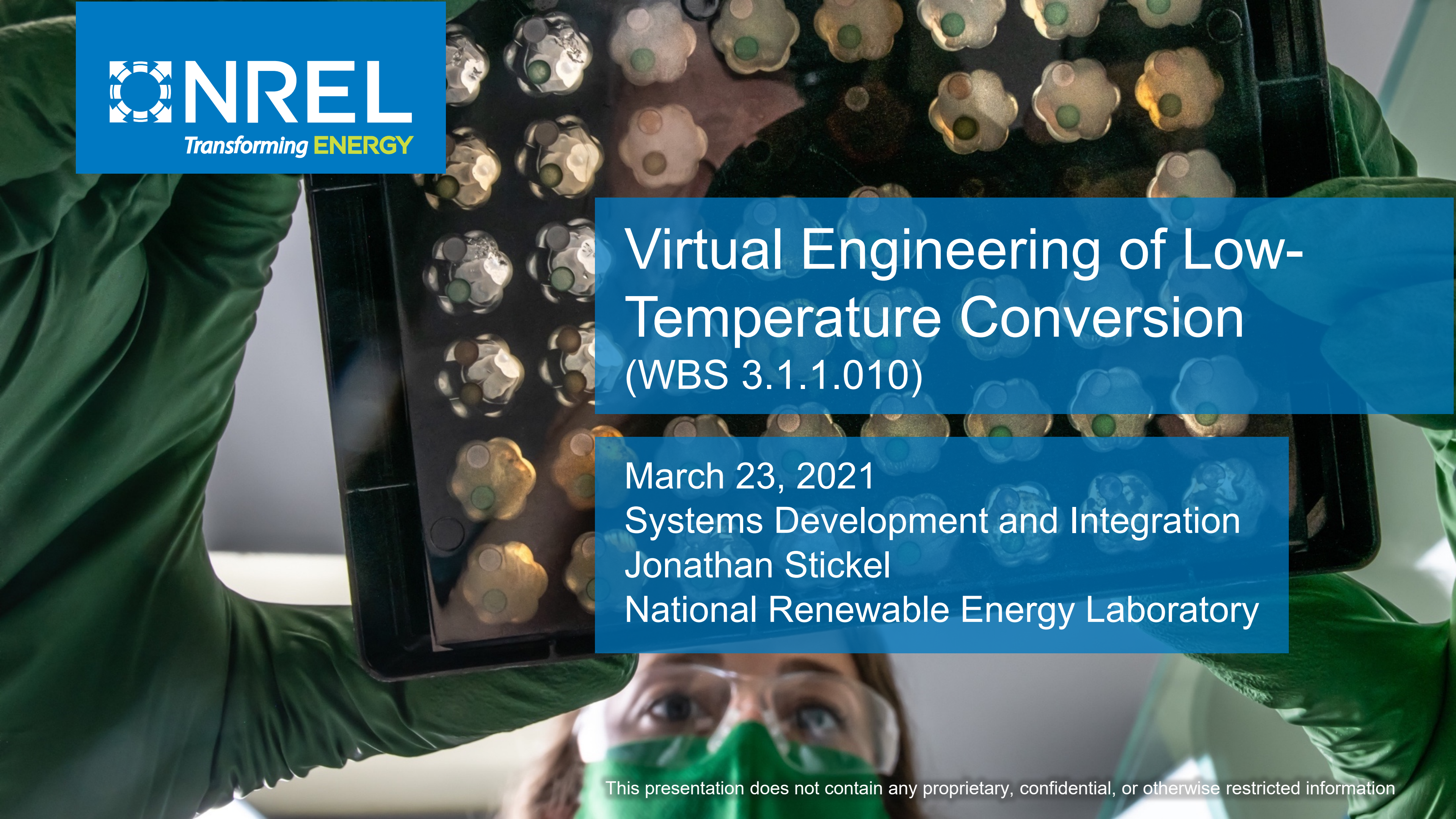


NREL Transforming ENERGY

Virtual Engineering of Low-Temperature Conversion (WBS 3.1.1.010)

