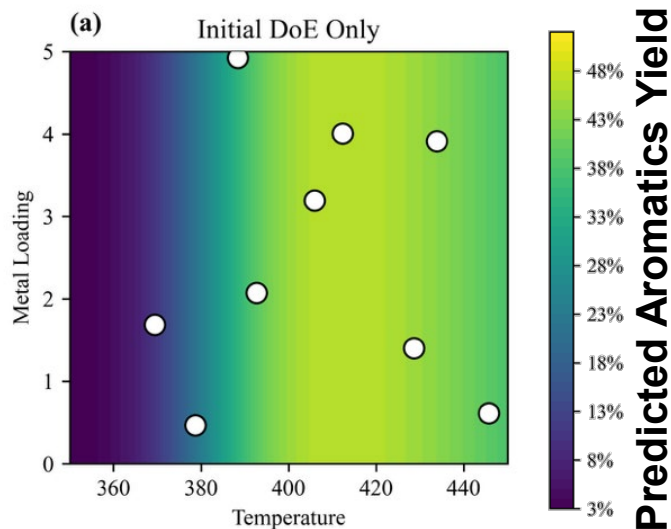
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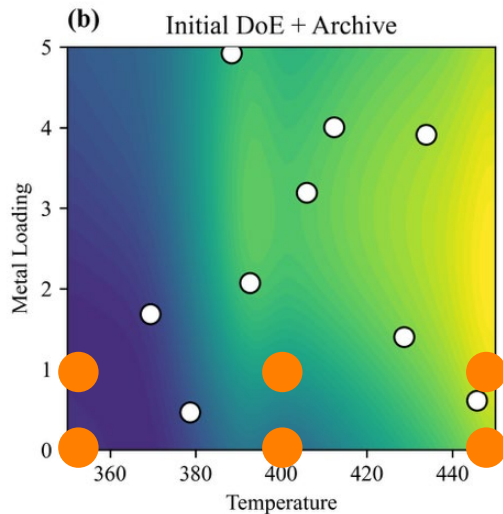
ALchemist recommended initialization points

Slice for 100% Zn, High acidity



Inject 1 μL 4-heptanone over 25 mg catalyst

- Collect 10 initial points identified by ALchemist to cover parameter space
- Add 9 experiments from previous work



Added experiments change prediction contours

Utilize ALchemist to evaluate cyclization of 4-heptanone

1. Define parameter space



2. Identify initial experiments



3. Train initial model

Model Initiation



4a. Evaluate acquisition function

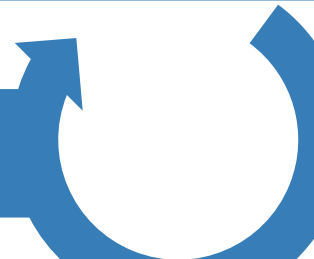
Experimental Iteration

- Exploit model to test predicted maxima
- Use model root mean squared error (RMSE) as convergence measure

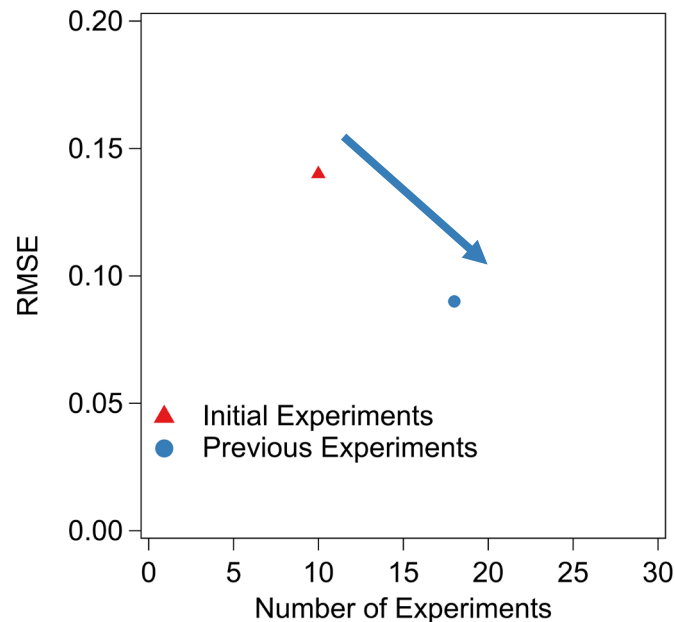
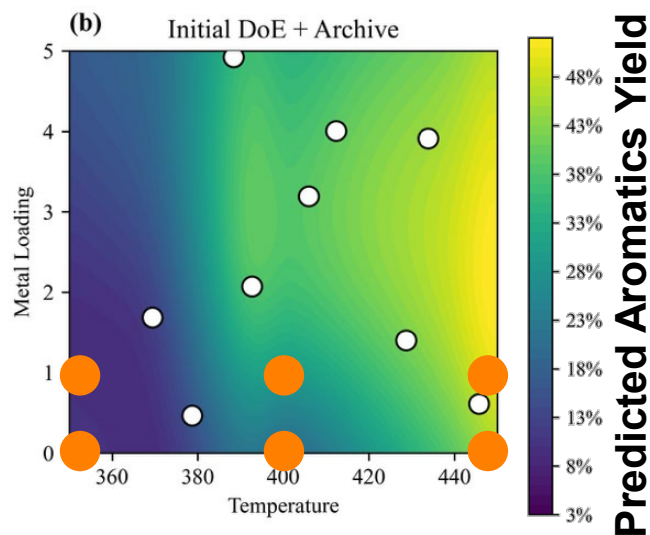
4d. Evaluate convergence

