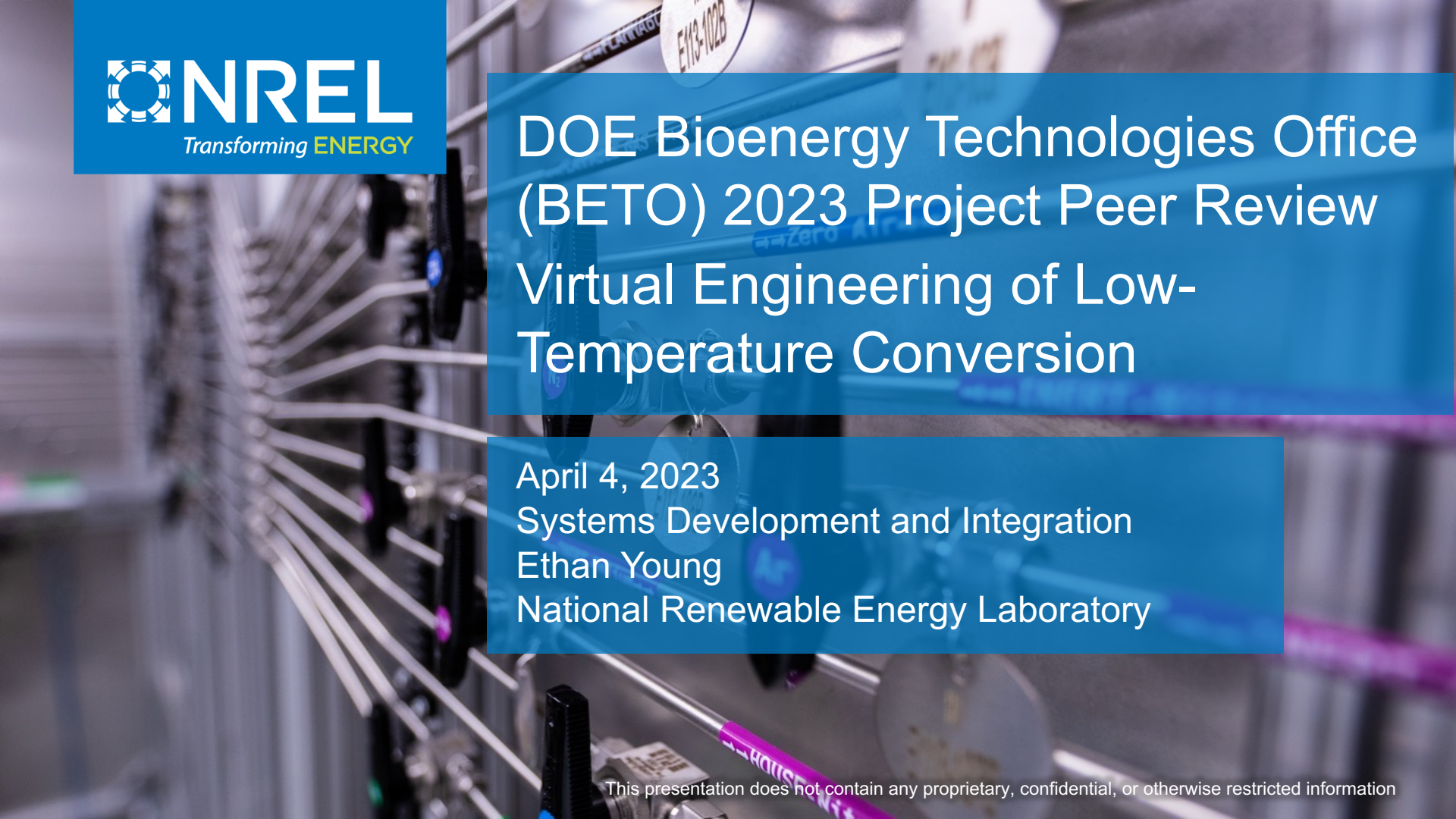


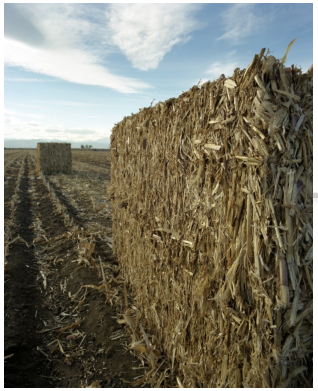
DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

Virtual Engineering of Low-Temperature Conversion

April 4, 2023

Systems Development and Integration
Ethan Young
National Renewable Energy Laboratory