March 23, 2021

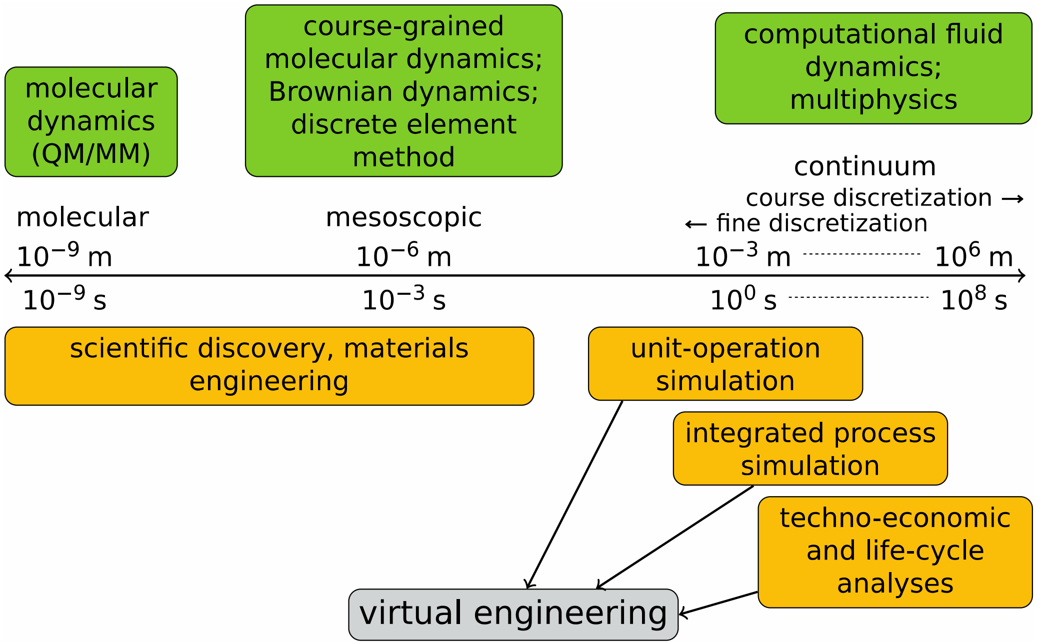
Systems Development and Integration

Jonathan Stickel
National Renewable Energy Laboratory

Project Overview

- **Virtual Engineering**: systematically integrates **mechanistic models** of unit operations and predicts outcomes for an **entire (bio-)chemical process**
- **Objective**: Develop **proof-of-concept** virtual-engineering software and **demonstrate** capabilities to evaluate and **optimize integrated-process performance**
- **Accelerate** development and **scale-up**
- Low-temperature biomass conversion (seed project)
- Currently, process-modeling TEA does not utilize state-of-the-art mechanistic models
- **Leverage** BETO-funded **pilot-scale** facilities and experiments

Computational science length and time scales



Virtual engineering is an extension of computational science

Market Trends

Product

- Anticipated decrease in gasoline/ethanol demand; diesel demand steady
- Increasing demand for aviation and marine fuel
- Demand for higher-performance products
- Increasing demand for renewable/recyclable materials

Feedstock

- Sustained low oil prices
- Decreasing cost of renewable electricity
- Sustainable waste management
- Expanding availability of green H_2
- Closing the carbon cycle

Capital

- Risk of greenfield investments
- Challenges and costs of biorefinery start-up
- Availability of depreciated and underutilized capital equipment

Social Responsibility

- Carbon intensity reduction
- Access to clean air and water
- Environmental equity

NREL's Bioenergy Program Is Enabling a Sustainable Energy Future by Responding to Key Market Needs

Value Proposition

- Virtual engineering integrates BETO-funded process modeling, TEA, and pilot-plant capabilities to accelerate development and reduce risk of market-relevant biomass conversion processes

Key Differentiators

- First-of-kind systems-modeling approach for biomass conversion (complex physicochemical phenomena)
- Broadly skilled NREL team with requisite software, computational, and domain-science expertise

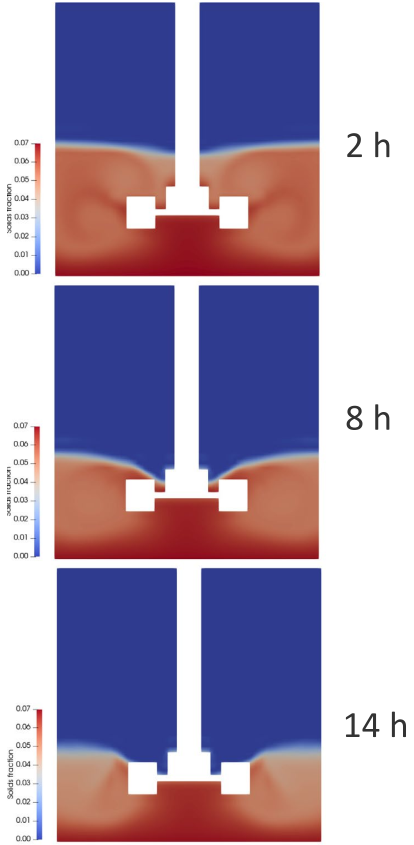
1. Management

Multidisciplinary team:

- Jonathan Stickel[1] (PI) **directs** the project
- Ethan Young[2] leads **programming** approach
- Andrew Glaws[2] leads **surrogate modeling**
- Andrew Bartling[3] leads **TEA integration**
- Hariswaran Sitaraman[2] provides expert advise for **unit-operation models**

Direct Collaboration:

- Bioprocess Modeling and Simulation (2.5.1.100)
- Biochemical Platform Analysis (2.1.0.100)
- Separations Development & Application (2.4.1.101)
- Biochemical Process Integration (3.4.2.201)



Solids volume fraction as predicted during CFD simulation of enzymatic hydrolysis

[1]Renewable Resources and Enabling Science, [2]Computational Science, [3]Catalytic Carbon Transformation & Scale-Up

Risk Management

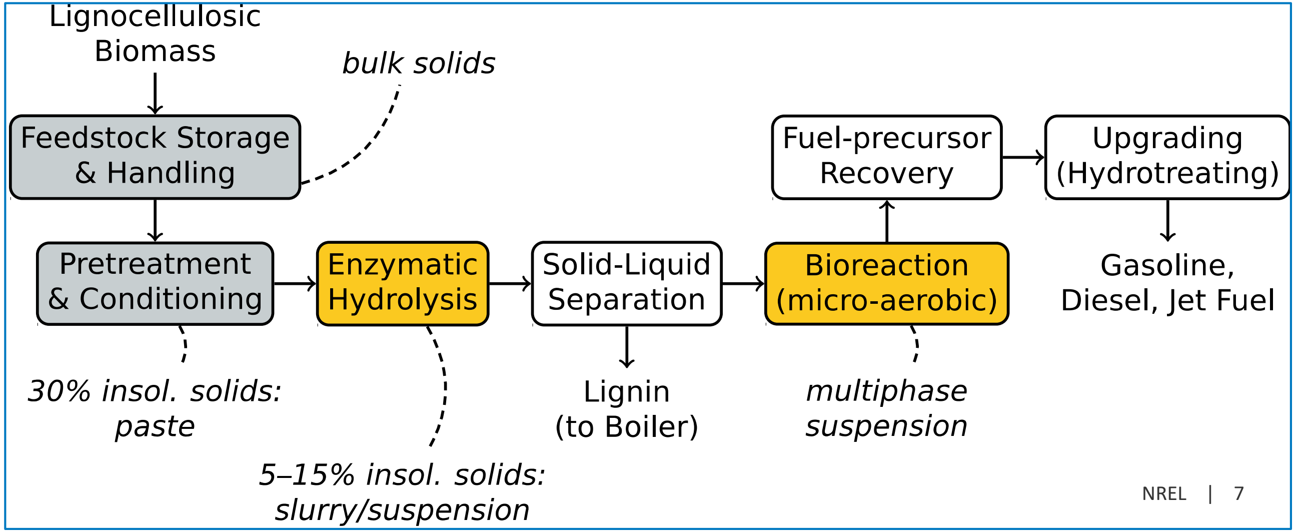
Risk Description	Response Plan	Severity	Status
Hiring of software engineer with requisite skills is delayed.	We will start the hiring process as soon as this project is confirmed for funding. If hiring is still significantly delayed, we will request a reschedule of project deliverables.	Moderate	**Complete**. Identified appropriate NREL staff instead.
Allocation of computing resource on NREL HPC (Eagle) is required for this work. Lack of allocation and inability to get jobs through the batch queue will delay results.	We follow NREL's HPC request process in order to receive adequate HPC node hours. If insufficient node hours are granted, we will request a reschedule of project deliverables.	Moderate	**Ongoing**. Sufficient allocation was received in FY20 and FY21.
Surrogate models do not adequately represent high-fidelity mechanistic models.	*If surrogate models are inadequate*, the optimization functionality will not be implemented. Instead, resources will be used to improve efficiency of once-through simulations and implement sensitivity analyses.	High	**In progress**. Surrogate models in development with milestones in FY21.