4b. Identify and run next experiment

4c. Update model



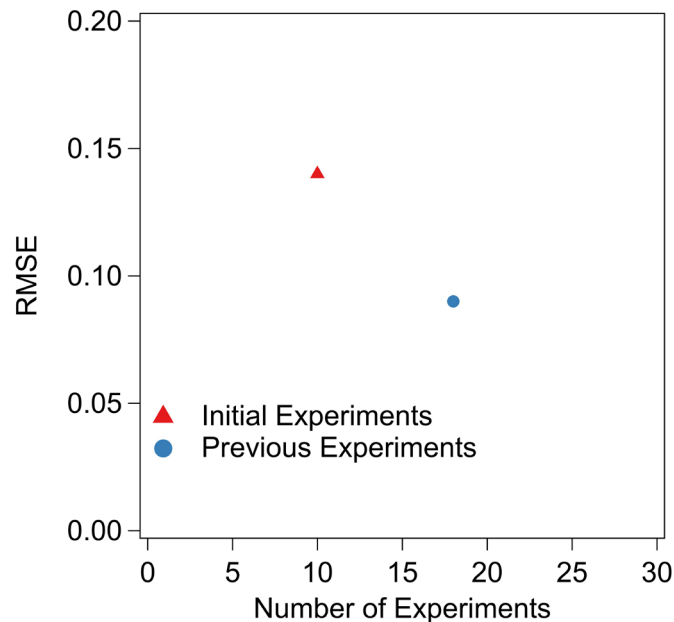
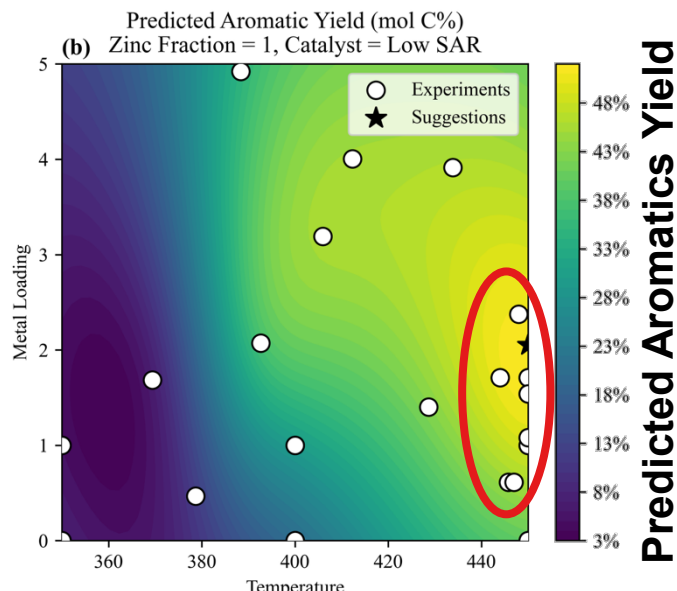
Track experimental performance using RMSE



