

# IDAES

Institute for the Design of  
Advanced Energy Systems

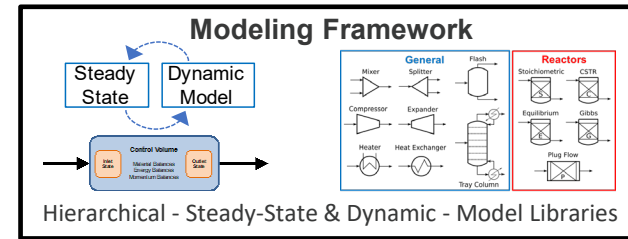
## IDAES for Advanced Users

Alejandro Garciadiego, Doug Allan, Miguel Zamarripa, Andrew Lee,  
Dan Gunter  
Stakeholder Summit 2023

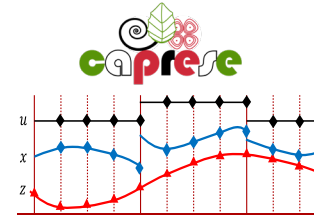


# IDAES for Advanced Users - Outline

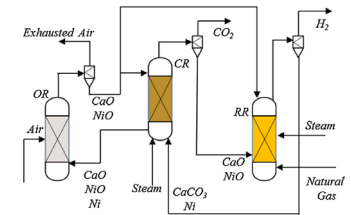
- Model, Flowsheet, Costing Libraries
- Dynamic and Controllable Models
- Surrogate Modeling
- Diagnostics & Visualization



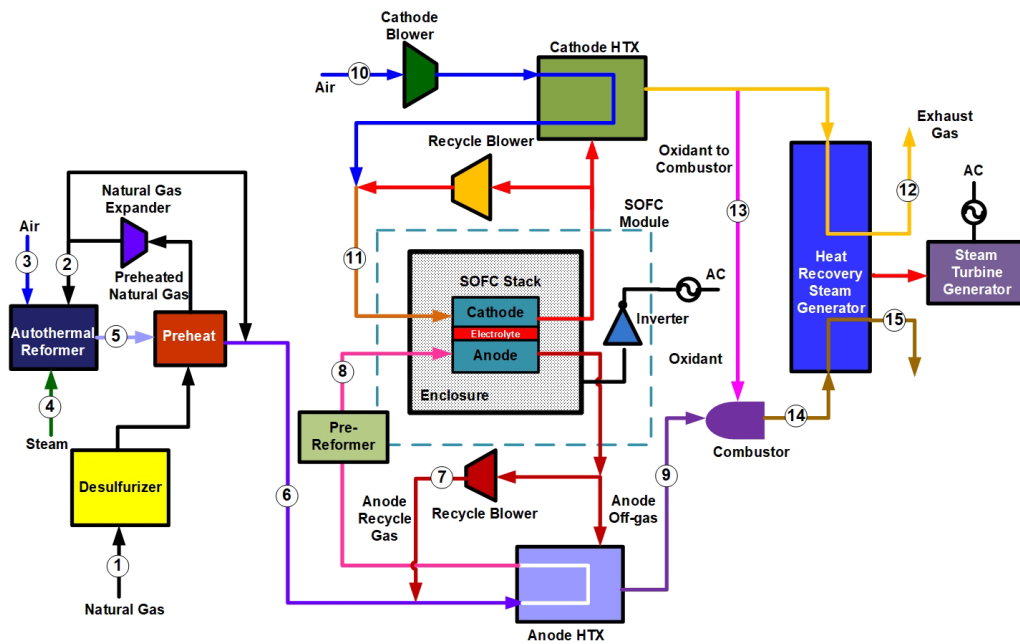
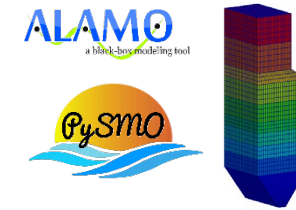
Process Operations  
Dynamics & Control



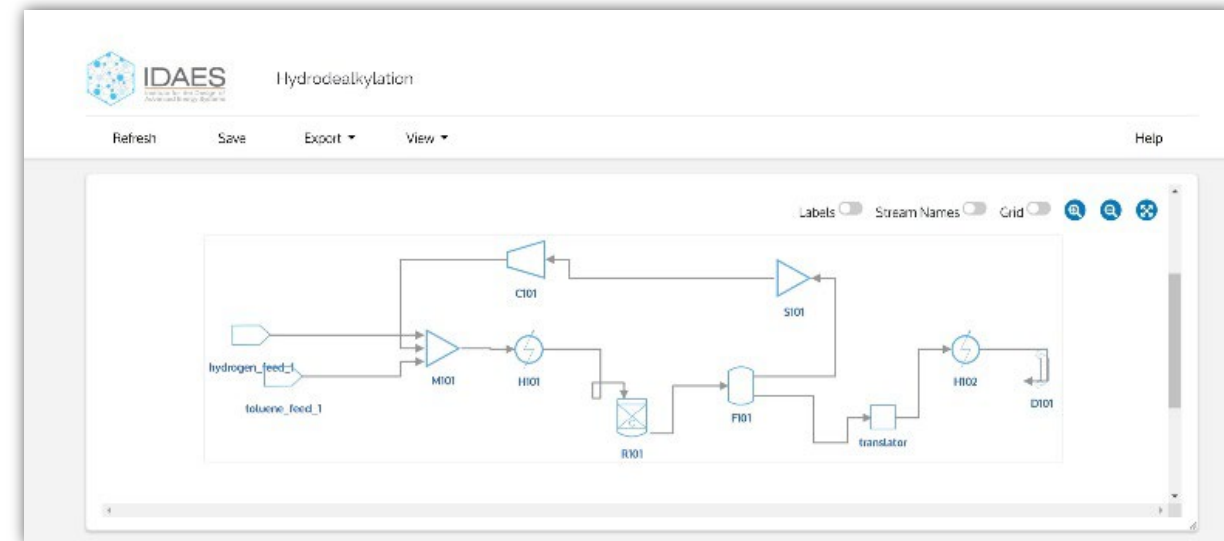
Plant Design  
Process Optimization



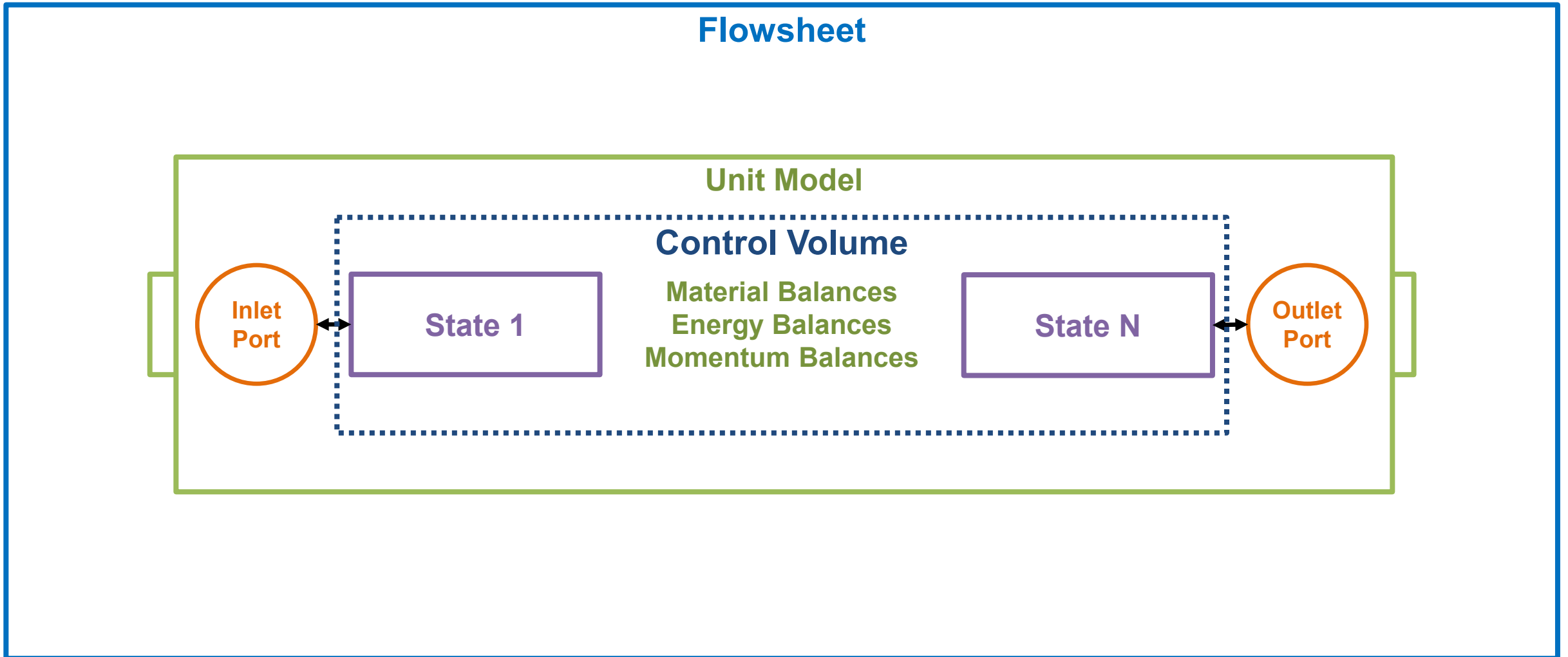
AI/ML  
Surrogate Modeling



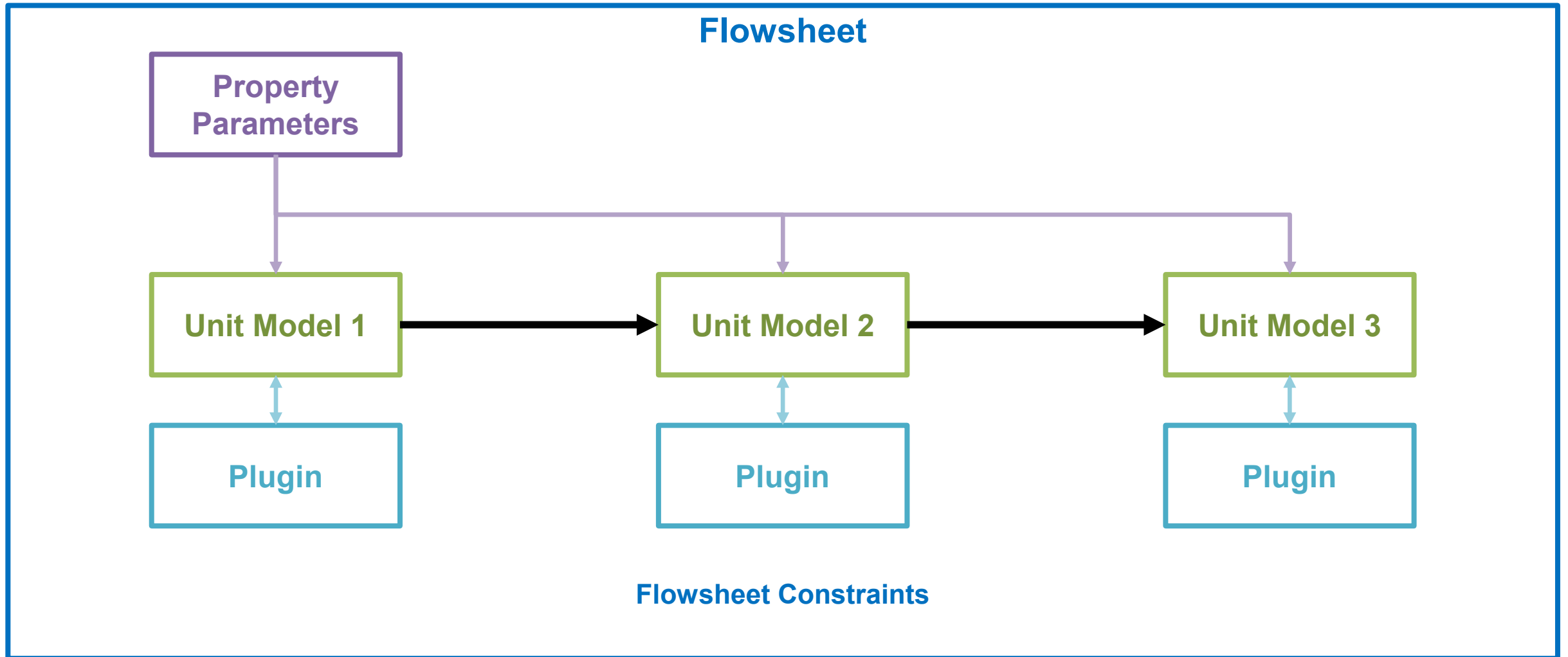
## Case Study – Solid Oxide Fuel Cell Flowsheet in IDAES



# Block Hierarchical Structure



# Block Hierarchical Structure



# IDAES Core Capabilities for Advanced Process Models

Unit Model Library



IDAES Unit **Model Library** provides basic unit models (i.e., mixers, splitters, flash drums) that can be used as building **blocks** for more **complex models**.