2. Approach

Systems-modeling architecture (*approach*)

- **Jupyter notebooks** and **Python programming** used to create a graphical user interface (**GUI**)
- The vebio Python package (developed in this project) contains functionality to create and interact with GUI elements and **facilitate information transfer** between **unit operation models**
  - Sub-models written in **different programming languages** and have **different computing needs**
  - **High-fidelity models** (CFD simulations) are automatically submitted to the **NREL HPC** scheduler, while **lower-fidelity models** and surrogates are run directly on the user's workstation.
- The economic outcomes of the process are evaluated through a programmatic interface to the **Aspen-Plus techno-economic analysis (TEA)** software.

Yellow: high-fidelity models used in this project
Gray: high-fidelity models available for future work
White: low-fidelity models available *or* Aspen-Plus

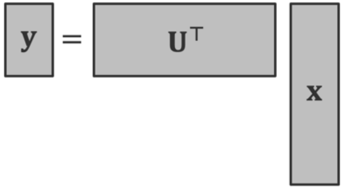


Surrogate modeling (*approach*)

Goal: develop efficient surrogate models for computationally expensive unit operations

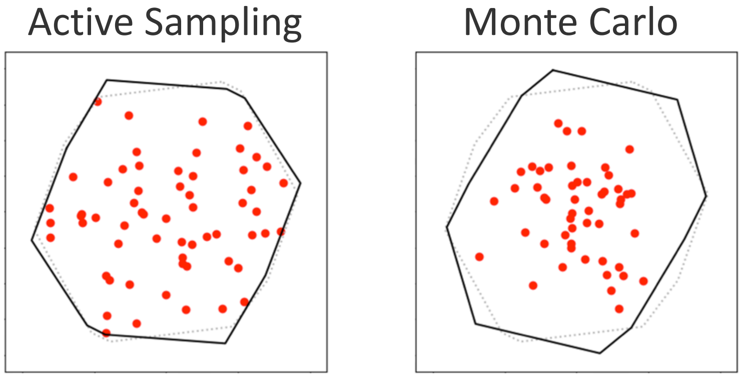
- Improve accuracy and reduce cost by performing dimension reduction

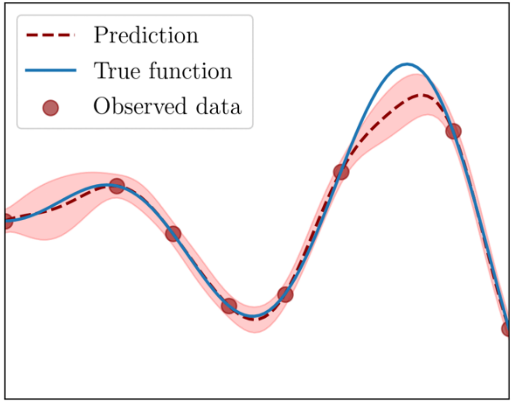
$$z = f(\mathbf{x}) \approx \tilde{f}(\mathbf{y})$$ where



- Important directions in $\mathbf{U}$ identified using polynomial ridge approximation [Hokanson & Constantine, 2018]
- Active importance sampling stretches samples along directions that maximize variation in $f(\mathbf{x})$
- Fit Gaussian process (GP) model to ridge subspace

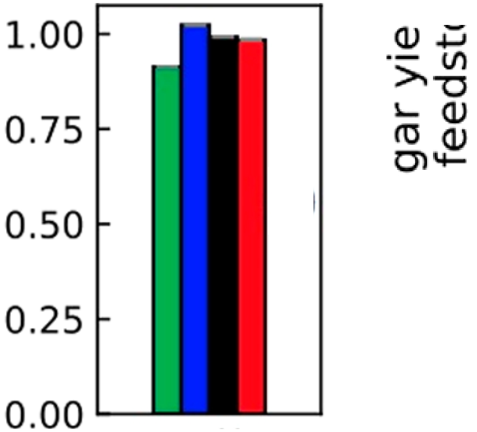
$$\tilde{f}(\mathbf{y}) \sim \mathcal{GP}\left(\mu(\mathbf{y}), k(\mathbf{y}, \mathbf{y}') + \alpha\delta_{ij}\right)$$