Adding previous experiments
reduced RMSE by over 30%

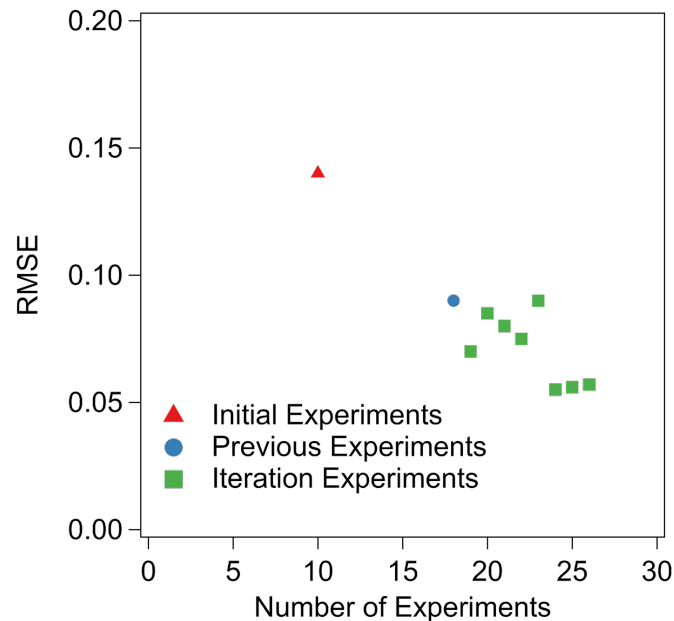
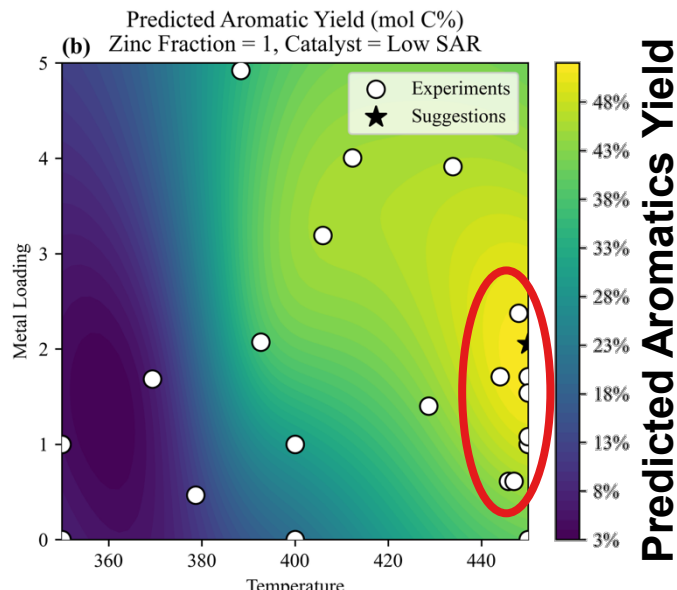
Track experimental performance using RMSE

Model identified high temperature and intermediate metal loading as attractive



Track experimental performance using RMSE

Model identified high temperature and intermediate metal loading as attractive



Iterative experiments lowered RMSE

Utilize ALchemist to evaluate cyclization of 4-heptanone

1. Define
parameter space



2. Identify initial
experiments



3. Train
initial model

Model Initiation



4a. Evaluate
acquisition function

**Experimental
Iteration**

5. Extract optimum



4d. Evaluate
convergence



4b. Identify and run
next experiment

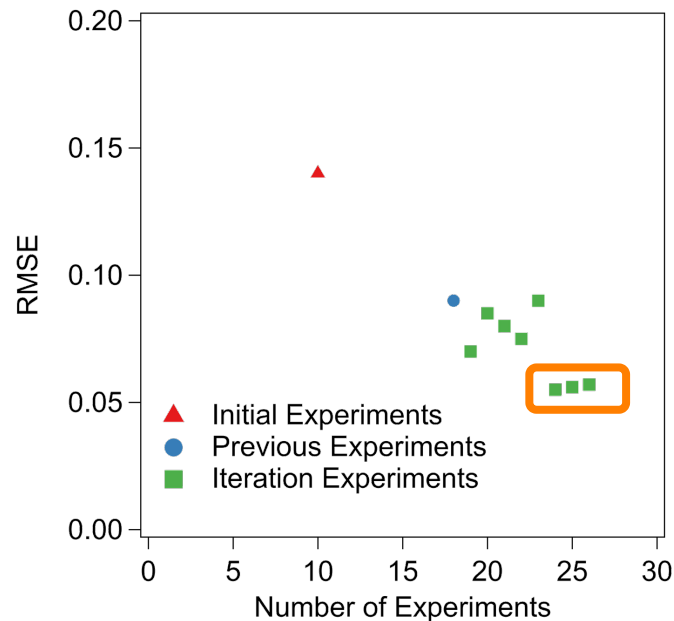
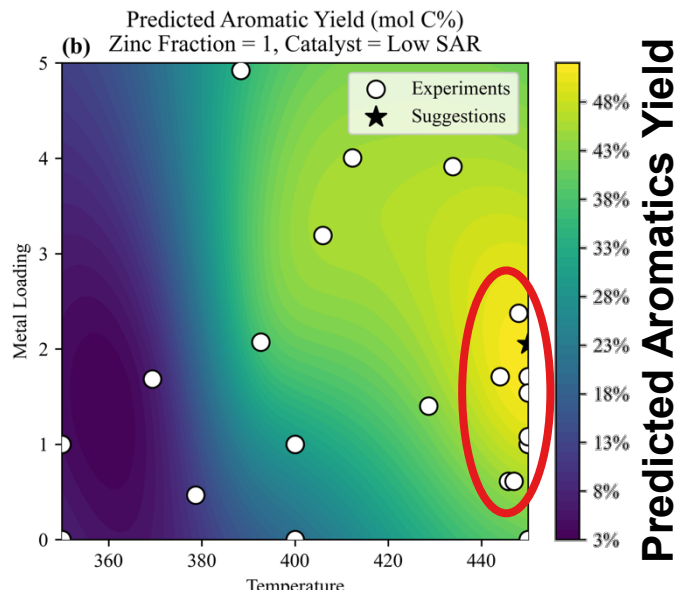