Property Blocks



## Properties:

- Implemented as modular blocks
- Flexibility to choose state variables
- Flexibility to use different property packages in same flowsheet
- Flexible formulation of equations

Ports

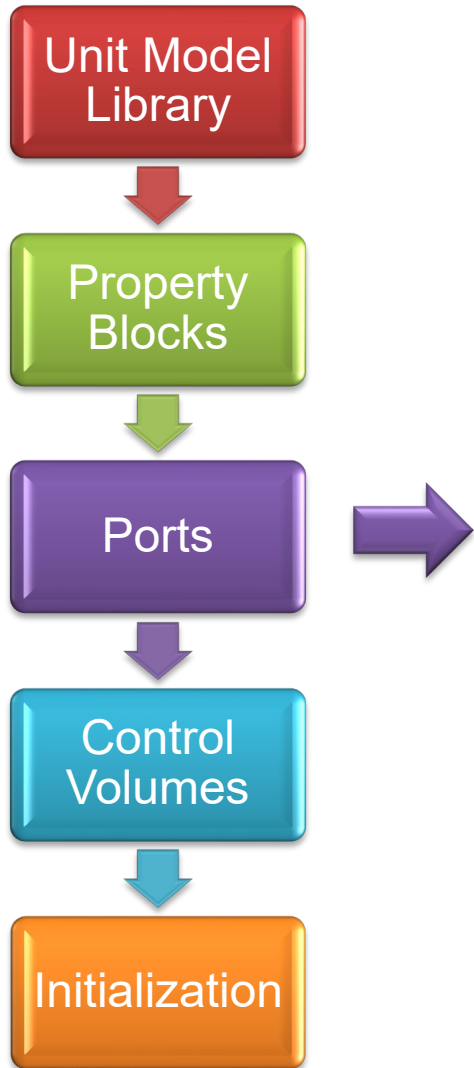
Control Volumes

Initialization

$$V = f(T, P, x) \quad h = f(T, x) \quad P_{sat} = f(T)$$

$$Cp = f(T) \quad y_i = K_i x_i \quad r = f(T, P, x)$$

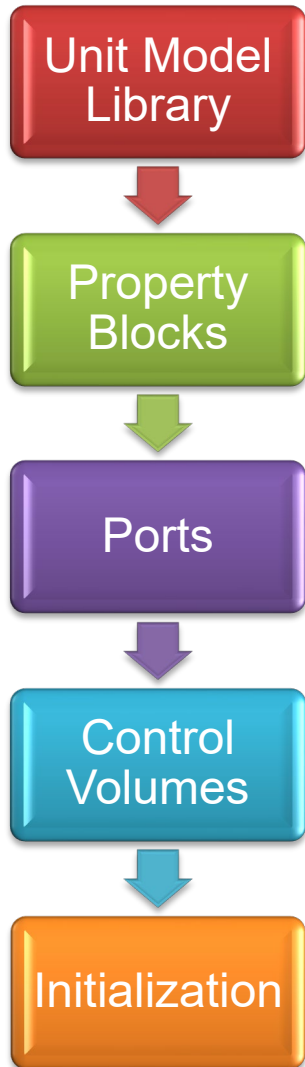
# IDAES Core Capabilities for Advanced Process Models



## Ports:

- Defined via the property package
- Can connect to any other Port with the same members automatically
- Translator blocks to connect Ports with different state variables

# IDAES Core Capabilities for Advanced Process Models



## Control Volumes:

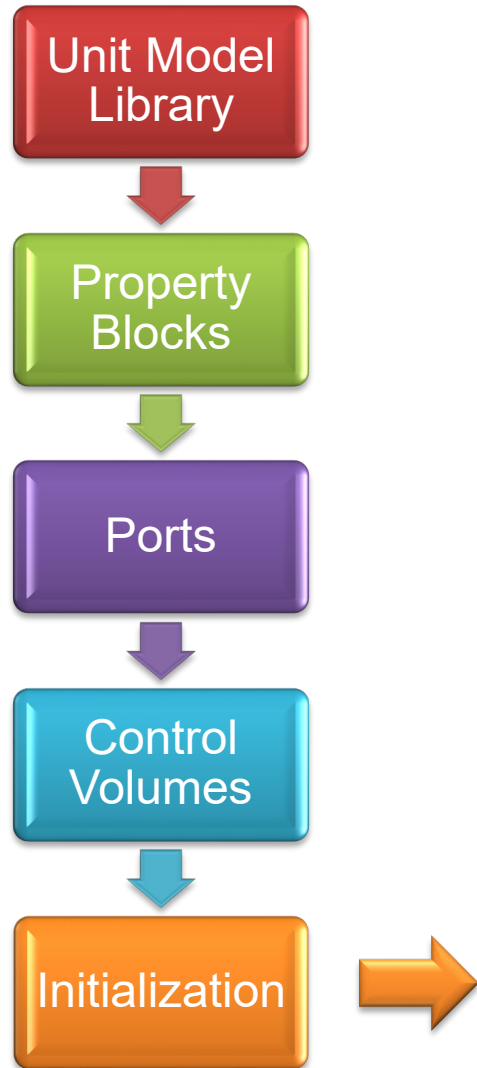
- Three types of Control Volumes available for different applications
  - 0-D (Inlet-Outlet type)
  - 1-D (Pipes, PFRs)
- Control Volumes can be connected together to develop complex multi-scale models
- Prebuilt **methods** for common forms of **balance equations**:

$$\frac{\partial M_j}{\partial t} = F_{in,j} - F_{out,j} + N_{rxn,j} + N_{eq,j} + N_{phase,j}$$

$$\frac{\partial E}{\partial t} = H_{in} - H_{out} + Q + W$$

$$0 = P_{in} - P_{out} + \Delta P$$

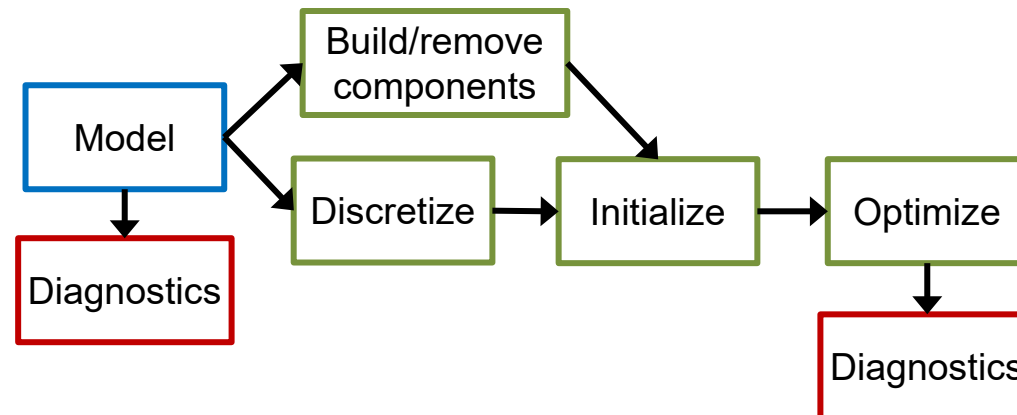
# IDAES Core Capabilities for Advanced Process Models



## Initialization:

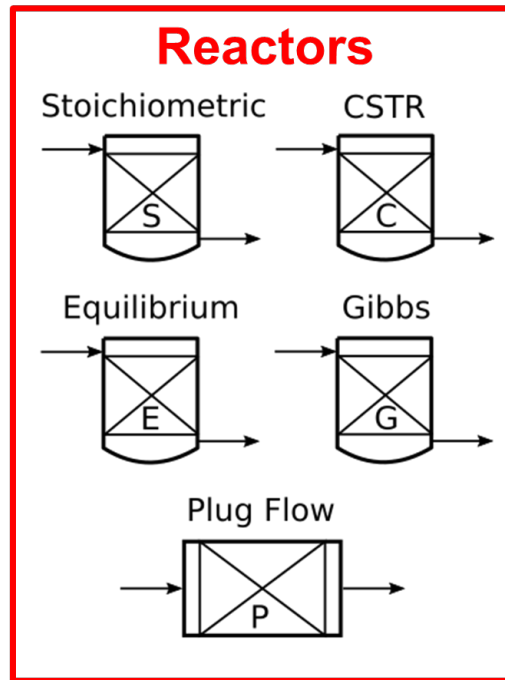
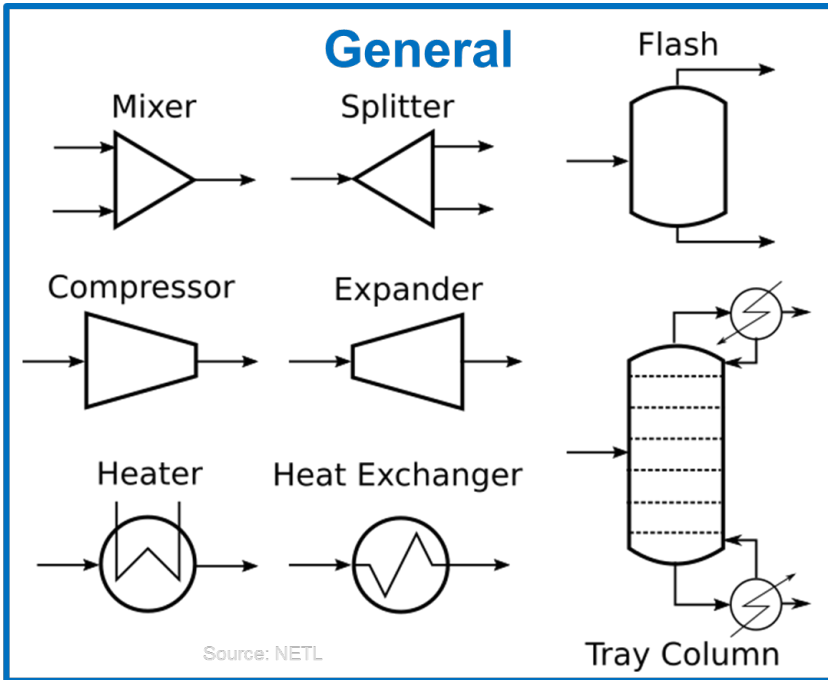
- Custom initialization routines
- IDAES developed tools for solving complex models
  - Decomposition solvers
  - Reliability and convergence tools
- IDAES diagnostics toolset (structural analysis, ...)

## Modular Framework



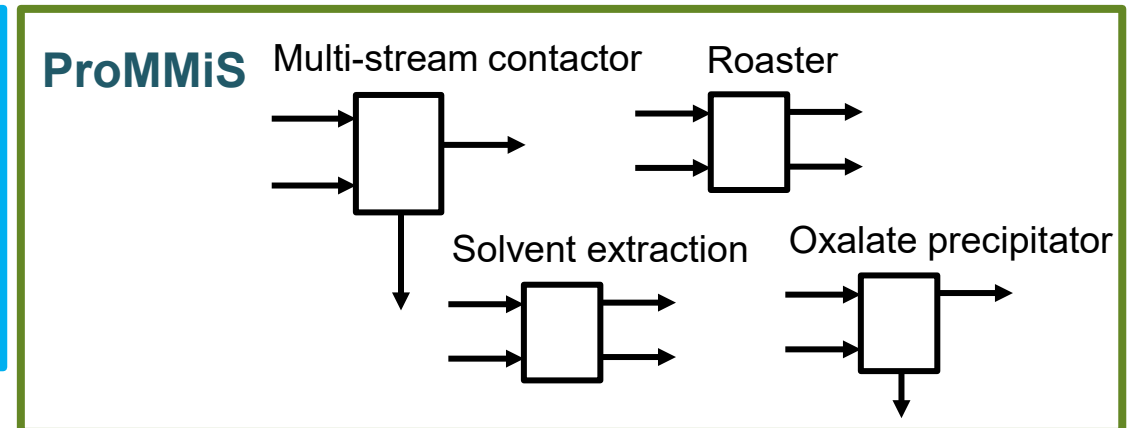
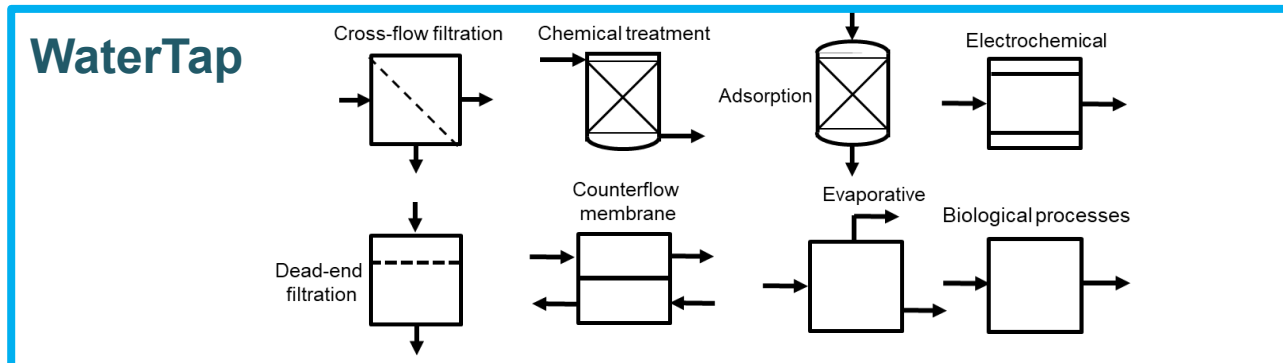