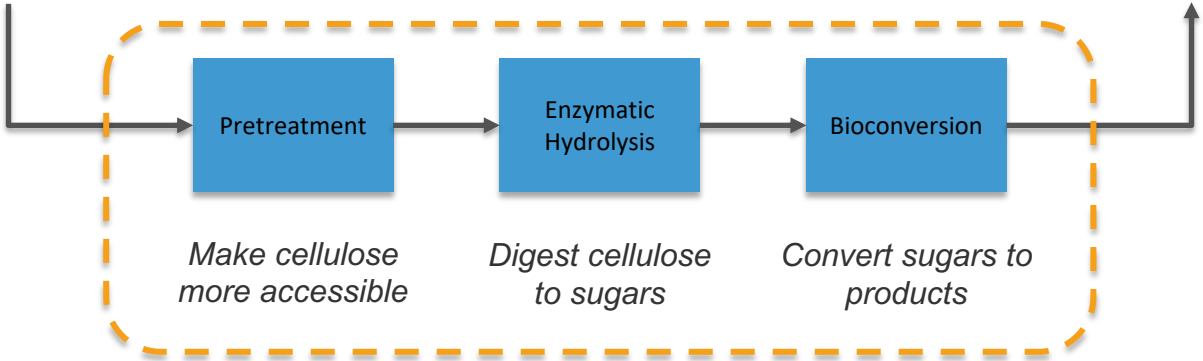
Project Overview: Motivation



Feedstock storage and handling

Catalytic upgrading

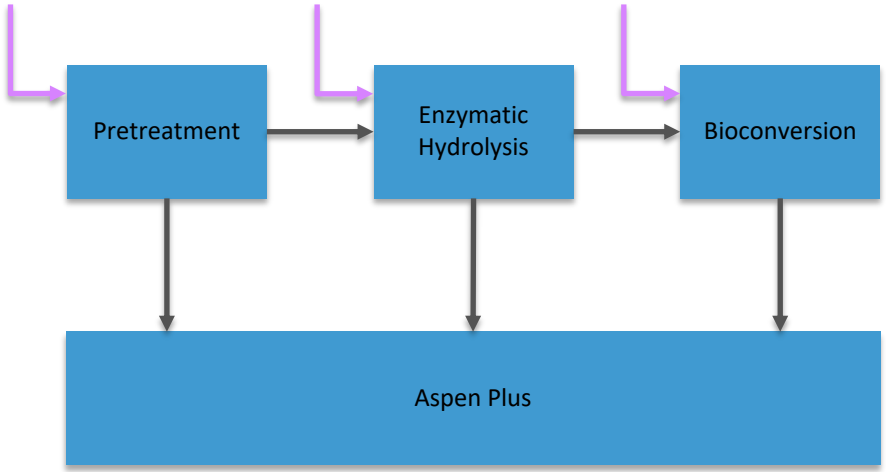
Project Scope



Project Overview: Motivation

Virtual Engineering (VE):

The process of connecting mathematical models of unit operations and **predicting outcomes for an *entire* chemical process to accelerate paths to biofuels**



Goal: Construct a linking framework and cutting-edge exemplar models to enable start-to-finish calculations while exposing key operating decisions to the user

Project Overview: Motivation

Virtual Engineering (VE):

The process of connecting mathematical models of unit operations and **predicting outcomes for an *entire* chemical process to accelerate paths to biofuels**

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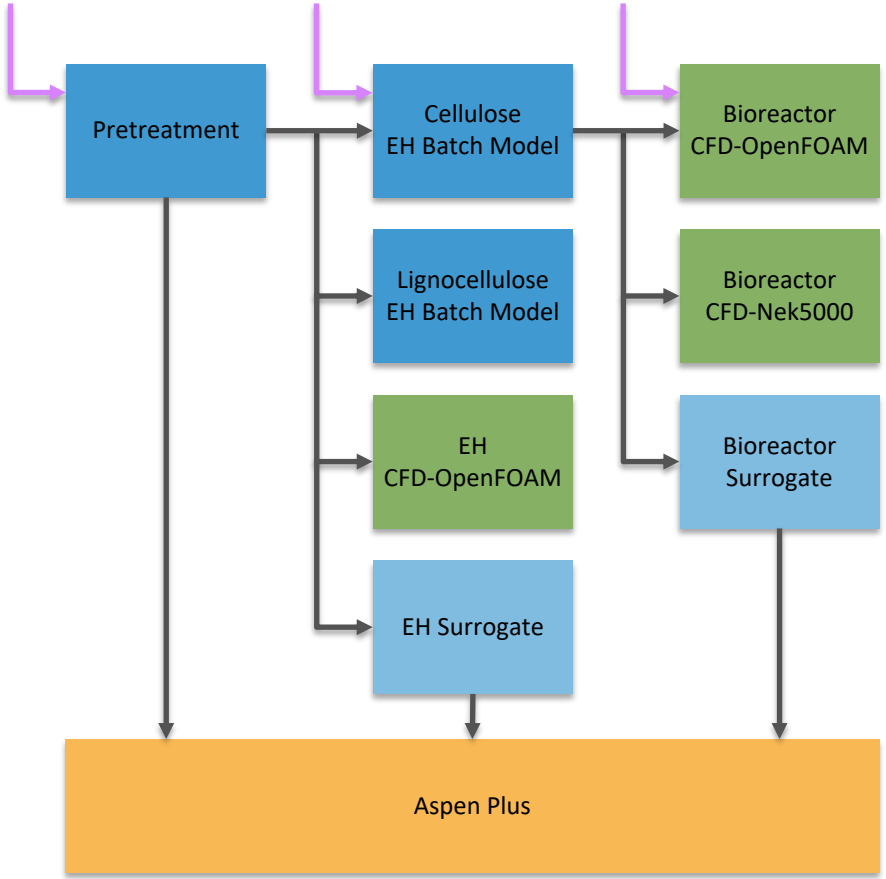