4c. Update model

Stop iterating when RMSE
stops improving and predicted
optimum stops changing

Track experimental performance using RMSE

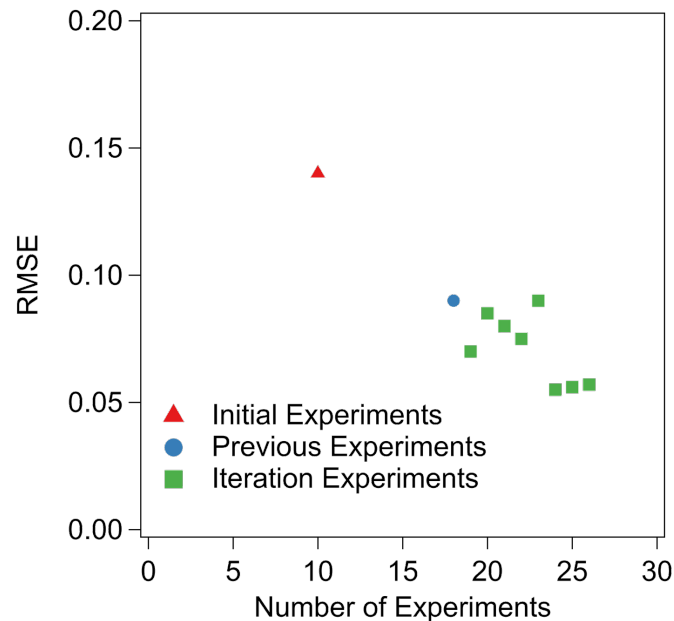
Model identified high temperature and intermediate metal loading as attractive



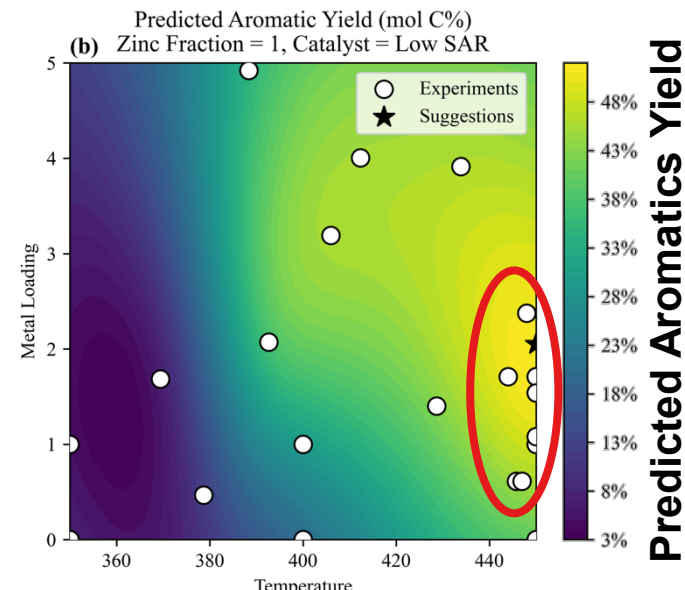
Iterative experiments lowered RMSE
Little improvement past 25 experiments