# Unit models developed

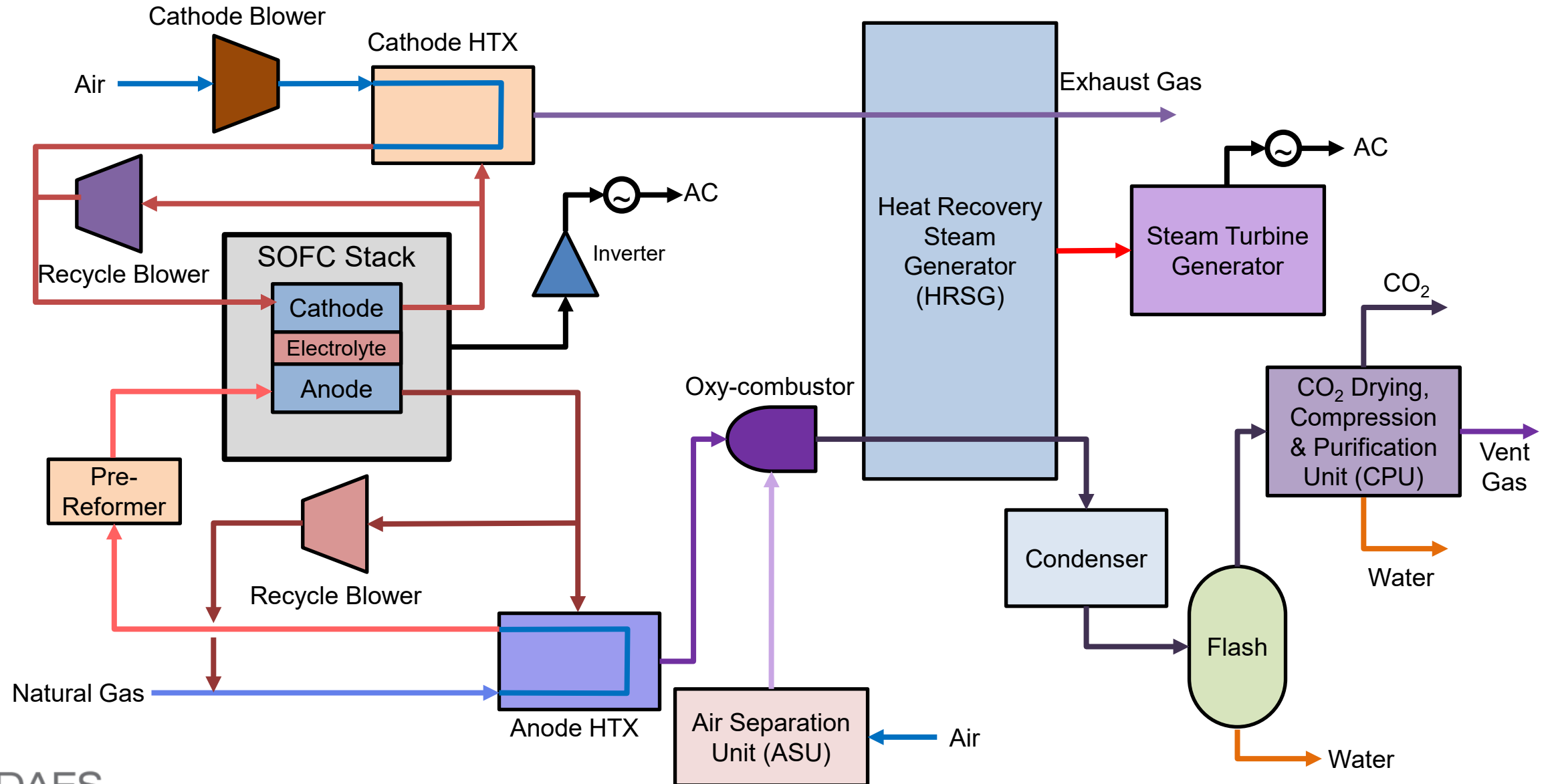


- Library of common thermodynamic models
  - Ideal
  - Cubic Equations of State
  - Helmholtz Equation of State
  - Electrolytes
- Extensive libraries for common unit operations
  - Mixers, Splitters, Heaters, Heat Exchangers, Pressure Changers, Reactors
  - Dynamics and Control
- Specialized Libraries for other equipment
  - Distillation, SOFC/SOEC, Power Generation, Gas-Solids Contactors, Gas-Liquid Absorption

## Project specific models developed leveraging IDAES:

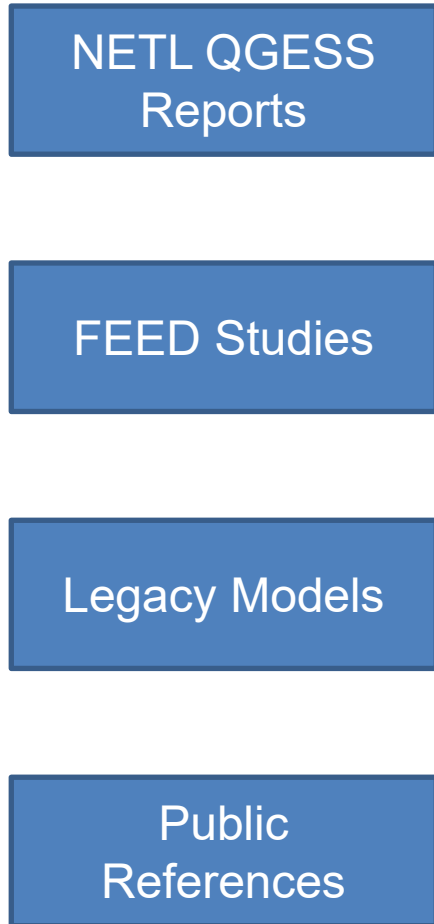


# Solid oxide electrolysis cell (SOFC) Flowsheet building



# Cost Optimization in IDAES using NETL's QGESS<sup>1</sup> Methodology

## Data Sources



## General Costing Library

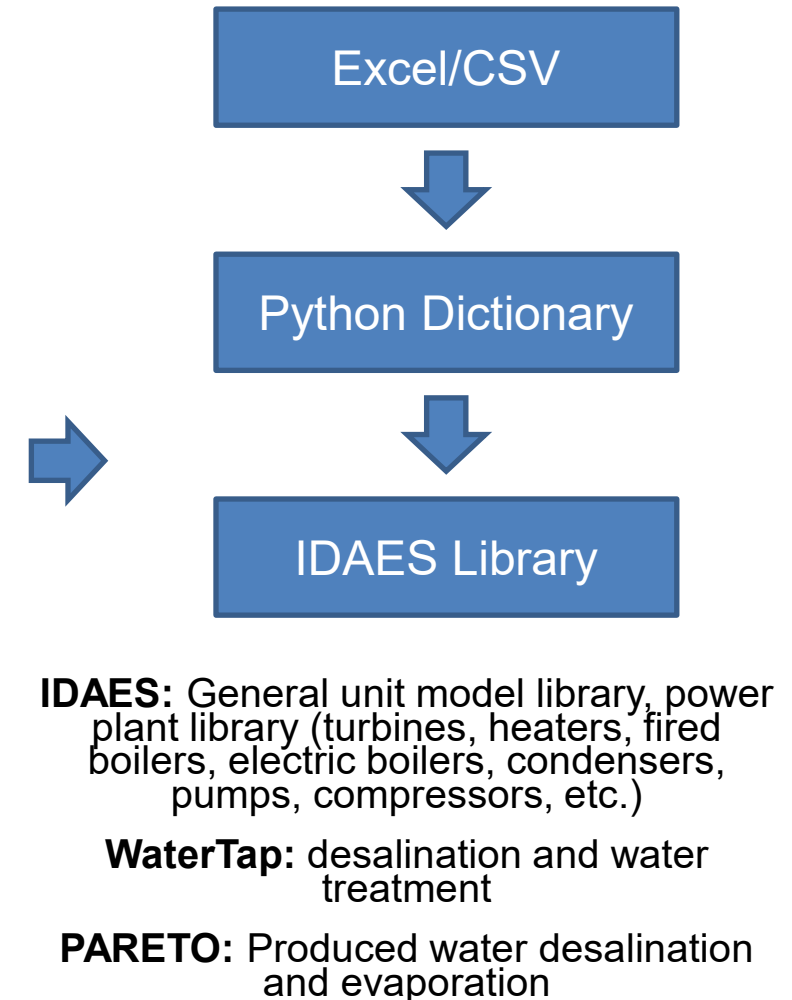
Unit	Cost Correlation	Basis
Heat Exchanger	$C_B = f(\text{area})$ $CP = (CE/500)F_D F_M C_B$	Area, Material, and pressure
Reactors, Flash, Vessel	$C_V = f(W)$ $C_{PL} = f(D, L)$ $CP = (CE/500)C_{PL} F_M C_V$	Material, Dimensions (length, diameter)
Compressor	$C_B = f(P_C)$ $CP = (CE/500)F_D F_M C_B$	$P_C$ - Theoretical reversible adiabatic power (horsepower)
Distillation column	$C_V = f(W)$ $C_{PL} = f(D, L)$ $C_{BT} = f(D)$ $CP = (CE/500)C_{PL} F_M C_V$	Material, Dimensions (length, diameter), number and type of trays.
...		

Scale costs as appropriate:

$$SC = RC \left( \frac{SP}{RP} \right)^{EXP}$$

SC: Scaled Cost  
 RC: Reference Cost  
 SP: Scaled Parameter  
 RP: Reference Parameter

## Implementation



<sup>1</sup> QGESS: Capital Cost Scaling Methodology Revision 4

# Summary

1. Developed unit models and property models in the IDAES framework
2. Contributed unit model and flowsheet examples to the IDAES open-source GitHub repository
3. Developed costing in IDAES based on NETL's QGESS<sup>1</sup> Methodology
4. Modeled and simulated an initial NGFC flowsheet without CCS in IDAES Core Modeling Framework (CMF)
5. Developed a natural gas property package in IDAES CMF
6. Compared initial NGFC flowsheet with state-of-the-art commercial simulators
7. Contributed NGFC example to the IDAES open-source GitHub repository

# Motivation: Dynamic Modeling, Simulation, and Optimization

- No plant is truly at steady state
- When optimization is used for design, resulting plant may not be **controllable**
  - Setpoint transition
  - Start up/shut down
- **Dynamic operation** of integrated energy systems (IES) can take advantage of dynamic electricity pricing
- **Equipment degradation** occurs over thousands of hours

