Virtual Engineering Software Framework for Integrated Biomass Conversion Modeling

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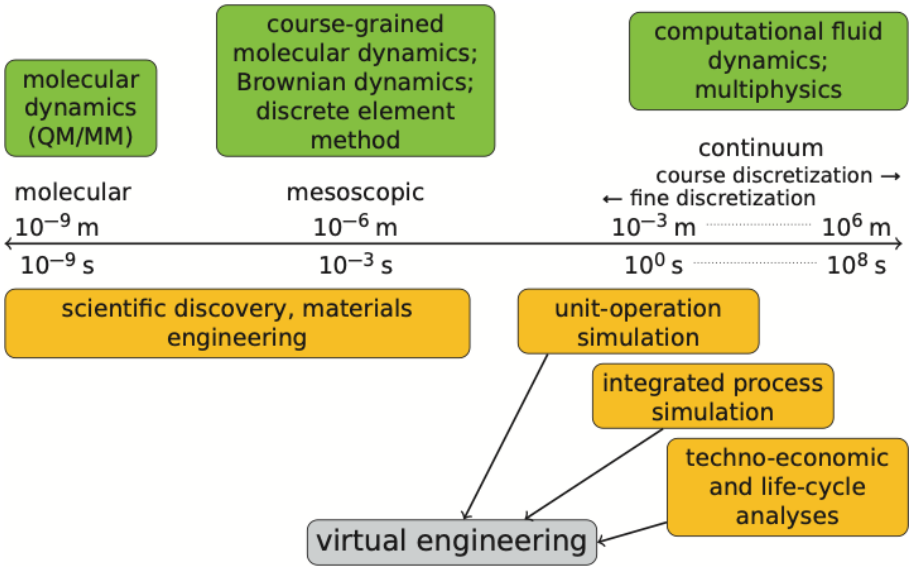
“Virtual Engineering”

Virtual Engineering (VE)

The process of connecting mathematical models of unit operations and predicting outcomes for an entire chemical process



VE Application

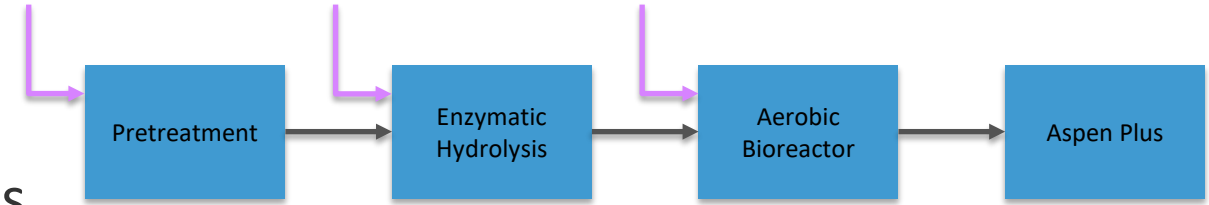
- We apply this VE approach to simulating the **low-temperature conversion of lignocellulosic biomass** to a fuel precursor
- Conversion of this challenging feedstock is modeled through three central unit operations: **pretreatment**, **enzymatic hydrolysis**, and **aerobic bioreaction**
- Numerical models of these operations are the subject of active research across diverse groups

Unit Operations

- **Pretreatment**: Opens up the biomass' resistant lignin shell to expose *more* cellulose chains to the hydrolysis step
- **Enzymatic Hydrolysis**: Enzymes digest the now-exposed cellulose and form sugars like glucose and xylose
- **Aerobic Bioreaction**: These sugars are converted into alcohols/fatty-acids via microbial action for eventual upgrading to fuels like ethanol or bio-diesel

VE Flowchart

Goal: Construct a framework to link together all the models to enable start-to-finish calculations while exposing key operating decisions to the user