Track experimental performance using RMSE

Model identified high temperature and intermediate metal loading as attractive

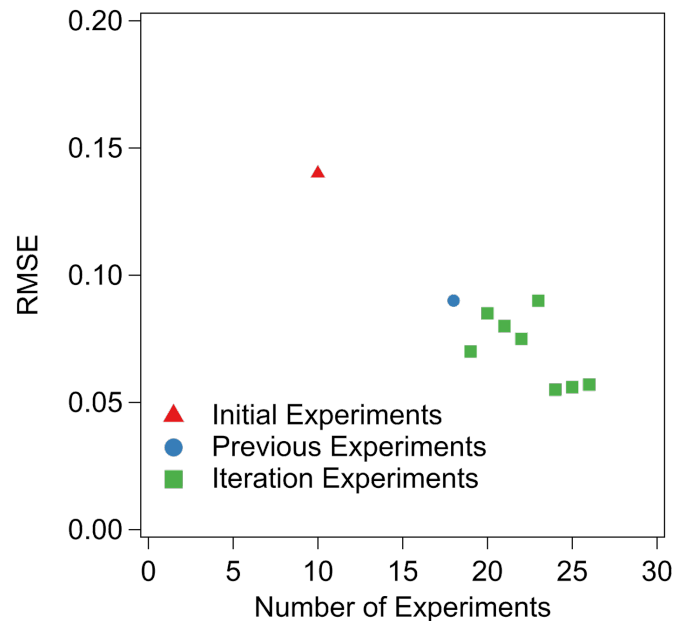


Identify optimum performance at 450 °C, 2 wt. % Zn

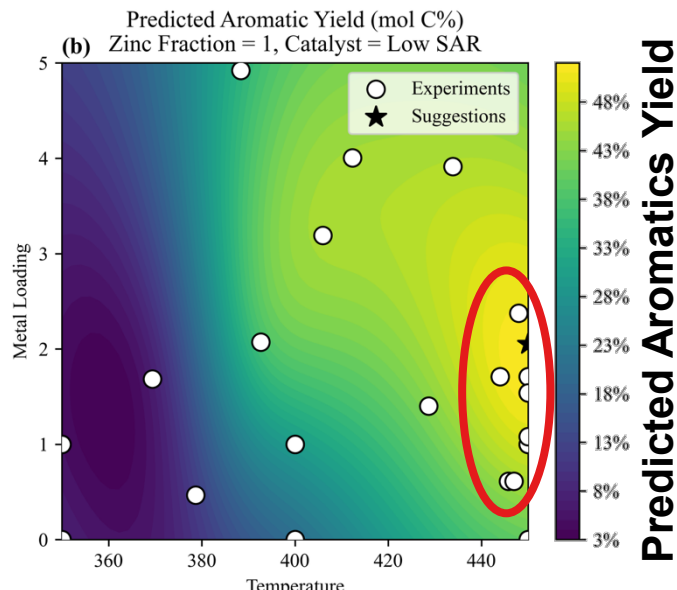


Track experimental performance using RMSE

Model identified high temperature and intermediate metal loading as attractive



Identify optimum performance at 450 °C, 2 wt. % Zn --> Scale up this catalyst



Modify baseline ZSM-5 catalyst to push selectivity towards aromatic products

Ketone cyclization is catalyzed by acid sites within ZSM-5

Consider modifying

1. Catalyst acidity – balance cyclization and cracking to lights
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Factorial Design of Experiments
with midpoints
would require 81 experiments



Achieved optimization in
less than half the
experiments of a factorial
DOE

Evaluate scaled up modified catalyst in a continuous reactor

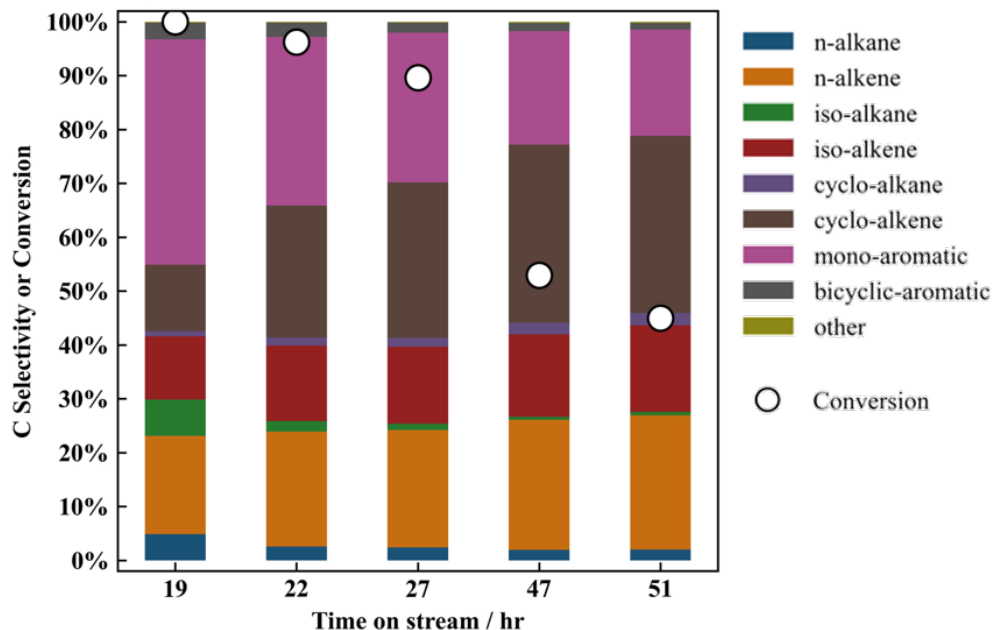
Test baseline and modified ZSM-5 in a continuous reactor