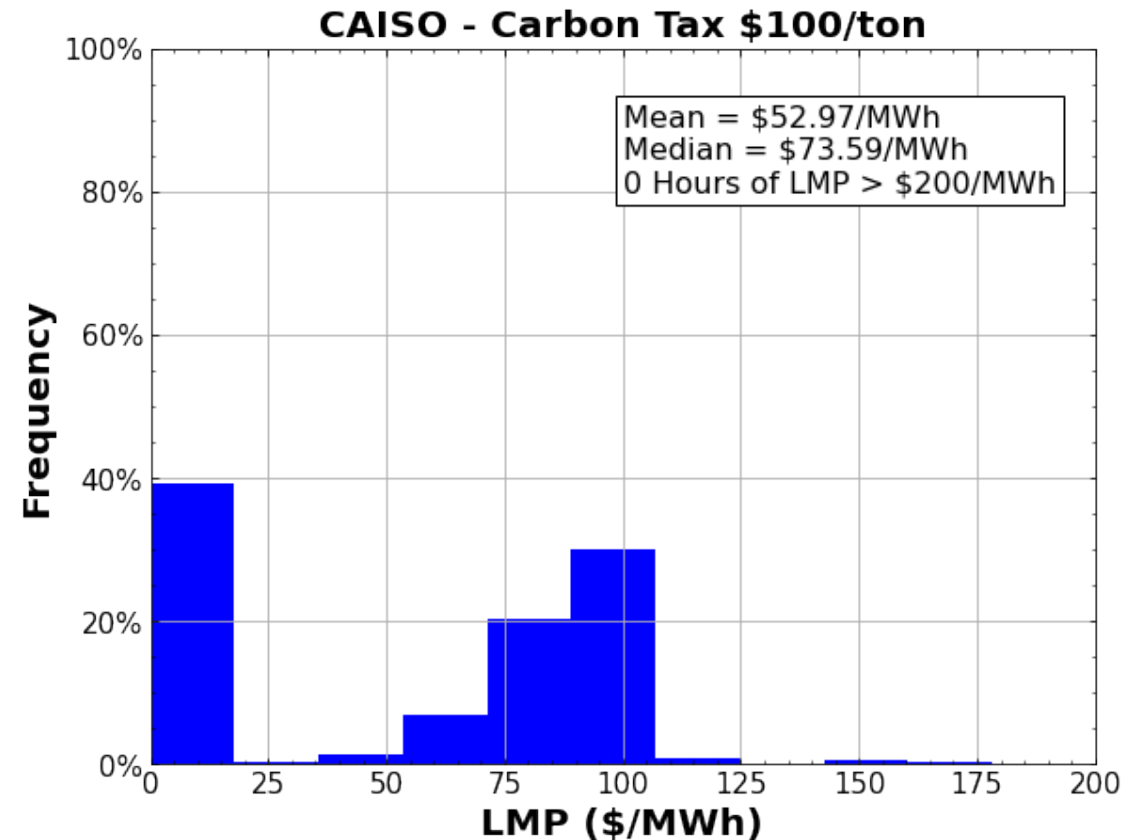
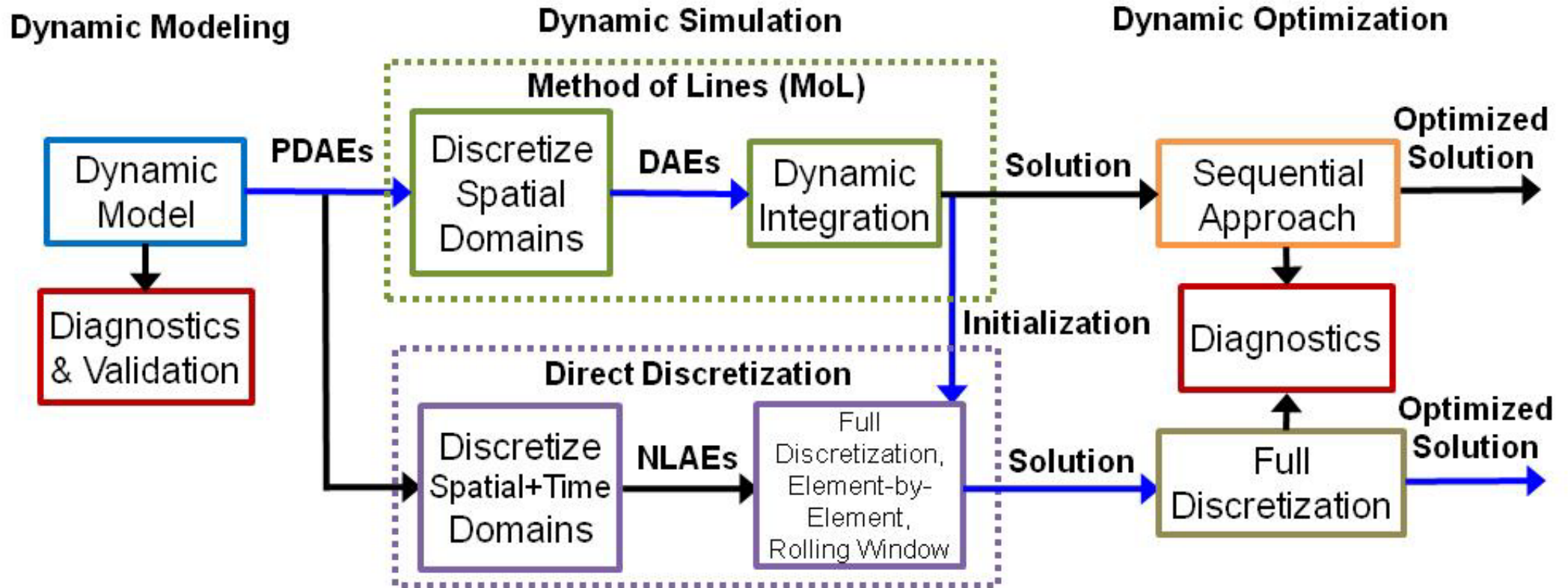


Figure from a presentation by Cortes et al.

(Price Signal Data): Cohen, Stuart; Durvasulu, Venkat (2021): NREL Price Series Developed for the ARPA-E FLECCS Program. National Renewable Energy Laboratory.

# IDAES Dynamic Modeling/Simulation/Optimization Workflow



# IDAES Dynamic Modeling/Simulation/Optimization Workflow

- **PYOMO DAE**

- Develop differential algebraic equation (DAE) model
- Apply diagnostic tools for structural/numerical analysis

- **IDAES**

- Set some/all unit models to be dynamic
- PID Controller implemented with anti-windup

- **Dynamic Simulation**

- **Method-of-Lines (MoL)** (AMPL/PETSc/TS)
- Direct Discretization

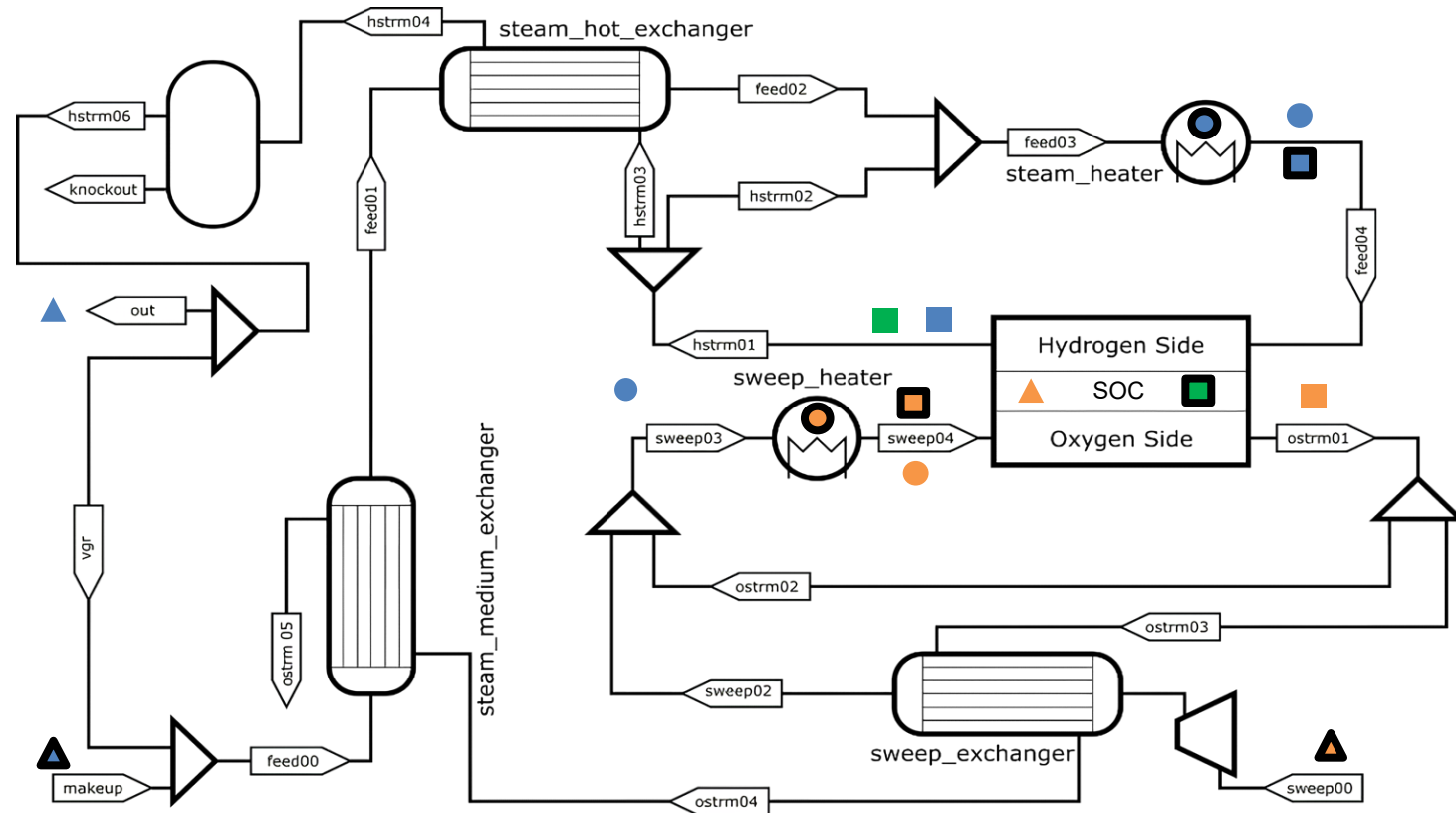
- **Dynamic Optimization**

- Full Discretization
- Can implement nonlinear model predictive control (NMPC)



# Case Study: Control of Solid Oxide Cell (SOC)-IES

Controller Type	Manipulated Variable (MV)	Controlled Variable (CV)
PI	Cell potential <span style="color: green;">■</span>	SOC fuel outlet H2 mole fraction <span style="color: green;">■</span>
P	Makeup feed rate <span style="color: blue;">▲</span>	Hydrogen production rate <span style="color: blue;">▲</span>
P	Sweep feed rate <span style="color: orange;">▲</span>	SOC stack core temperature <span style="color: orange;">▲</span>
PI (C1I)	Steam heater duty <span style="color: blue;">●</span>	Steam heater outlet temperature <span style="color: blue;">●</span>
PI (C2I)	Sweep heater duty <span style="color: orange;">●</span>	Sweep heater outlet temperature <span style="color: orange;">●</span>
P (C1O)	Steam heater outlet temperature setpoint* <span style="color: blue;">■</span>	SOC feed outlet temperature <span style="color: blue;">■</span>
P (C2O)	Sweep heater outlet temperature setpoint* <span style="color: orange;">■</span>	SOC sweep outlet temperature <span style="color: orange;">■</span>



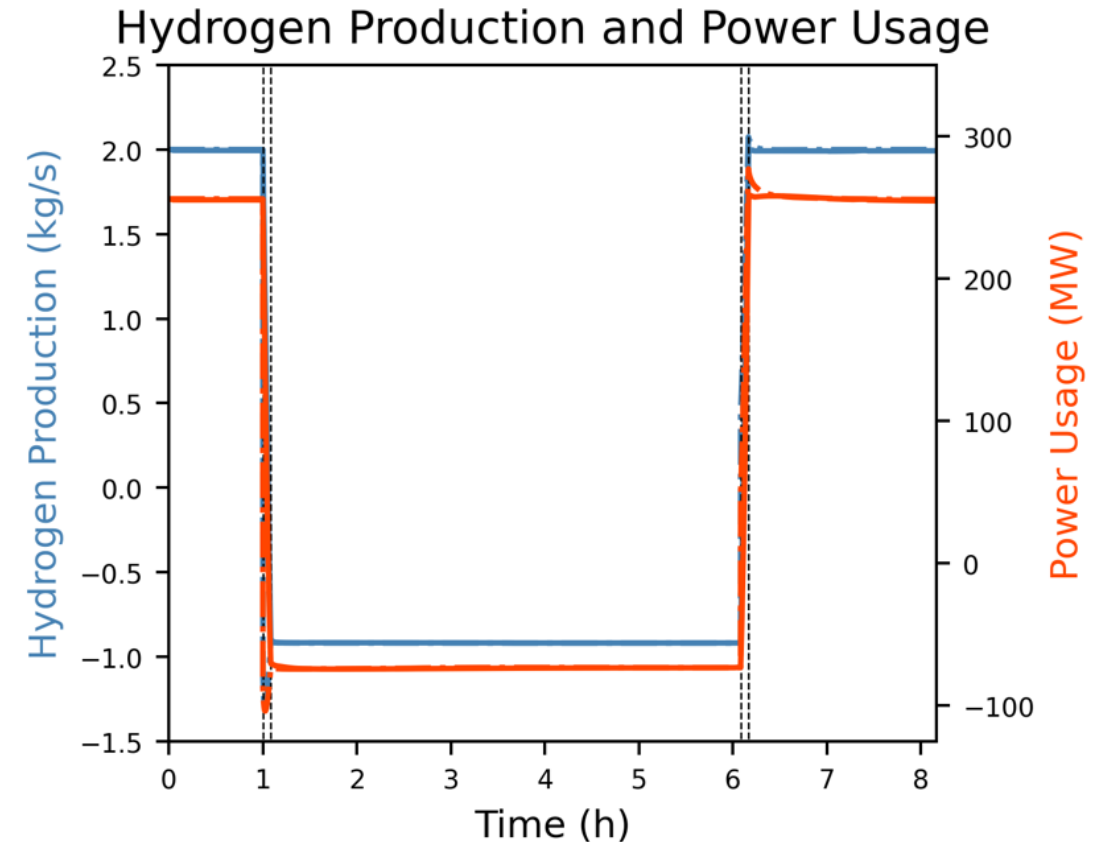
- Plantwide **PI control** setup with **cascade control**
- Compare to **NMPC**, which is better able to handle **variable interactions** and **constraints**