Approach: Management

Multidisciplinary Team:

- **Ethan Young**[1] (PI) HPC workflow expertise and core VE developer
- **Olga Doronina**[1]: Software development and optimization expert
- **Andrew Glaws**[2]: Surrogate model developer and machine learning expert
- **Hari Sitaraman**[1]: Continuum modeling/simulation expertise and domain guidance
- **Nick Carlson**[3]: TEA integration and domain guidance

Dev Group (Weekly)

Large Group (Monthly)

Risk: Pretreatment unit cannot be refactored into Python solver

Mitigation: Modify the original unit operation definition to be carried out using a simplified set of physics or computational models, e.g., relax a governing equation, use a different FEM shape function, or construct a surrogate model

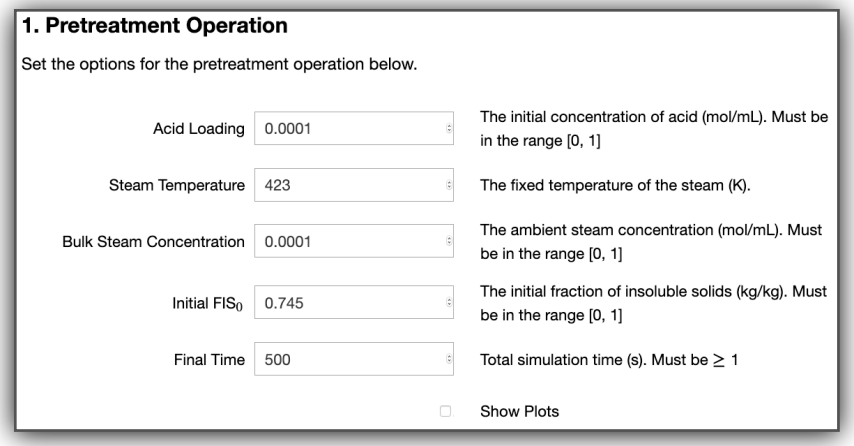
1. High Performance Algorithms and Complex Fluids Group, NREL
2. AI, Learning and Intelligent Systems, NREL
3. Economic, Sustainability, and Market Analysis, NREL

Note: There was no DEI plan associated with this project's initial 2019 AOP but we are interested in pursuing an internship through NREL's STAR program.

1. Approach: VE Framework

- We chose **Python** for the VE package for its flexibility and wide selection of APIs for interfacing with other languages/systems
- The user-facing code is deployed in a **Jupyter Notebook**[1] for the ability to deploy both GUI elements and code on different hardware and operating systems
- A **Conda environment** makes sharing this package with users and developers relatively easy
- *Milestones satisfied: FY20 Annual, Go/No-Go, FY22 Annual*

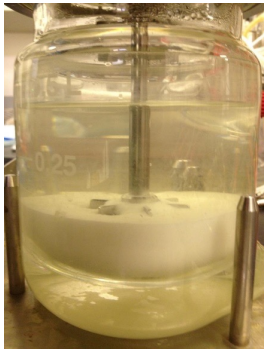
```
# Create the collection of widgets
pt_options = wf.WidgetCollection()

# Add option for Acid Loading
pt_options.initial_acid_conc = widgets.BoundedFloatText(
   value = 0.0001,
   max = 1.0,
   min = 0.0,
   description = 'Acid Loading',
   description_tooltip = 'The initial concentration...'
)
```

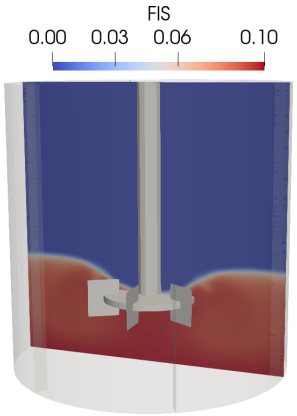


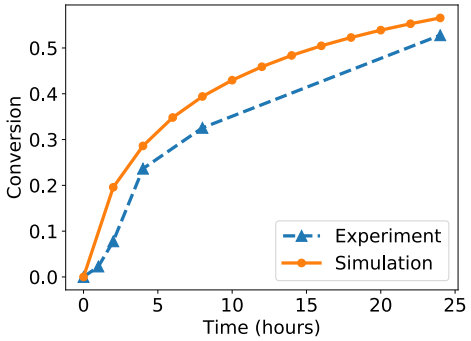
1. E. Young et al., "Virtual Engineering", Computer Software, 2022, doi:10.11578/dc.20220418.2