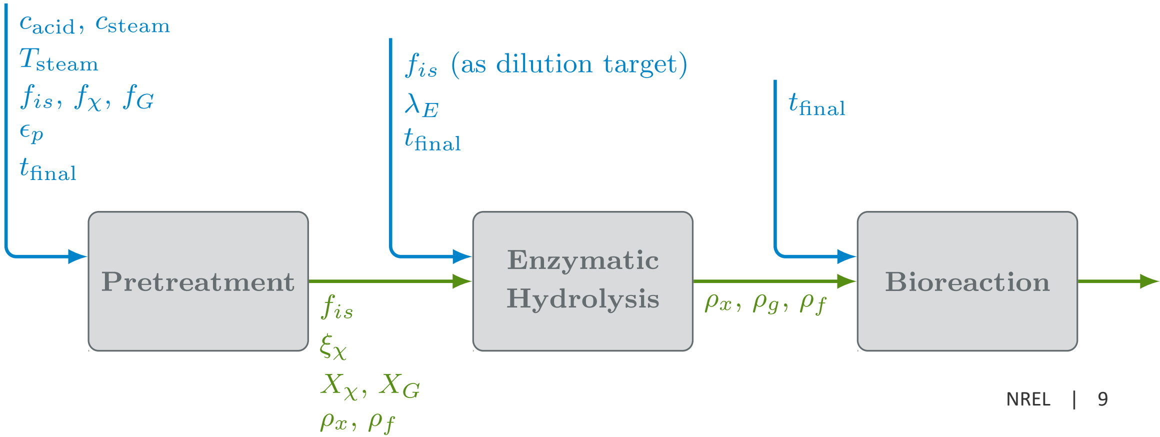


Experimental Validation (*approach*)

- Can the mechanistic models sufficiently represent pilot-plant processes?
- Are the information handoffs between models sufficient to achieve agreement with pilot-plant experiments?
- Use data from connected experiments where possible
  - pretreatment and enzymatic hydrolysis
- Validation of aerobic bioreaction model likely standalone
- Agreement within 30% at Go/No-go (03/2020); within 10% at End-of-Project (09/2021)



Pretreatment and enzymatic hydrolysis total conversion, FCIC baseline runs [ACS Sustainable Chem. Eng. (2020) **8:**2008]



3. Impact

- **Virtual engineering** integrates BETO-funded *process modeling*, *TEA*, and *pilot-plant* capabilities to accelerate development and reduce risk of market-relevant biomass conversion processes
- First-of-kind systems-modeling approach for biomass conversion
  - complex physicochemical phenomena require state-of-the-art multiphysics and multiscale models
- Will be useful to BETO and industry to evaluate and optimize integrated-process performance
- *Seed project*: proof-of-concept software infrastructure being developed—follow-on developments expected to enable production use:
  - Choice of unit-operation features, equipment type
  - High-quality visualizations and reports
- Software will be released *open-source* as a git repository

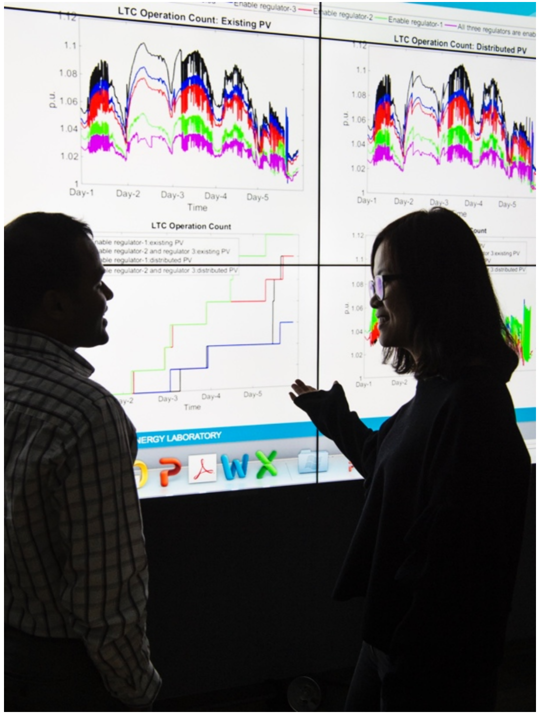


Photo by Dennis Schroeder, NREL 49009

4. Progress and Outcomes

Systems-modeling (*progress/outcomes*)