# SOC-IES Case Study: Comparison of PI control to NMPC

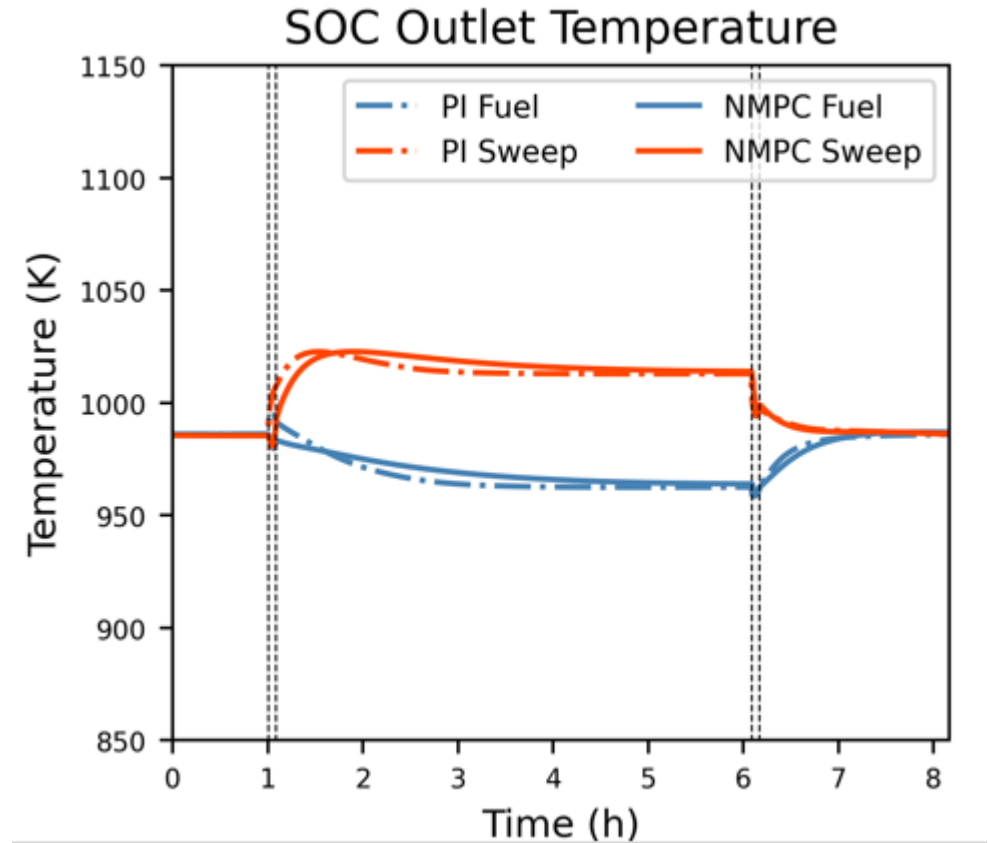
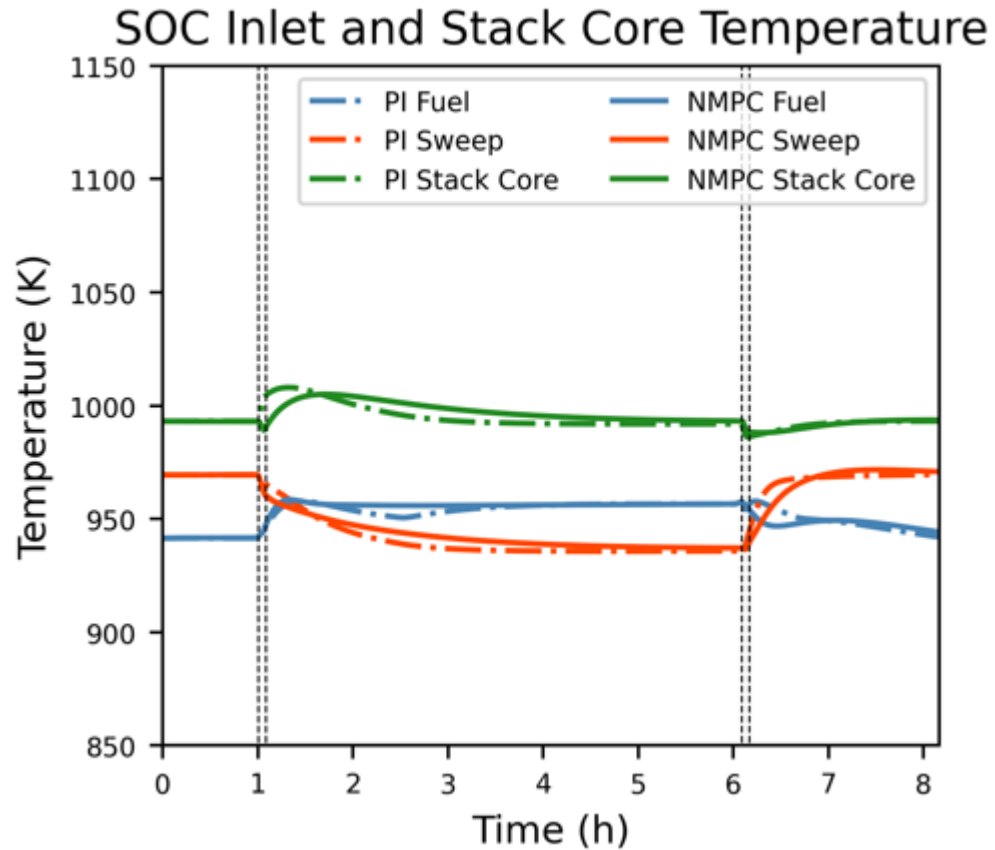
- Both PI and NMPC quickly transition between setpoints for maximum H<sub>2</sub> production to power generation (within 5-10 minutes) and back
- PI overshoots on power usage, whereas NMPC does not
  - Possibly able to be smoothed over by a local battery
- Both control methods are able to achieve a rapid transition

NMPC work by Mingrui (Michael) Li, Vibhav Dabadghao, and Lorenz (Larry) Biegler from CMU, more details on poster



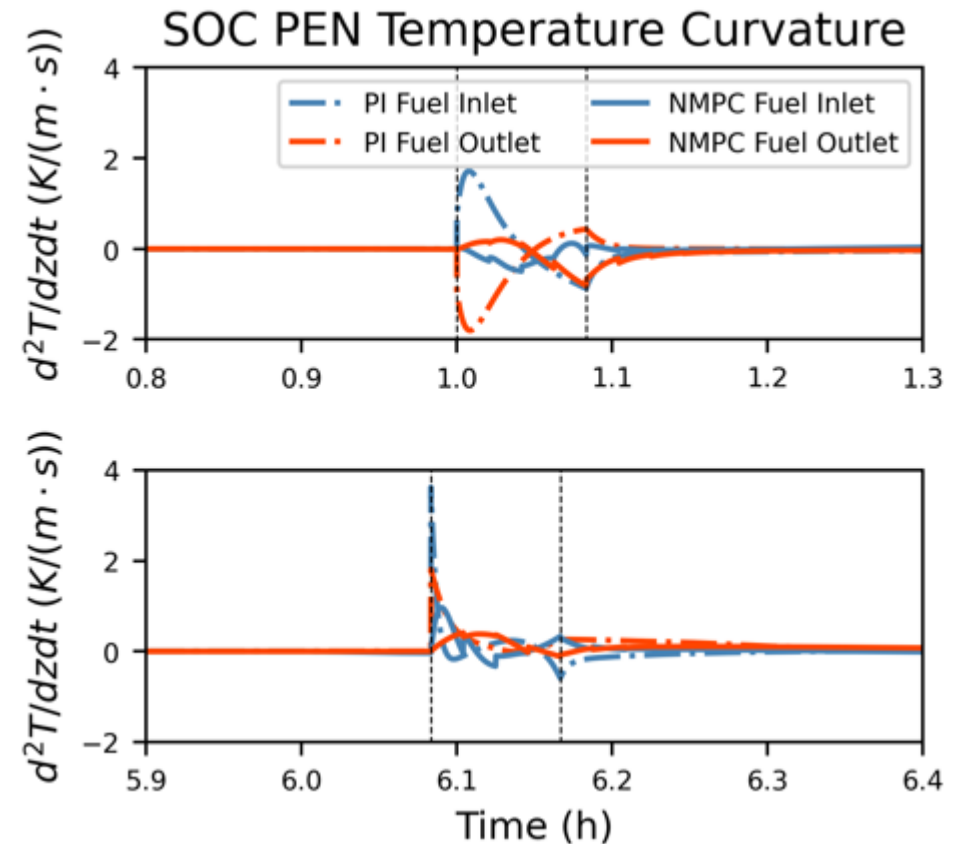
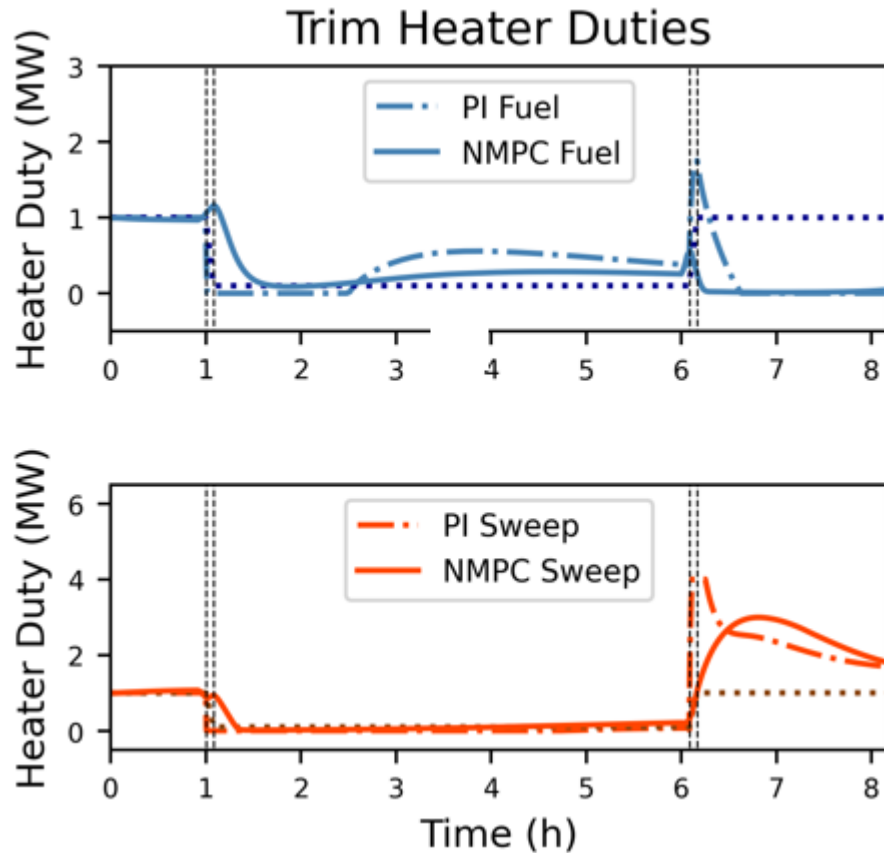
NMPC --- solid line  
PI --- dashed line

# SOC-IES Case Study: Slow thermal dynamics



- H<sub>2</sub> production responds immediately, but temperature takes hours to settle