1. Approach: Continuum Simulations

- As part of developing the VE framework, we have developed high-fidelity, computational fluid dynamics **(CFD) simulations of enzymatic hydrolysis[2] and aerobic bioreaction[3]**
- These jobs can be easily modified, compiled, and **launched on the HPC from the Notebook GUI**
- CFD wall clock time is roughly *3-4 days on HPC resources*
- *Milestones satisfied: FY21 Q3, Q4*



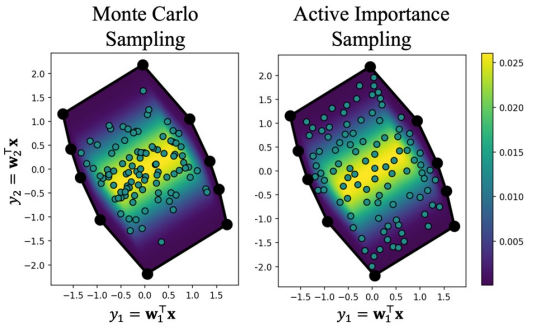


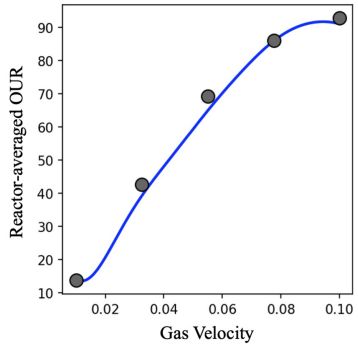


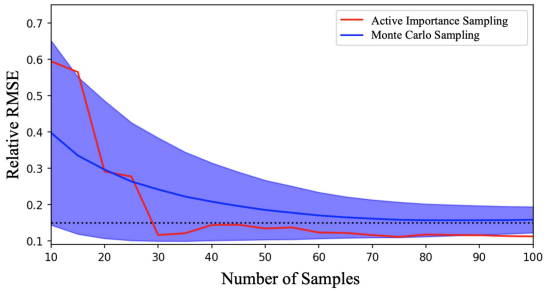
2. H. Sitaraman et al., "Coupled CFD and chemical-kinetics simulations of cellulosic-biomass enzymatic hydrolysis…", Chemical Engineering Science, 2019
3. M. Rahimi et al., "Computational fluid dynamics study of full-scale aerobic bioreactors…", Chemical Engineering Research and Design, 2018

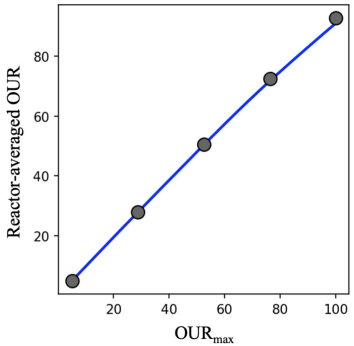
1. Approach: Surrogate Modeling

- Surrogate models are constructed by sampling our CFD simulations
- We leveraged **subspace-based dimension reduction** techniques and **active importance sampling**[4] to ensure an efficient and comprehensive exploration of the parameter space relative to Monte Carlo samples
- These models capture the complex physics of the CFD simulations **accurately and quickly (~260,000x speedup)**
- *Milestones satisfied: FY21 Q3, Q4*