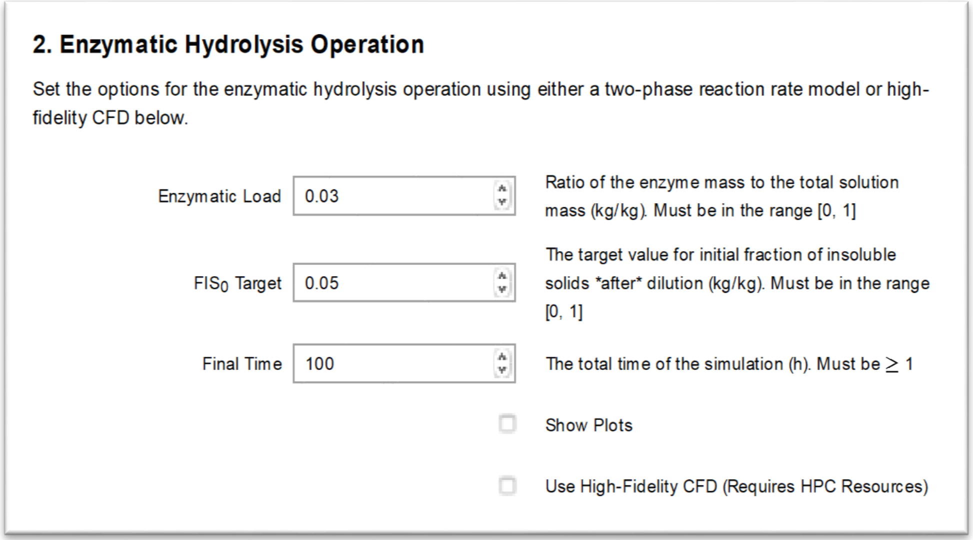
Virtual Engineering Notebook:

1. Explains inputs of unit operations to the user
2. Obtains and validates user-input values
3. Executes operations sequentially, transferring and parsing data between operations as necessary
4. Displays plots and prints results

- Programmatic interfaces with models written in different languages:
  - Pretreatment: in-house f90 solver (workstation)
  - Enz. hydrolysis: nek5000 FEM solver (HPC)
  - Bioreactor: OpenFOAM C++ FVM solver (HPC)

Future work:

- Infrastructure for process optimization
- Improved reporting of results and visualizations

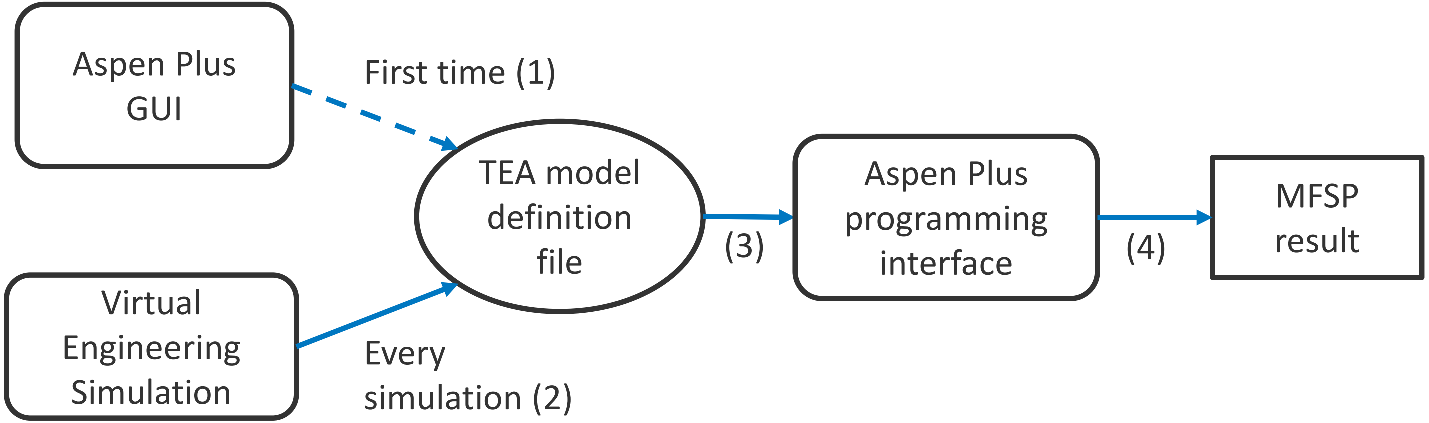



```
Running Enzymatic Hydrolysis Model

INPUTS
Lambda_e = 0.0300
FIS_0 = 0.0500
yF0 = 0.4911
t_final = 100.0000

FINAL OUTPUTS (at t = 100.0 hours)
rho_g = 21.4285
Total Conversion = 0.8149


Finished Enzymatic Hydrolysis
```