# SOC-IES Case Study: Trim heaters and mixed partials

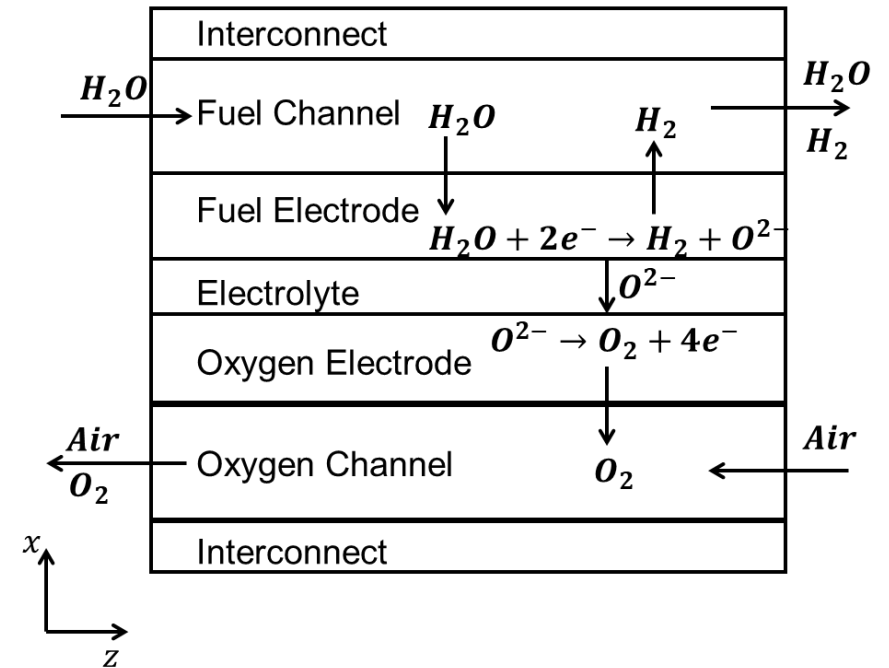


- Trim heaters are still engaged at end of time period, indicating the entire system is not at steady state yet
- NMPC can minimize magnitude of time derivative of cell temperature gradient (mixed partial) in order to reduce thermal failure probability

# Case Study: SOEC Degradation Modeling

- Due to degradation, **SOC performance is time-varying**.
- Optimize SOC system performance over **cell's entire lifespan** to maximize net present value (NPV)
- Cell experiences both **physical** and **chemical degradation**.
- Due to mass and heat integration, it is desired that the entire SOC-IES be considered.
- Results presented are for **electrolysis mode only**.
- Long timescales (up to 20,000 hours) mean that **everything in IES besides cell is at steady-state**

SOC degradation work by Nishant Giridhar, Quang Minh Li, and Debangsu Bhattacharyya at WVU, more details on poster



## Planar fuel electrode supported SOEC

### Materials

- Fuel electrode – Ni-YSZ
- Oxygen electrode – LSM-YSZ
- Electrolyte – YSZ

### Modeling details

- First principles dynamic 2-D, non-isothermal equation-oriented model
- Capable of SOFC and SOEC operation
- This work - SOEC

# SOEC Microstructure Degradation Modeling

- Degradation occurs over thousands of hours

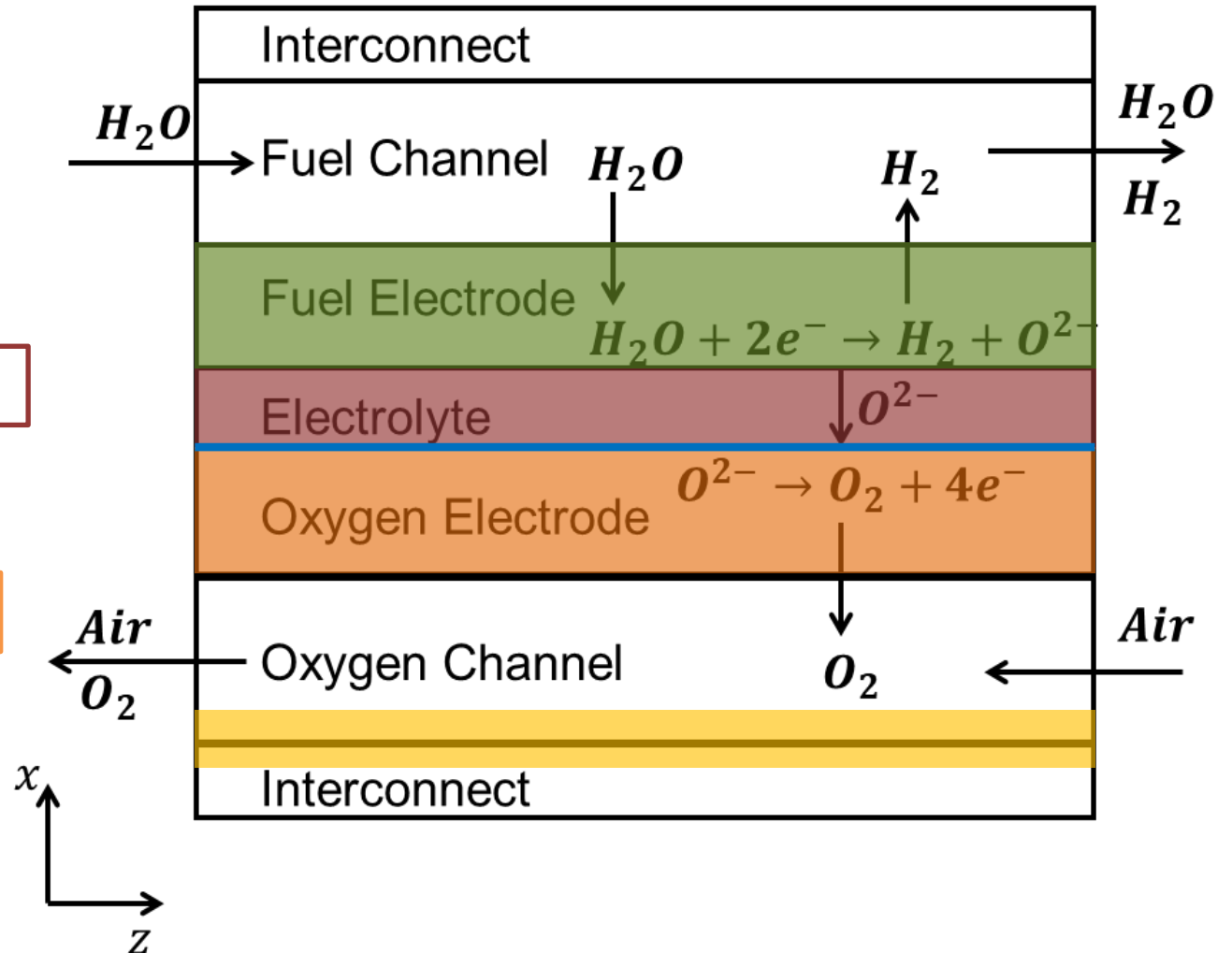
Fuel electrode Ni agglomeration

YSZ electrolyte phase transformation

LSM-YSZ phase coarsening

Lanthanum zirconate scale growth

Chromium oxide scale growth



# Optimizing Long-Term SOEC System Operation

## Case 0: Constant Temperature

- Constant H<sub>2</sub> production rate at 1.5 kg/s
- Constant temperature at SOC inlets

## Case 1: Maximize Integral Efficiency

- Constant H<sub>2</sub> production rate at 1.5 kg/s
- Objective: Maximize integral efficiency for the flowsheet.

## Case 2: Minimize Final Degradation

- Constant H<sub>2</sub> production rate at 1.5 kg/s
- Objective: Minimize resistance growth for oxygen electrode

Decision variables at each time point:

1. Feed heater duties
2. Sweep heater duties
3. Sweep blower flowrate
4. Feed exchanger flowrate
5. Feed recycle ratio
6. Sweep recycle ratio

$$\max \frac{1}{t_f} \sum_{t=0}^{t_f} \eta_{th,t} \Delta t$$

st.

$$h(x) = 0$$

$$\frac{dR}{dt} = f_R(x, t)$$

$$j_t = j_0 \quad \forall t$$

$$\eta_{th,t} = \frac{HHV(H_2, t)}{P_{in,total,t}}$$

$$\min \frac{R_{t_f}}{\Delta t}$$

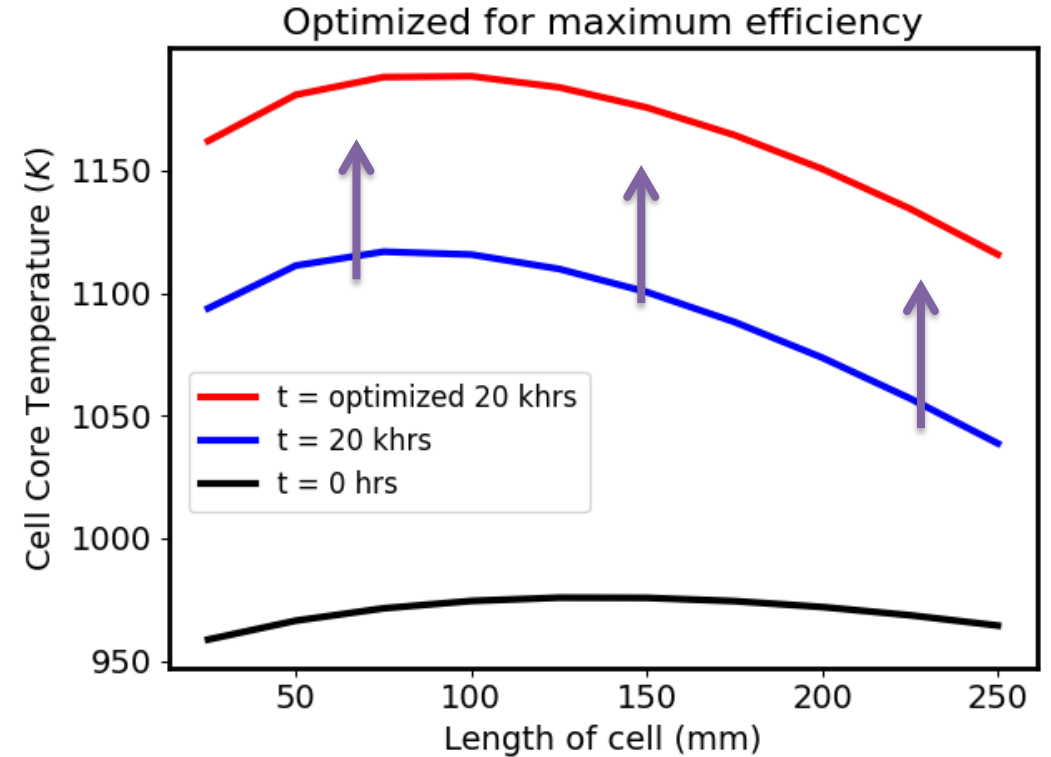
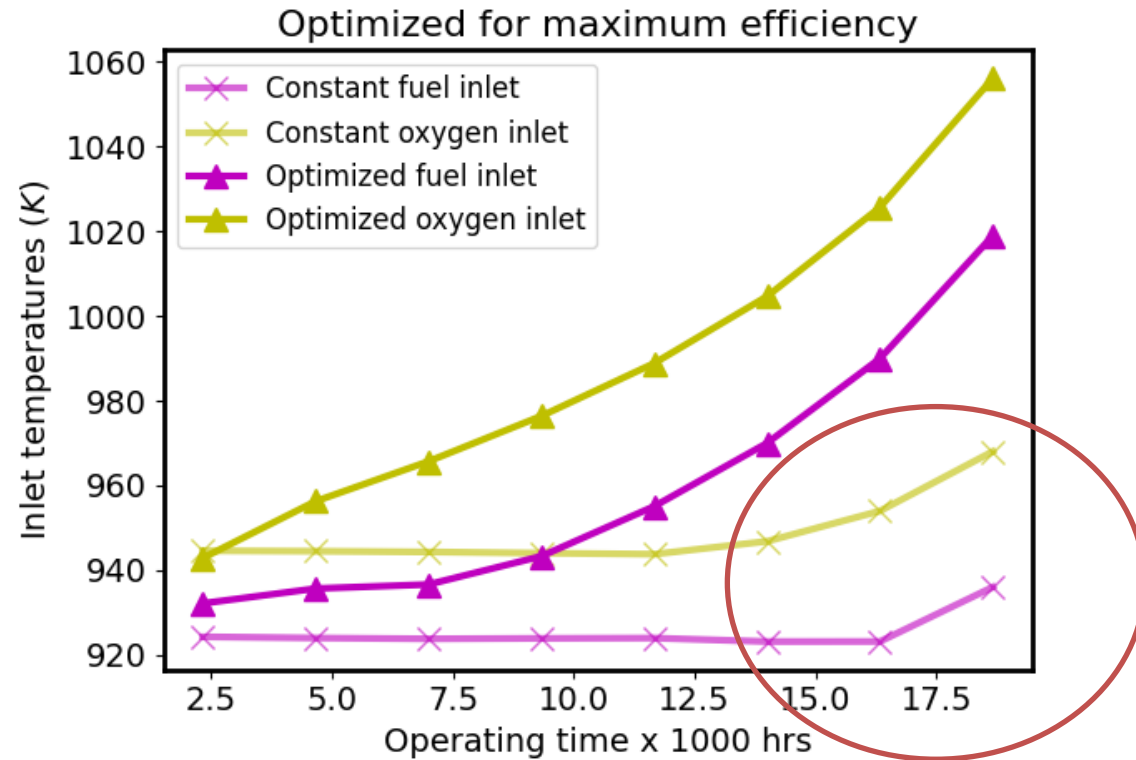
st.