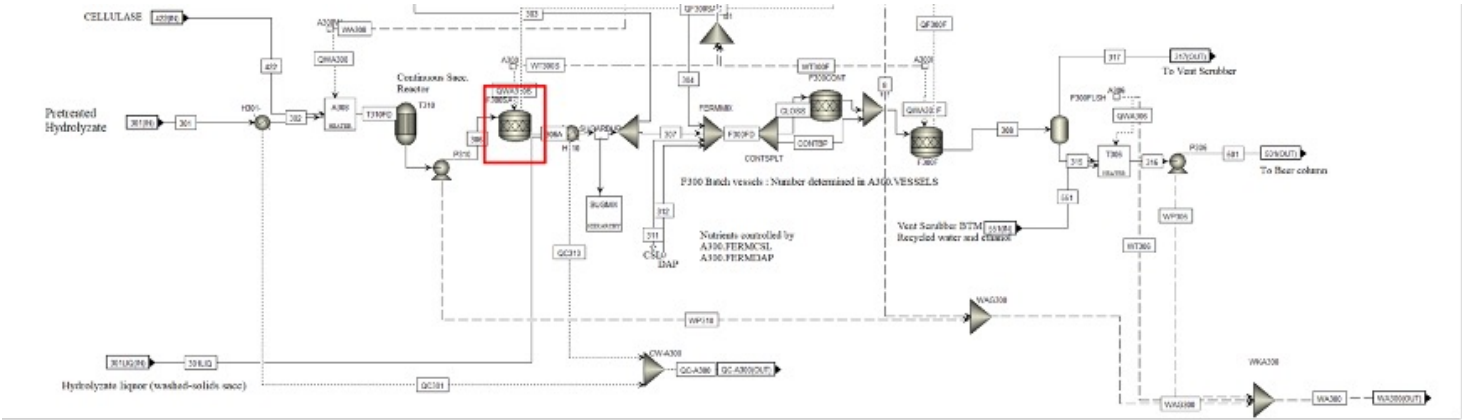




4. A. Glaws et al., "Active Importance Sampling for Efficient Surrogate Modeling…", 16th U.S. National Congress on Computational Mechanics, 2021

1. Approach: TEA Interface

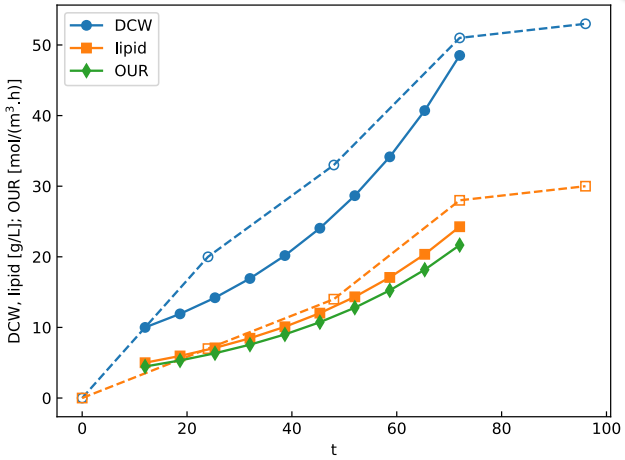
- Connections to Aspen Plus are made using a set of file-writing functions
- A backup file exported using the Aspen Plus GUI can be **edited through targeted file-writing operations**
- This edited Aspen Plus definition can be deployed directly from the command line using the `pywin32` package
- *Milestones satisfied: FY20 Q3, FY22 Q2*



2. Progress and Outcomes: Validation

- Data from the FCIC baseline runs of Sievers et al.[5] are used to validate pretreatment and enzymatic hydrolysis
- Data from Fei et al.[6] is used to validate bioreaction
- In most cases, we show **<10% relative error** between experimental data produced in pilot plants and our models
- Instances of larger disagreement are typically outliers or occur in transition regimes

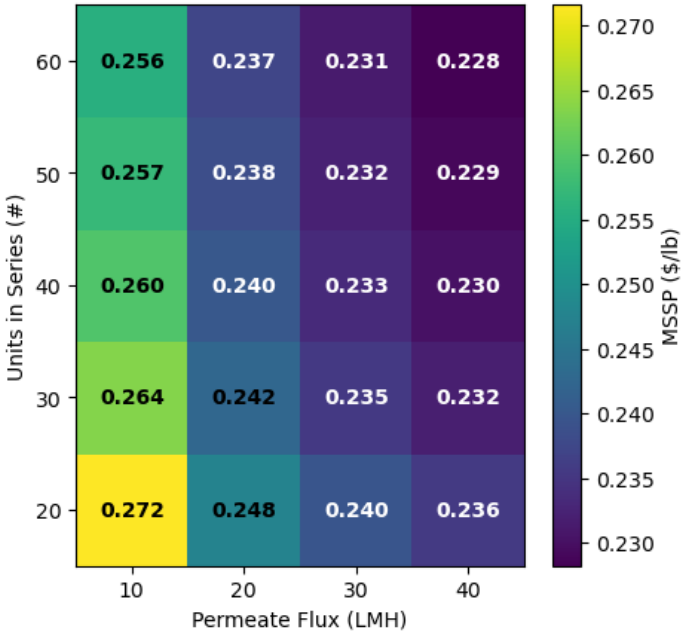
Operation	Quantity	Experiment	Simulated	% Err
Pretreatment	FIS (%)	26	25	-3.8
	xylan (g/g)	0.078	0.05	-35.9
	glucan (g/g)	0.5	0.48	-4.0
	xylose (g/L)	53	56	5.7
	xylan conversion (%)	82	81	-1.2
EH	FIS (%)	7.6	6.9	-9.2
	glucose (g/L)	64	63	-1.6
	xylose (g/L)	38	44	15.8
	glucan conversion (%)	88	80	-9.1



5. D. A. Sievers et al., “Throughput, reliability, and yields of a pilot-scale conversion process…”, ACS Sustainable Chemistry and Engineering, 2020
6. Q. Fei et al., “Enhanced lipid production by rhodosporidium toruloides…”, Biotechnology for Biofuels, 2016