- 450 °C, 1 g catalyst, WHSV = 2.9 h⁻¹
- Feed 4-heptanone through a HPLC pump
- Condense liquid products for GCMS analysis

Evaluate scaled up modified catalyst in a continuous reactor

Test baseline and modified ZSM-5 in a continuous reactor

Unmodified ZSM-5

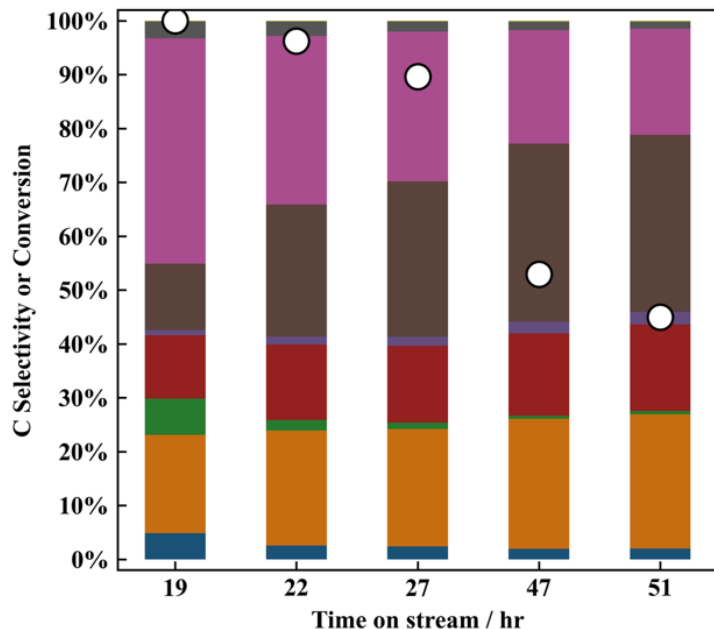


Unmodified catalyst deactivated with time on stream and lost aromatics selectivity to alkenes

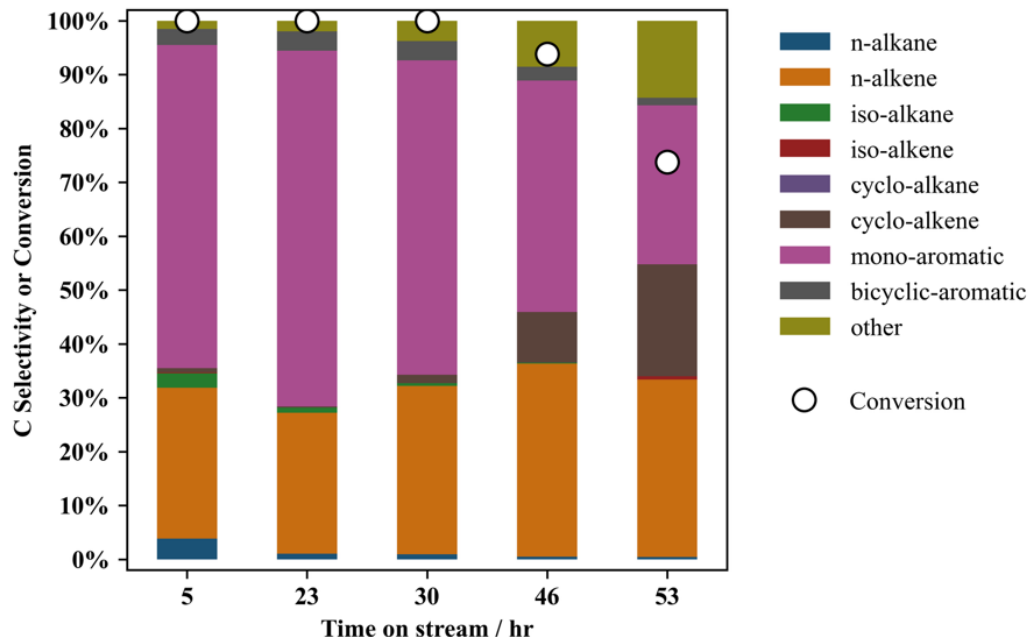
Evaluate scaled up modified catalyst in a continuous reactor