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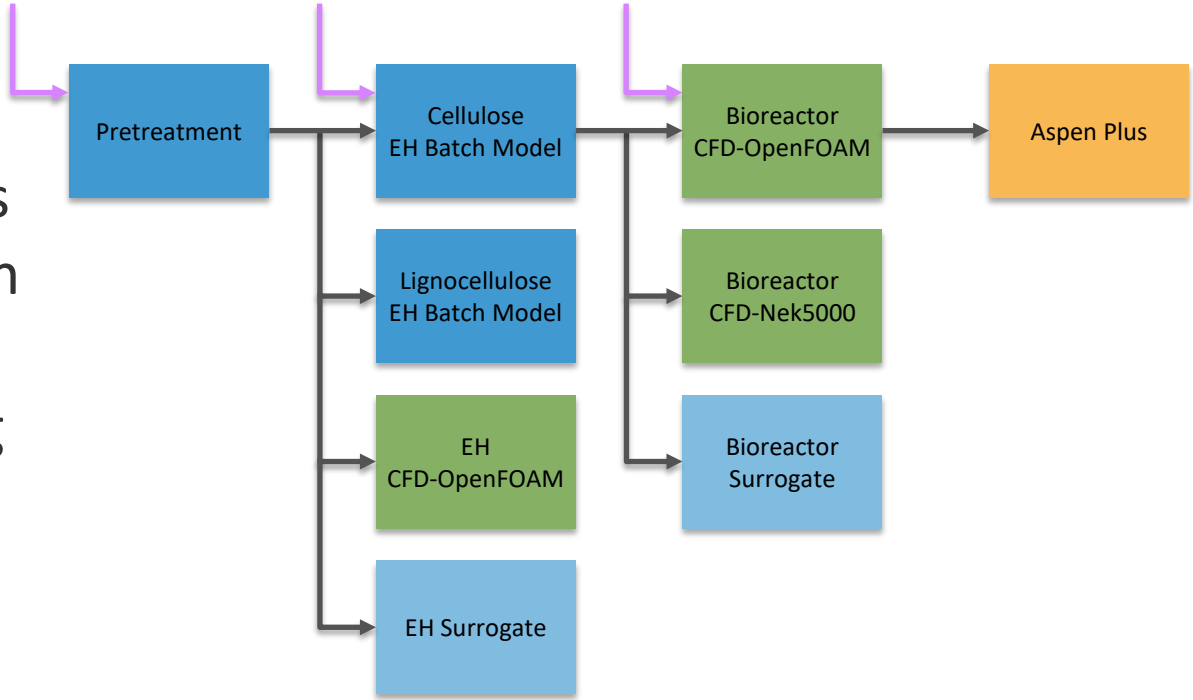


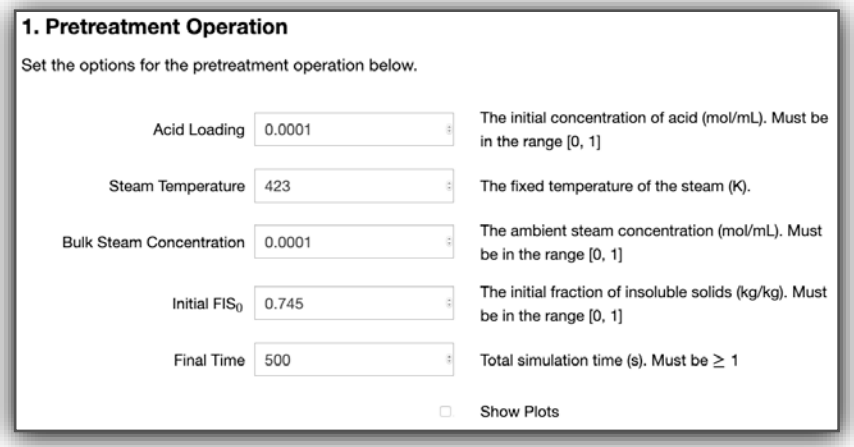
Python + Notebook

- 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** for the ability to deploy both markdown and code on different hardware, including Mac/Windows/Linux laptops and HPC
- A **Conda environment** makes sharing this package with users and developers relatively easy

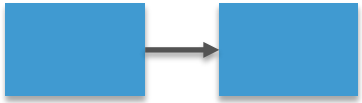
ipywidgets

Using **ipywidgets** within the Notebook provides an easy way to solicit user input for key parameters in the conversion process

```
# 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...'
)
```



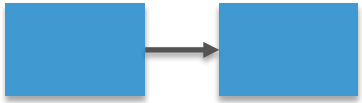
Linking Python Units



- All unit models communicate through a shared YAML file
- At the beginning/end of each step, values are transferred between the YAML file and a Python dictionary

```
pretreatment_input:
  initial_acid_conc: 0.0001
  steam_temperature: 416.0
  bulk_steam_conc: 0.0001
  initial_solid_fraction: 0.75
  final_time: 500.0
  show_plots: false
pretreatment_output:
  fis_0: 0.24501120794572953
  conv: 0.7497337597062437
  X_X: 0.0819860235910653
  X_G: 0.4982436778338859
  rho_x: 79.35199267597184
  rho_f: 0.36666211248901875
```