TEA Integration (*progress/outcomes*)

Key outcome to date

- TEA model-definition file generated by Aspen Plus GUI (1)
- VE software modifies definition file based on mechanistic modeling simulation results (2)
- VE software then initiates Aspen Plus (via programming interface, *no GUI*) (3) to compute MFSP for the modified TEA model (4)
- Workflow can be iterated for sensitivity studies (complete) and optimization (future work)
- Example: VE simulation with varied EH loading and time:
  - MFSP range $3.96/GGE – $4.32/GGE *



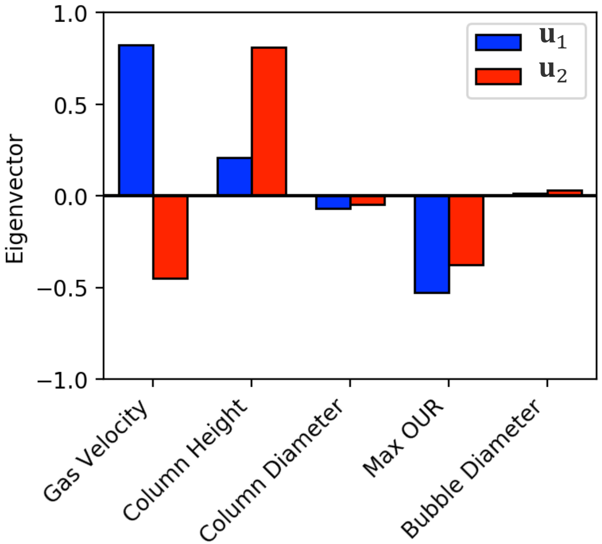
*preliminary and unvalidated model results

Surrogate modeling (*progress/outcomes*)

Bubble Column Bioreactor

Quantity	Lower Bound	Upper Bound
Gas Velocity $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$	0.01	0.1
Column Height (m)	10	50
Column Diameter (m)	1	6
Max Oxygen Uptake Rate $\left(\frac{\mathrm{mol}}{\mathrm{m}^3\ \mathrm{hr}}\right)$	5	100
Bubble Diameter (m)	0.003	0.008

Quantity of Interest: reactor-averaged **oxygen concentration**

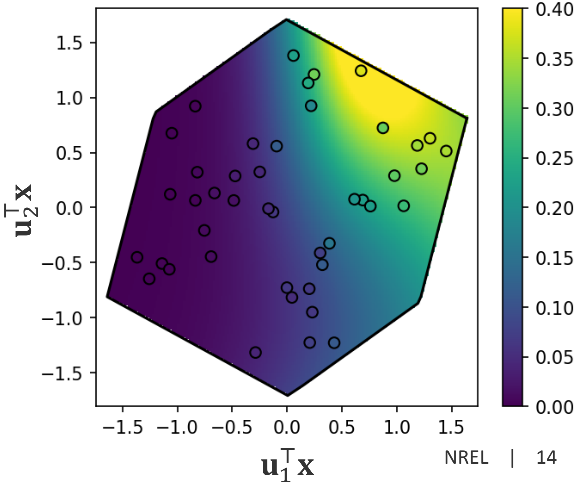


5 input parameters reduced to 2 active variables $\rightarrow$ $\mathbf{y} = \mathbf{U}^\top \mathbf{x}$

- Basis vectors $\mathbf{U}$ provide input sensitivity insights

Fit a GP in the reduced subspace

- Flexible model can be fit on irregular domain
- Active samples explore low-dimension subspace well



Future work:

- Rigorous investigation of testing accuracy
- Surrogate model for enzymatic hydrolysis
- Achieve agreement (within 15%) with high-fidelity model