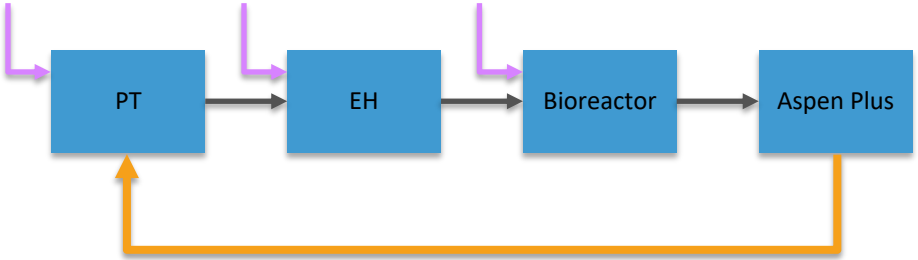
2. Progress and Outcomes: TEA Automation

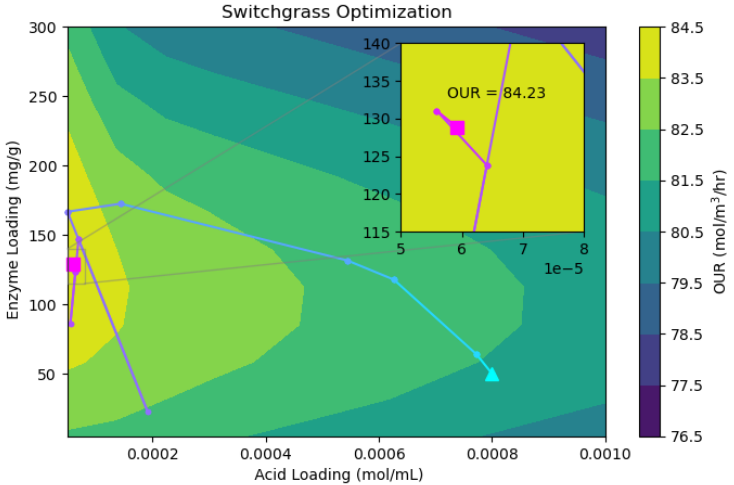
- Developed a workflow where continuous enzymatic hydrolysis (CEH) model definitions could be varied programmatically (**WBS 2.4.1.101**)
- These inputs affected the calculated values of **reactor size, membrane area, and conversion** which were in turn used as **inputs to Aspen Plus** to predict a minimum sugar selling price (MSSP)
- Ability to support multiple once-through simulations and connect to a variety of different unit models; in this case, ***a unit model not originally included in the VE roadmap***



2. Progress and Outcomes: Optimization

- Optimization problems defined by specifying objectives, controls, and constraints through VE Notebook widgets
- **`SciPy` optimization** algorithms (L-BFGS-B, SLSQP) used to identify optimal solutions
- **Example**: **Maximize oxygen uptake rate (OUR)**, a measure of the sugars-to-fuel conversion rate, by adjusting the acid loading in pretreatment and enzyme loading in enzymatic hydrolysis.
- *Milestones satisfied: FY22 Q3*