Linking Python Units



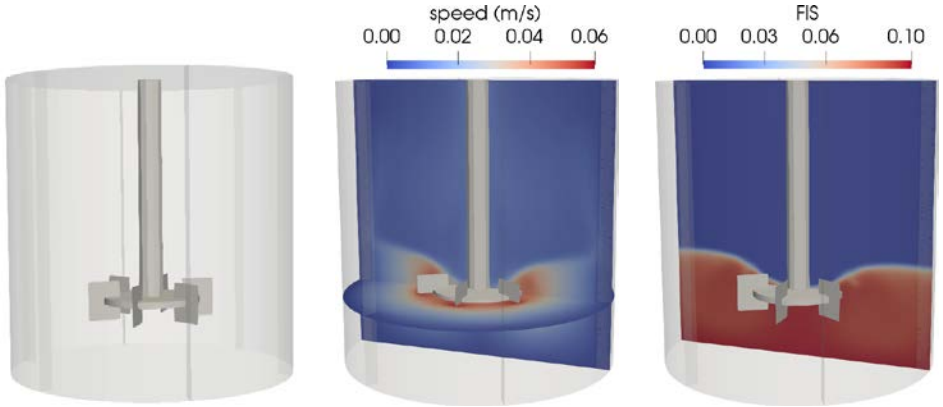
- Minimal function calls at beginning and end of Python models manage this IO

```
from vebio.Utilities import yaml_to_dict, dict_to_yaml

params_filename = sys.argv[1]
ve_params = yaml_to_dict(params_filename)

# Code for unit operation
# ...

dict_to_yaml([ve_params, output_dict], params_filename)
```

- Depending on the level of code abstraction, these values may need to be manually assigned

Linking HPC Jobs

- Variables in the YAML file are written to input files defining either Nek5000 (Fortran) or OpenFOAM (C++) simulations
- These may require as many as 6 days to solve on HPC resources



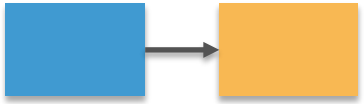
Schematic of EH stir-tank reactor, velocity magnitude of fluid, and FIS contours after 10 hours of hydrolysis

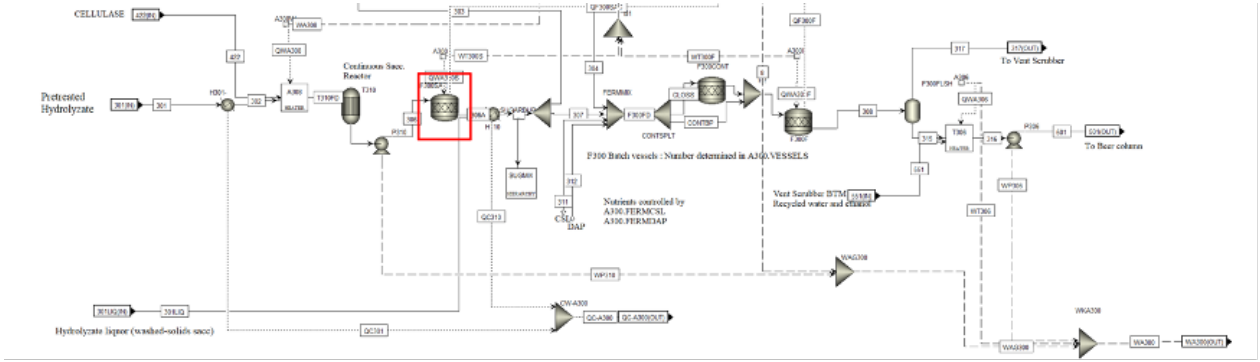
Linking HPC Jobs

- Jupyter Notebook server can be **launched from an HPC compute node** accessed via SSH tunnel
- Enable CFD units based on available resources, fall back to computationally simpler models where necessary

```
In [164]: nodeid_list = !srun hostname

          for nodeid in nodeid_list:
              print()
              !scontrol show node {nodeid}


          NodeName=r3i4n26 Arch=x86_64 CoresPerSocket=18
             CPUAlloc=36 CPUTot=36 CPULoad=0.01
```

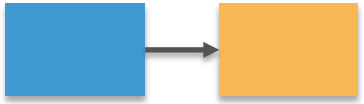
Linking Aspen Jobs





- Connections to Aspen Plus are made using another file-writing technique
- A backup file exported using the Aspen Plus GUI can be **edited through targeted file-writing operations**

Linking Aspen Jobs



- This edited Aspen Plus definition can be deployed directly from the command line using the `pywin32` package
- Spreadsheet macros/calculations can be carried out after the Aspen Plus solve in this same fashion