$$h(x) = 0$$

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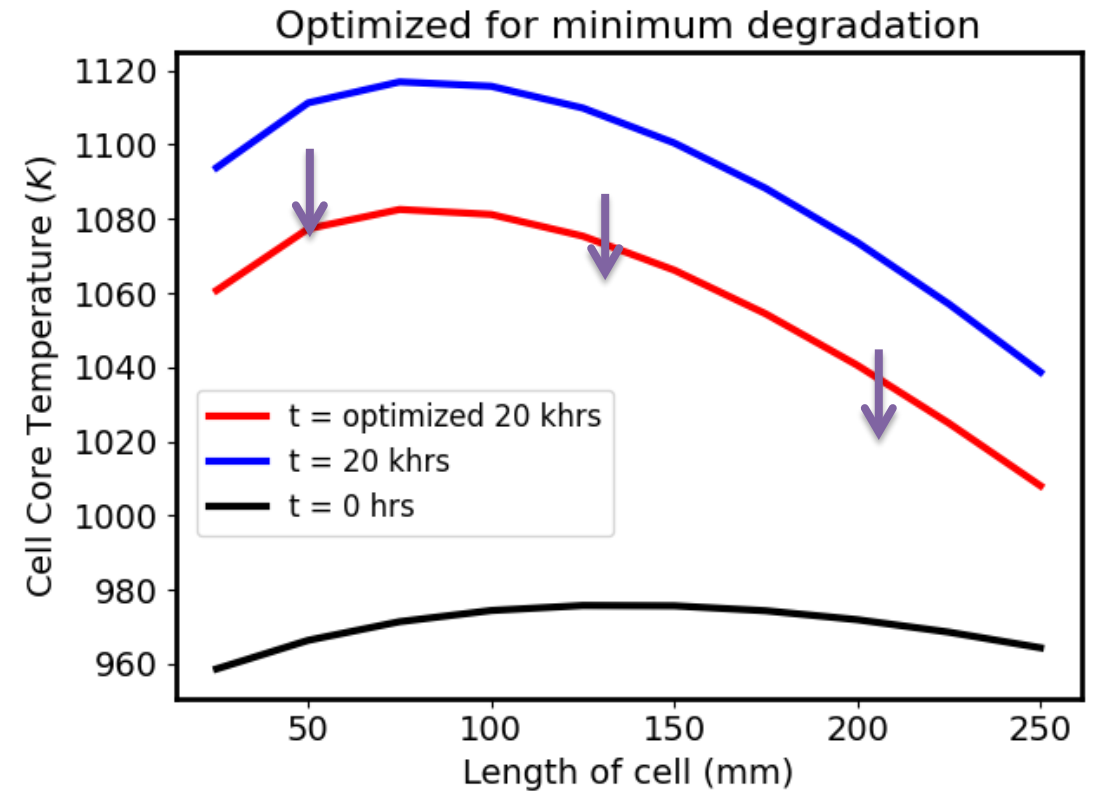
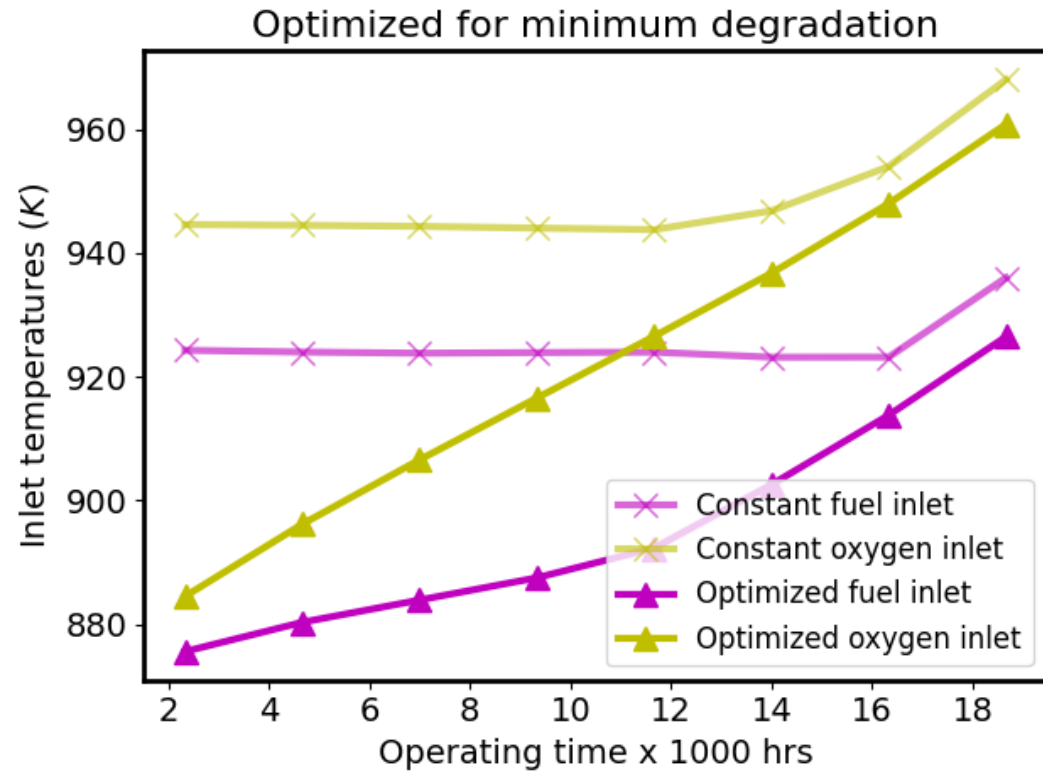
# Case 1. Maximize SOEC Efficiency over 20,000 hrs of Operation



## Inlet temperatures for maximizing efficiency:

- ~~Inlet temperature increases to~~ **Constant inlet temperature** to **reduce resistive losses**
- ~~Increased Joule heating in cell causes air blower to hit a bound, so~~ **Increased temperature comes at a price of increased chemical degradation**  
temperature must increase.

# Case 2. Minimize SOEC Degradation over 20,000 hrs of Operation

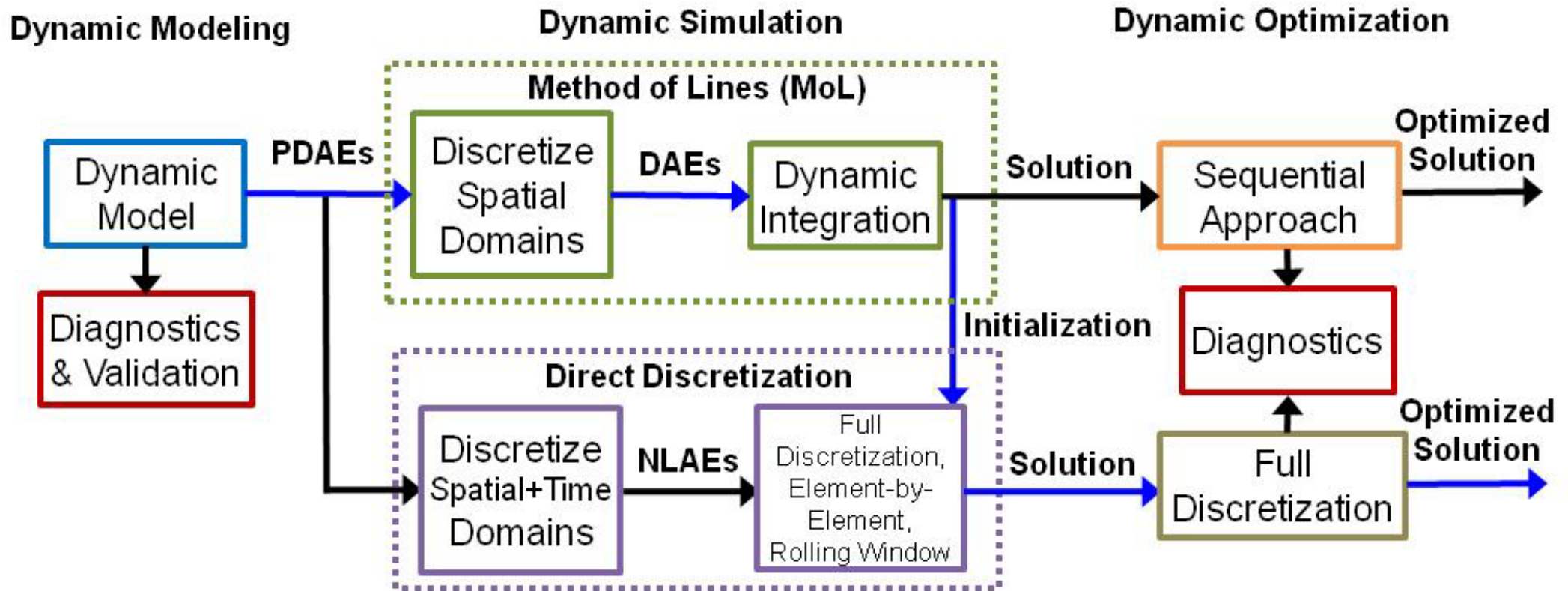


## Inlet temperatures for minimizing degradation:

- **Inlet temperatures remain low** throughout the operating period.
- **Cell core temperatures** about 60 K **lower** than the constant temperature case.



# Dynamics Questions



Questions about Pyomo/IDAES dynamic capabilities?

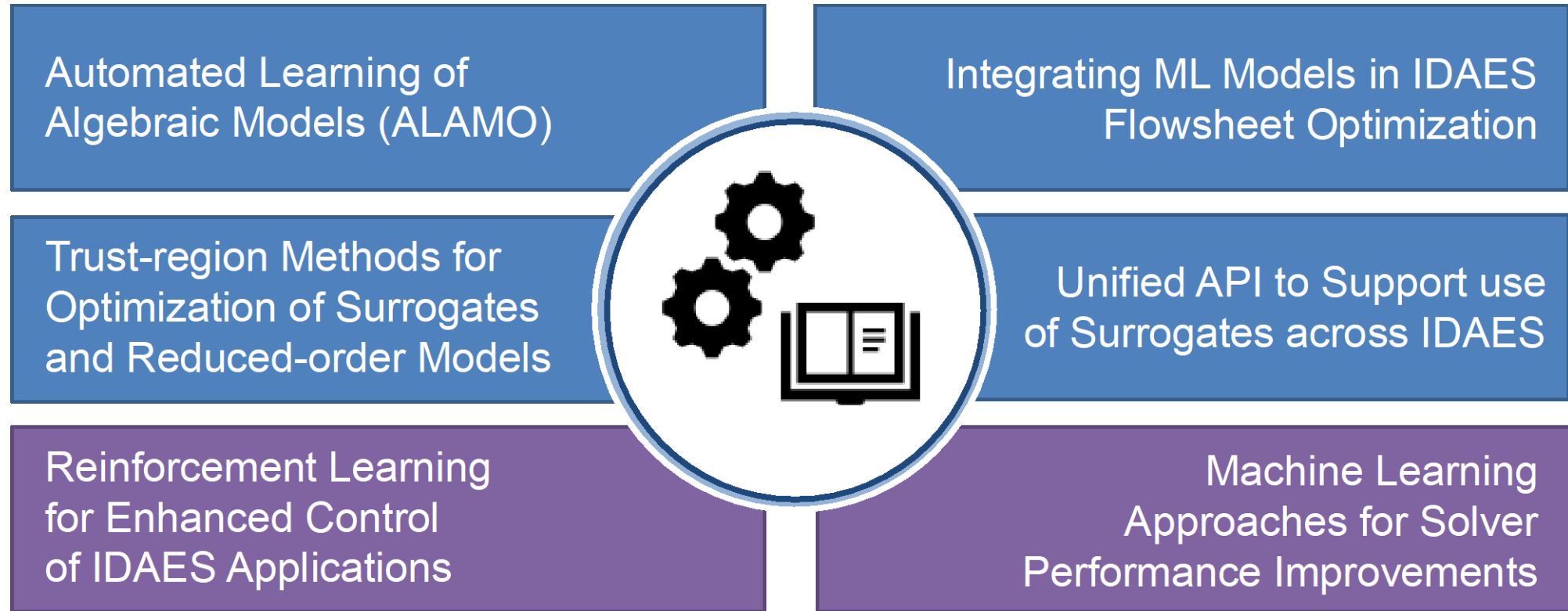
# Surrogate Modeling in IDAES

## What it is new?

Development: Trust region framework, examples, notebooks,

Application: market integration, SOFC examples, etc.