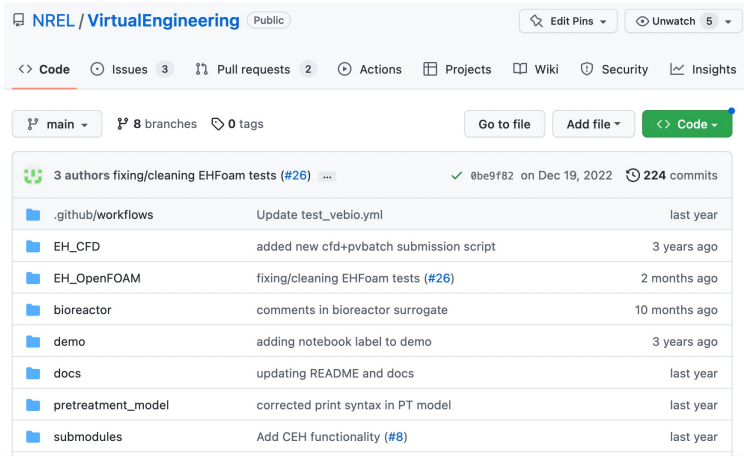


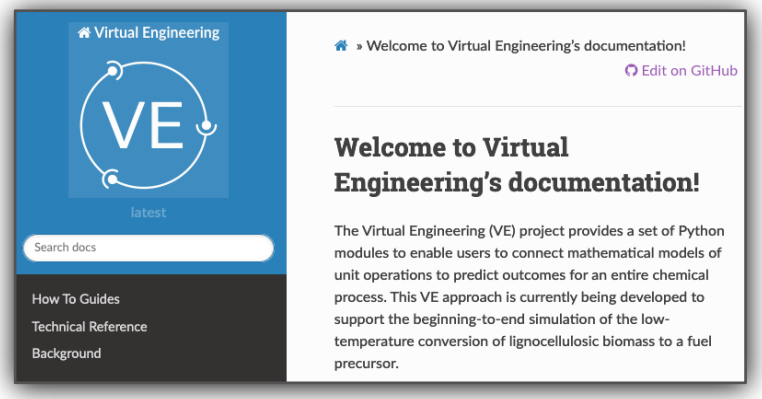


3. Impact

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

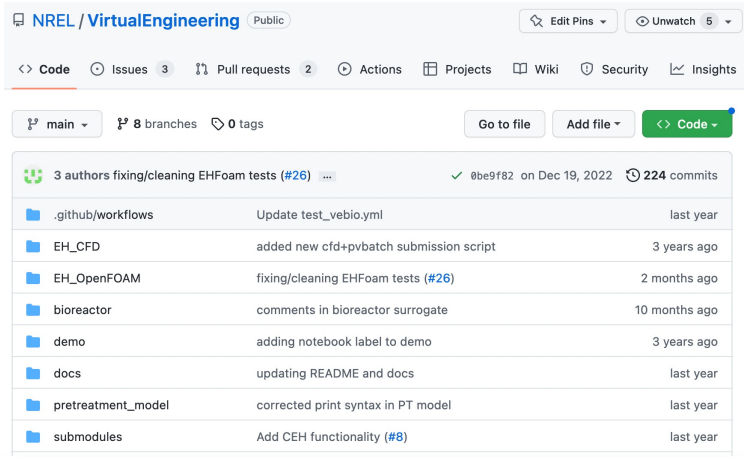
- State-of-the-art multiphysics and multiscale models
- Proof-of-concept software infrastructure being developed, follow-on developments expected to enable production use
- **Software is freely available on our public GitHub repository:** github.com/NREL/VirtualEngineering

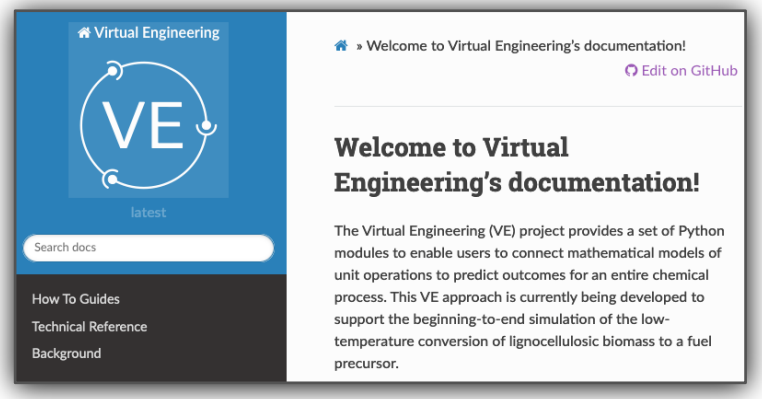




3. Impact

- Cross-platform enabling outcomes including connections with active work in the CO2 Consortium and thermochemical conversion
- We demonstrate the VE approach on a biomass workflow but have **designed each component in a way that can easily support new domains and feedstocks**
- Enable acceleration to commercialization for billions of gallons of sustainable aviation fuels (SAF)
- De-risk technologies toward commercialization and deployment





Summary

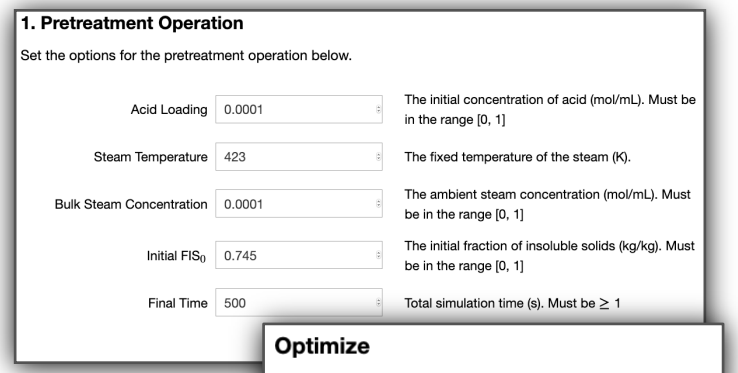
We have developed a proof-of-concept software package and a library of supporting models and tools:

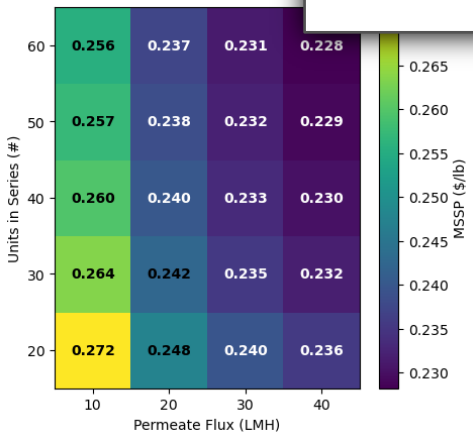
(1) The use of **Notebooks to provide an intuitive GUI** for studies