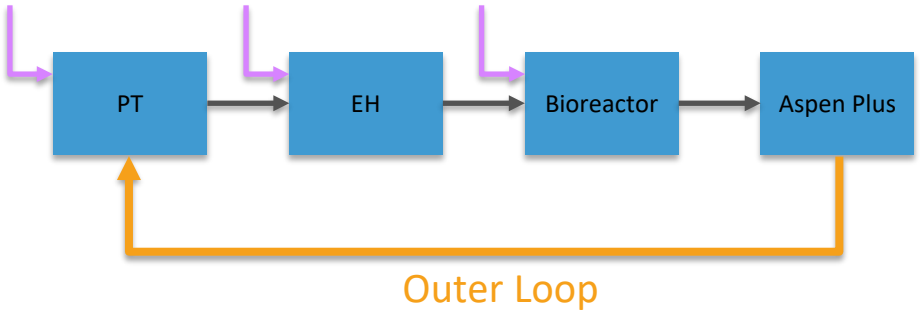
Estimated Glucan Conversion		Enzymatic Hydrolysis Time (hr)				
		72	78	84	90	96
Enzyme Loading (mg/g)	10			0.710		
	15			0.751		
	20	0.765	0.774	**0.782**	0.790	0.797
	25			0.808		
	30			0.830		

MFSP ($/GGE)		Enzymatic Hydrolysis Time (hr)				
		72	78	84	90	96
Enzyme Loading (mg/g)	10			3.96		
	15			4.03		
	20	4.13	4.13	**4.12**	4.11	4.09
	25			4.22		
	30			4.32		

Demo of VE Notebook for 3-Unit Simulation

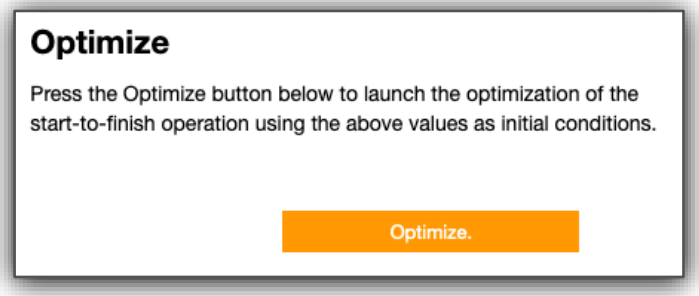
Optimization Studies

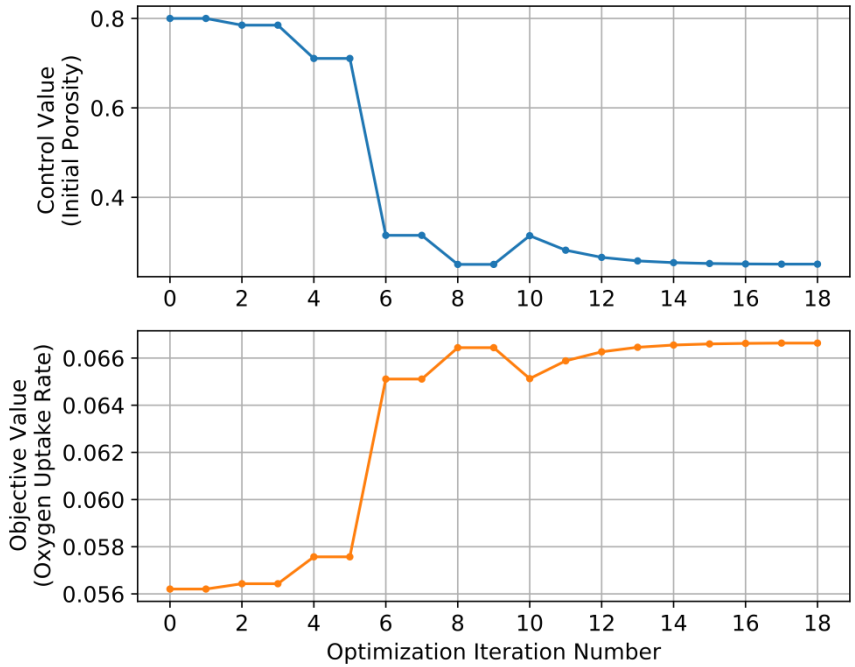
- `SciPy` optimization algorithms (L-BFGS-B, SLSQP) can be used for outer-loop optimization studies
- Objectives, controls, and constraints can be directly defined through Notebook widgets



Optimization Studies

As a proof of concept, we maximize an output of the aerobic bioreactor by adjusting the feedstock's initial porosity subject to constraints





Concluding Remarks

- Connected simple Python scripts, CFD simulations, and Aspen Plus calculations with `vebio`
- For future optimization studies, **accurate surrogate models** will take on even greater importance
- We're currently developing documentation and examples as part of enabling collaboration with new projects and **moving toward a public software release**

Questions?

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