Test baseline and modified ZSM-5 in a continuous reactor

Unmodified ZSM-5



2.0 wt. % Zn ZSM-5

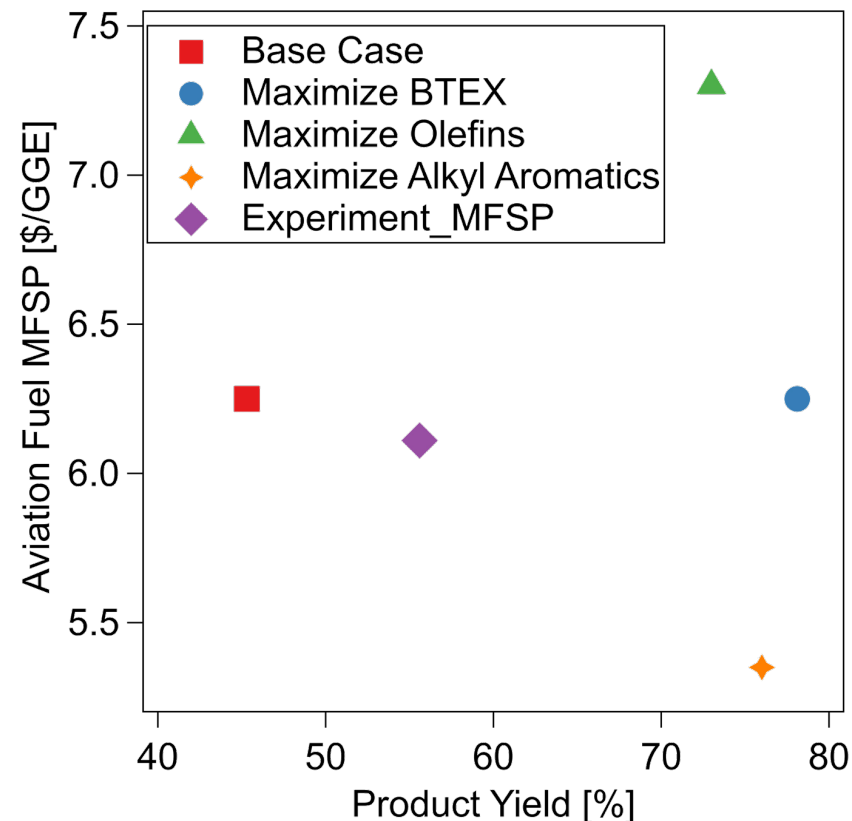


Zn addition maintains activity longer and has ~20-40% higher selectivity to aromatics (H-transfer from Zn)

Use updated experimental results to update TEA calculations

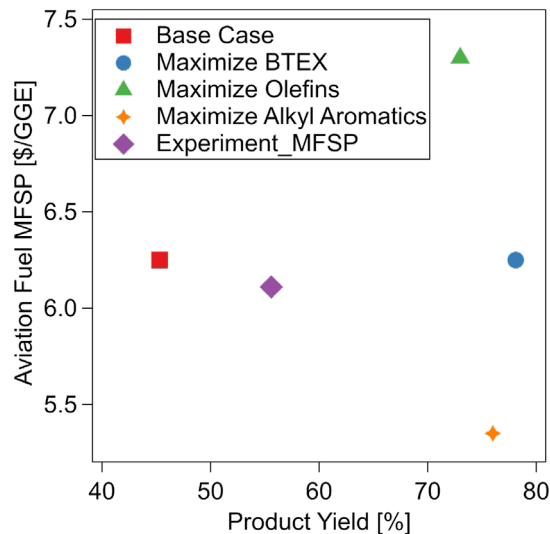
Modified ZSM-5 achieves a 2% decrease in aviation fuel MFSP

- Double BTEX yield to ~40% (less valuable fixed value product) aviation fuel yield improves by 3%