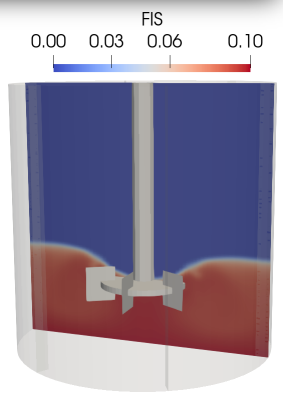
(2) Interface with **high-fidelity CFD** or computationally lightweight **surrogate models** informed by precursor CFD solves.

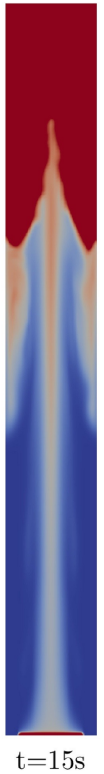
(3) Interface with **TEA automatically** from the command line

(4) Perform both once-through simulations and **iterative optimizations with minimal modifications**









Thank You

www.nrel.gov

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A portion of the research was performed using computational resources sponsored by the Department of Energy's Office of Energy Efficiency and Renewable Energy and located at the National Renewable Energy Laboratory.

Additional Slides

Quad Chart Overview

Timeline

- Start: October 1, 2019
- End: September 30, 2023

	FY22 Costed	Total Award
DOE Funding	172,581	275,000 (year 1) 300,000 (year 2) 325,000 (year 3) 257,000 (year 4)

TRL at Project Start: 4
TRL at Project End: 6

Project Goal

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

End of Project Milestone

Demonstration of large-dimension optimization problem composed of >2 controls with TEA outcomes in the loop. Presentation of results with a focus on new models and overarching VE methodology.

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

- Peer review comment #1:
  - **Regarding our software implementation vs. using Aspen Plus:** Aspen Tech makes great software for the dedicated purpose of simulating process systems, typically steady-state, in the petrochemical and other well-established industries. However, it is not designed to be a flexible platform for simulating novel unit-operation models written in different programming languages nor interfacing with HPC resources. Rather than using Aspen Plus, it was more straightforward for us to implement our own VE software using the Python programming language. We are also implementing surrogate models in our VE software rather than integrating them into Aspen, thus keeping the same VE software interface for multiple use cases.

Responses to Previous Reviewers' Comments

- Peer review comment #2:
  - **Regarding the purpose of the HPC models:** We are currently implementing CFD models, requiring HPC resources, for enzymatic hydrolysis and bioreaction. Yes, low-order models exist that do not require the HPC, and the VE software is setup to automatically fall back to those models when no HPC hardware is detected. These low-order models are "zero-dimensional" and presume the reactors are well-mixed, a condition that can require an impractical amount of energy to achieve. The CFD models are able to predict the relationship between mixing speed and/or aeration rate (and hence energy costs) with reactor performance (productivity/yield).

Responses to Previous Reviewers' Comments

- **Go/No-Go Overview**: Our 18-month Go/No-Go milestone report summarizes the VE software capabilities that have been developed so far:
  - A comprehensive working version of VE software has been implemented that includes mechanistic models for pretreatment, enzymatic hydrolysis, and bioreaction.
  - High-fidelity CFD simulations that use HPC resources have been enabled for enzymatic hydrolysis and bioreaction.
  - Data from FCIC Baseline runs were used to evaluate pretreatment and enzymatic hydrolysis (Sievers et al., 2020), while data from Fei et al. (2016) was used to evaluate bioreaction. Agreement between simulation and experimental results were all within 30% difference (agreement for many metrics were better than 10%).
  - Integration of techno-economic analysis(TEA) was performed previously (Young and Bartling, 2020) and is not described in detail here.
  - Altogether, we have developed a complete working version of VE software and have met the quantitative metrics for this Go/No-Go decision point.

Publications, Patents, Presentations, Awards, and Commercialization

- Glaws, H. Sitaraman, E. Young, and J. Stickel, “Active Importance Sampling for Efficient Surrogate Modeling of Unit Operations in the Biochemical Conversion Process”, 16th U.S. National Congress on Computational Mechanics July 29, 2021.
- E. Young, H. Sitaraman, A. Glaws, A. Bartling, J. Lischeske, and J. Stickel, “Keynote: Virtual Engineering Software Framework for Integrated Biomass Conversion Modeling”, 2021 AIChE Annual Meeting, November 10, 2021.
- E. Young, H. Sitaraman, A. Glaws, A. Bartling, J. Lischeske, and J. Stickel, “Virtual Engineering Software for Integrated Biomass Conversion Modeling”, NREL Adaptive Computing Workshop, June 14, 2022.