Summary

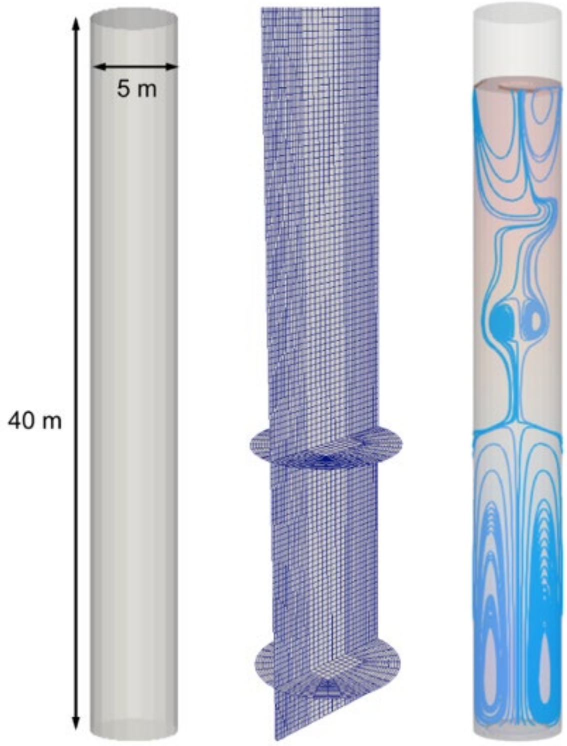
Overview: Virtual engineering integrates BETO-funded *process modeling*, *TEA*, and *pilot-plant* capabilities to accelerate development and reduce risk of market-relevant biomass conversion processes

Management: Diverse team (scientists, engineers, mathematicians, programmers) is working together to creatively achieve successful implementation of VE software

Approach: Develop software to perform systems modeling with high-fidelity mechanistic models, surrogate models, and TEA integration

Impact: Will be useful to BETO and industry to evaluate and optimize integrated-process performance and reduce-risk of commercialization

Progress: Working VE software with GUI developed, TEA integration implemented, and surrogate models in progress; process optimization to be demonstrated



Market Trends

Product	Anticipated decrease in gasoline/ethanol demand; diesel demand steady
Product	Increasing demand for aviation and marine fuel
Product	Demand for higher-performance products
Product	Increasing demand for renewable/recyclable materials
Feedstock	Sustained low oil prices
Feedstock	Decreasing cost of renewable electricity
Feedstock	Sustainable waste management
Feedstock	Expanding availability of green H_2
Feedstock	Closing the carbon cycle
Capital	Risk of greenfield investments
Capital	Challenges and costs of biorefinery start-up
Capital	Availability of depreciated and underutilized capital equipment
Social Responsibility	Carbon intensity reduction
Social Responsibility	Access to clean air and water
Social Responsibility	Environmental equity

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Value Proposition

- Virtual engineering integrates BETO-funded process modeling, TEA, and pilot-plant capabilities to accelerate development and reduce risk of market-relevant biomass conversion processes

Key Accomplishments

- Programmatic infrastructure, including TEA integration, and GUI created
- Surrogate modeling development shows promise
- Will be useful to BETO and industry to evaluate and optimize integrated-process performance

Thank You

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Transforming **ENERGY** through computational excellence

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Additional Slides

Quad Chart Overview

Timeline
- Start: October 1, 2019
- End: September 30, 2022

	FY20	Active Project
DOE Funding	$245,000	$835,000

AOP Project Partners
- Bioprocess Modeling and Simulation (2.5.1.100)
- Biochemical Platform Analysis (2.1.0.100)
- Separations Development & Application (2.4.1.101)
- Biochemical Process Integration (3.4.2.201)

Barriers addressed:
- ADO-A. Process Integration
- ADO-D. Technology Uncertainty of Integration and Scaling

Project Goal
Develop proof-of-concept virtual-engineering software and demonstrate capabilities to evaluate and optimize integrated-process performance

End of Project Milestone
A comprehensive software implementation of virtual engineering, capable of simulating and optimizing the low-temperature conversion process of lignocellulosic biomass to fuel, including a graphical user interface. Our framework will be validated against pilot plant data within an accuracy of 10%.

Funding Mechanism
FY19 Lab Call

Advanced Development and Optimization
- Modeling/ hardware co-development to improve biomass processing/ handling inside the plant

Responses to Previous Reviewers' Comments

- First peer review for this project
- Go/No-Go, March 2021: *Initial working version of VE software. The simulations results will agree within 30% of pilot-plant experimental data.*

Publications, Patents, Presentations, Awards, and Commercialization

Publications

- Young E., Stickel J.J., Bartling A., Sitaraman H., Glaws, A., Lischeske, J., (2021) Toward a virtual engineering environment for the simulation and optimization of low-temperature biomass conversion, 2021, Computers & Chemical Engineering, *In Preparation.*

Presentations

- Glaws, A., et al. “Active importance sampling for efficient surrogate modeling of unit operations in the biochemical conversion process”. 16th U.S. National Congress on Computational Mechanics (USNCCM), July 2021, *Abstract Submitted.*