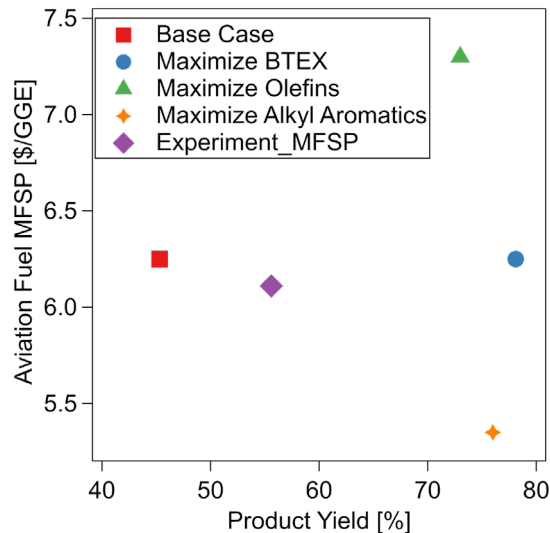
Light ketone cyclization provides a demonstration case for the value of active learning in catalyst development

Utilize TEA to identify attractive products to target

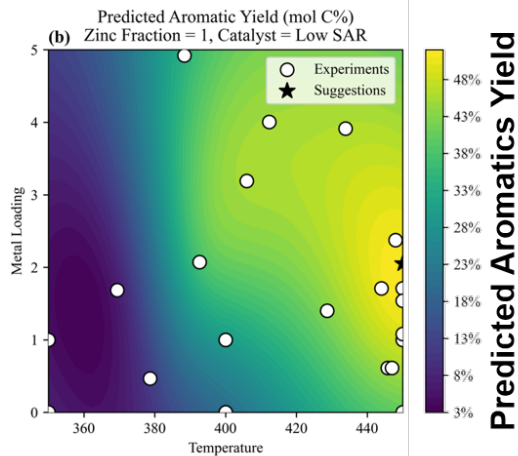


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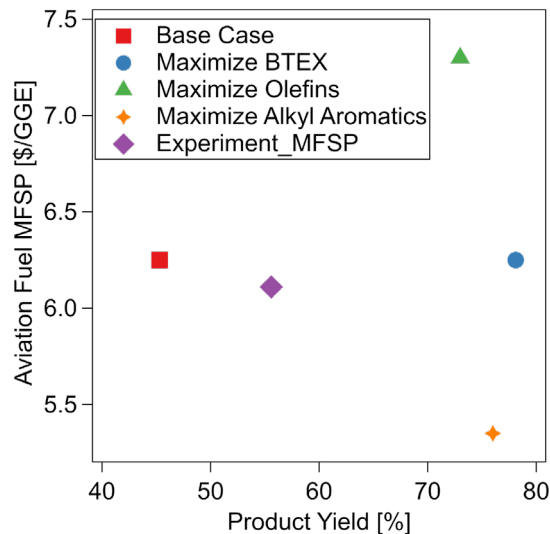


Utilize ALchemist to accelerate catalyst development

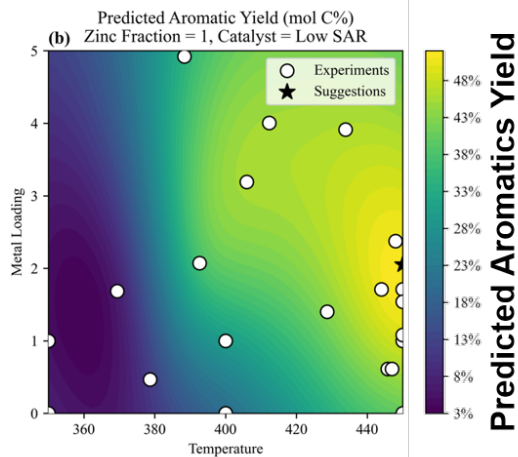


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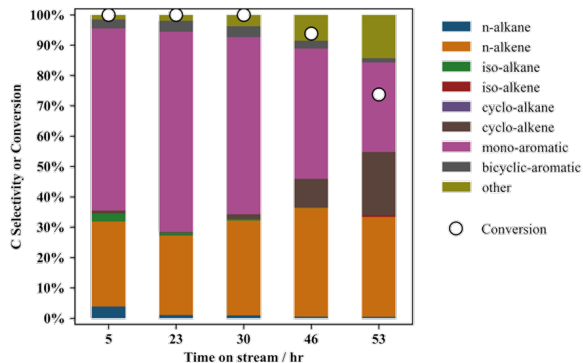
Utilize TEA to identify attractive products to target



Utilize ALchemist to accelerate catalyst development



Achieve a 20% relative improvement in product selectivity



Acknowledgements



Caleb Coatney



Matt Wiatrowski



Jacob Dempsey



ALchemist



ChemCatBio
Chemical Catalysis for Bioenergy



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Accelerating catalyst development for wet waste to aromatic aviation fuels using active learning

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TCBiomass 2026

8/27/2026

Thank you

www.nlr.gov

NLR/PR-5100-101572

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