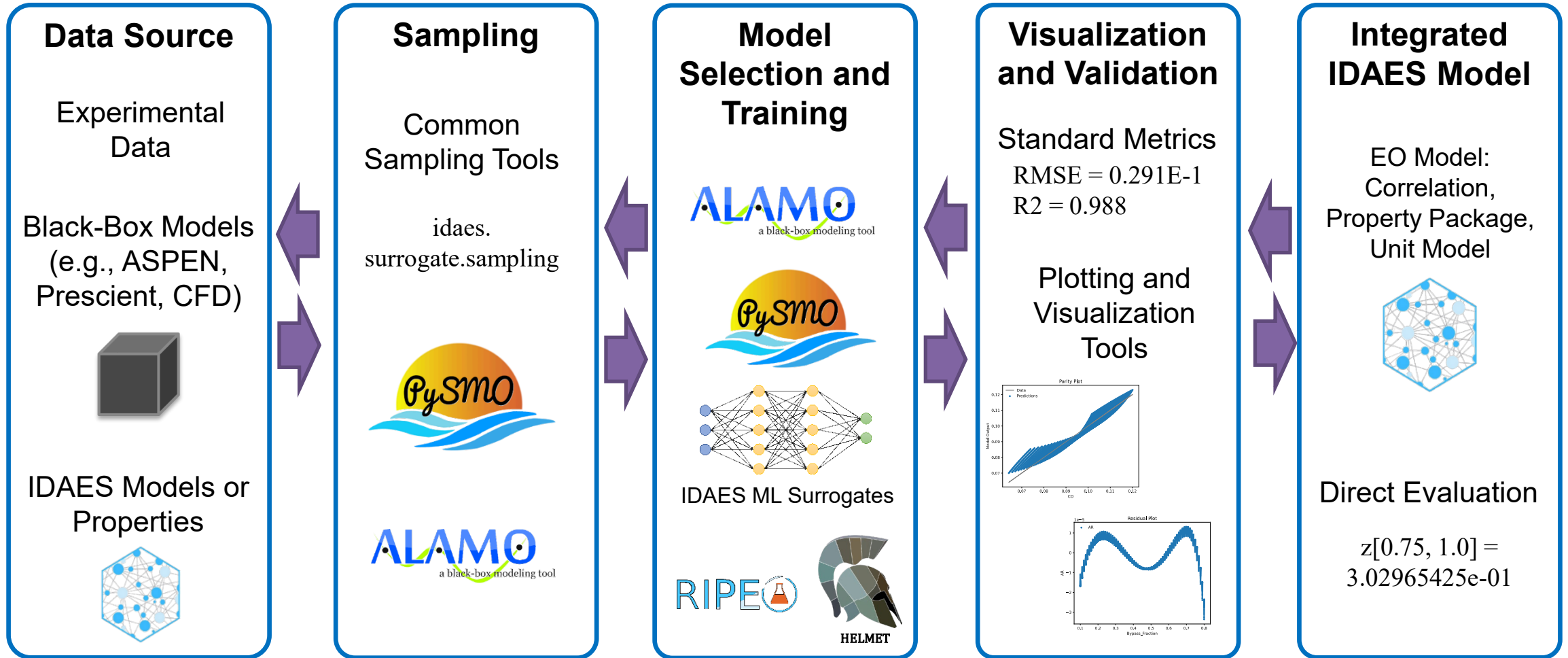
# Machine Learning and AI for Optimization



Fundamental Tools Enabling Workflows Across IDAES Team

**“Consistent Framework to Validate/Verify ML/AI Tools for Optimization”**

# IDAES Framework: Surrogates for Optimization



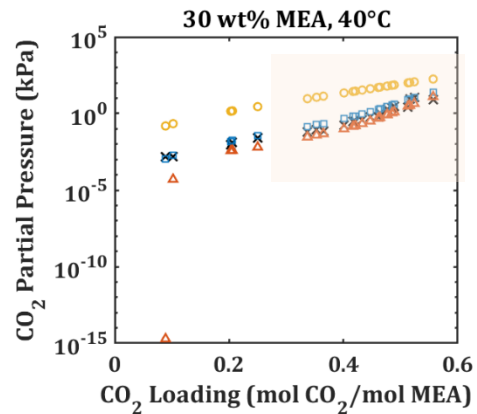
Validate solution against rigorous model or data

# 1.- Data Source “Best Practices”



Ensure **quantity and quality**

- Experiments: visualize data to guarantee sampling distribution
- Simulation: ensure model robustness



80% of data is between 0.4 and 0.6 CO<sub>2</sub> loading

## 2.- Sampling “Best Practices”



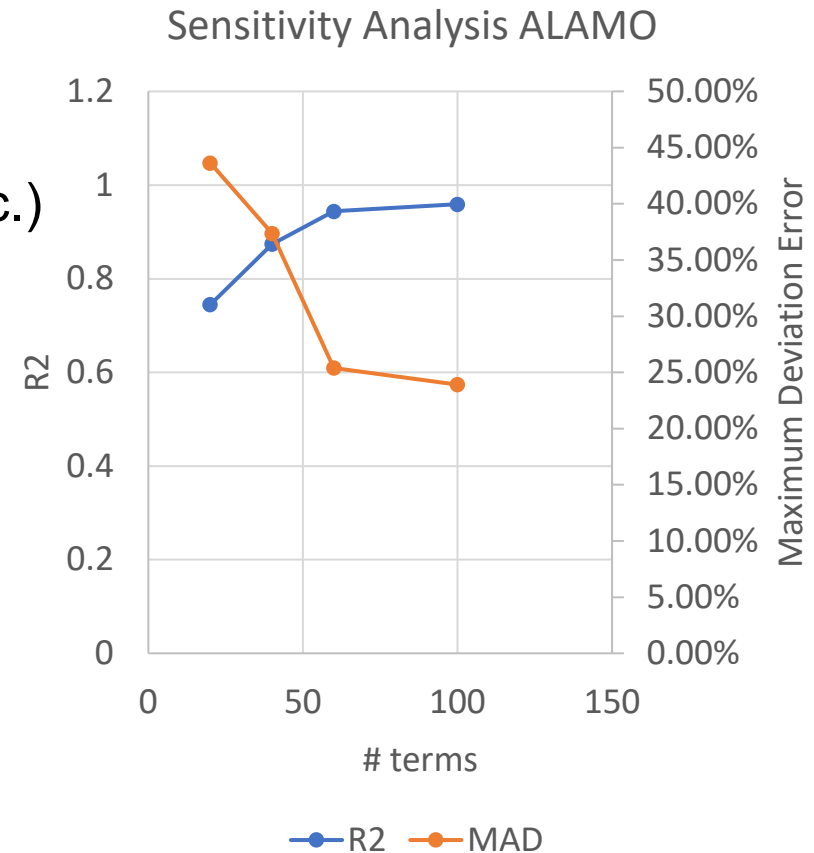
- Identify samples within the Population
  - Remove “bad data”
  - Remove infeasible operating conditions
- Training data and Validation data

```
df = pd.read_excel(fname, sheet_name='data_set.xlsx')
n_data = df[input_labels[0]].size
df_training, df_validation = split_training_validation(df, 0.8, seed=n_data)
```

# 3.- Model Selection “Best Practices”



- ALAMO provides flexible models
  - Mallows CP, Bayesian Information Criterion (BIC), ...
  - Flexible models (monomial powers, multi, ratio combinations, etc.)
  - Constrained regression and custom basis functions
  - Adaptive sampling (systematic approach to interrogate models)
- PySMO
  - Flexible models (polynomials, radial basis functions, kriging)
  - Native Pyomo tool (open-source)
- Neural Networks (open source tensorflow.Keras)
  - Correlated output variables
  - Flexible NN (Sigmoid, Relu, etc.)



## 4.- Model Verification/Validation



- The IDAES framework developed several tools for validating and verifying the surrogate models.
  - Plotting tools provide visual verification (parity, scatter errors, ...)
  - Model statistics provide a good idea of model fitting and errors ( $R^2$ , RMSE, MAD, etc.)



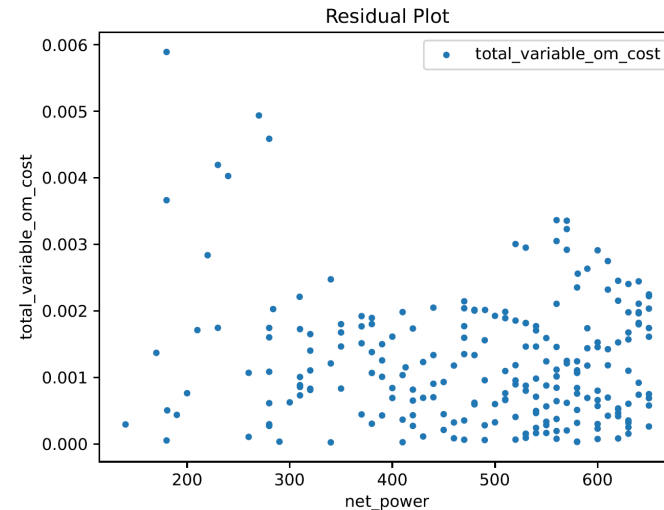
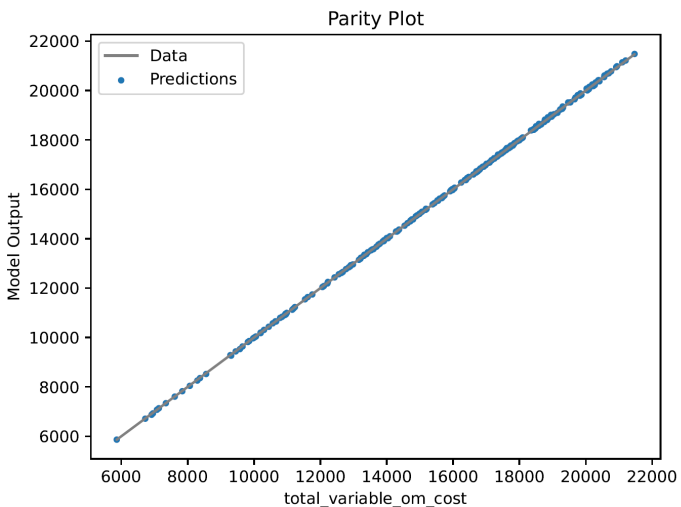
# 4.- Model Verification/Validation

```
df_training, df_validation = split_training_validation(df, 0.8, seed=n_data)
# Train surrogate (this will call to Alamo through AlamoPy)
success, alamo_surrogate, msg = trainer.train_surrogate()

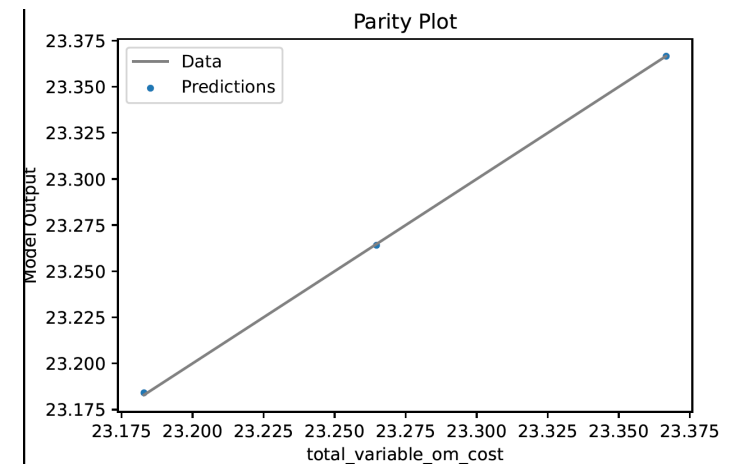
# Display the metrics of fit
metrics = compute_fit_metrics(alamo_surrogate, df_validation)
# Generate residual and parity plots
surrogate_residual(alamo_surrogate, df_validation, filename=fname, relative_error=True)
surrogate_parity(alamo_surrogate, df_validation, filename=fname)
surrogate_residual(alamo_surrogate, df_training, filename=fname, relative_error=True)
surrogate_parity(alamo_surrogate, df_training, filename=fname)
```

80% of data for training  
20% for validation

## Training Data Set



## Independent Data Set



# 5.- Surrogates for Optimization



- Two main aspects: 1.- integrating the surrogate models in the mathematical model, and 2.- robustness of the final mathematical model.

Automated surrogate modeling implementation

```

# create the IDAES model
m = ConcreteModel()
m.fs = FlowsheetBlock(default={"dynamic": False})
m.variable_OM_costs = Var(initialize=20, doc='variable OM costs in $/MW')
m.net_power = Var(initialize=650, doc='net power or rated capacity in MW')
m.h2_production = Var(initialize=5, doc='hydrogen production in kg/s')
m.ng_flowrate = Var(initialize=27, doc="natural gas flowrate in kg/s")
m.surrogate = SurrogateBlock()
m.var_cost_d_hrs = Var(doc='variable OM costs in $/hr')
inputs = [m.net_power, m.h2_production] # MW, kg/s
outputs = [m.var_cost_d_hrs, m.ng_flowrate] # $/hr, kg/s
m.surrogate.build_model(alamo_surrogate,
                        input_vars=inputs,
                        output_vars=outputs)
m.power_con_min = Constraint(expr= m.net_power >= Pmin)
m.power_con_max = Constraint(expr= m.net_power <= Pmax)
  
```

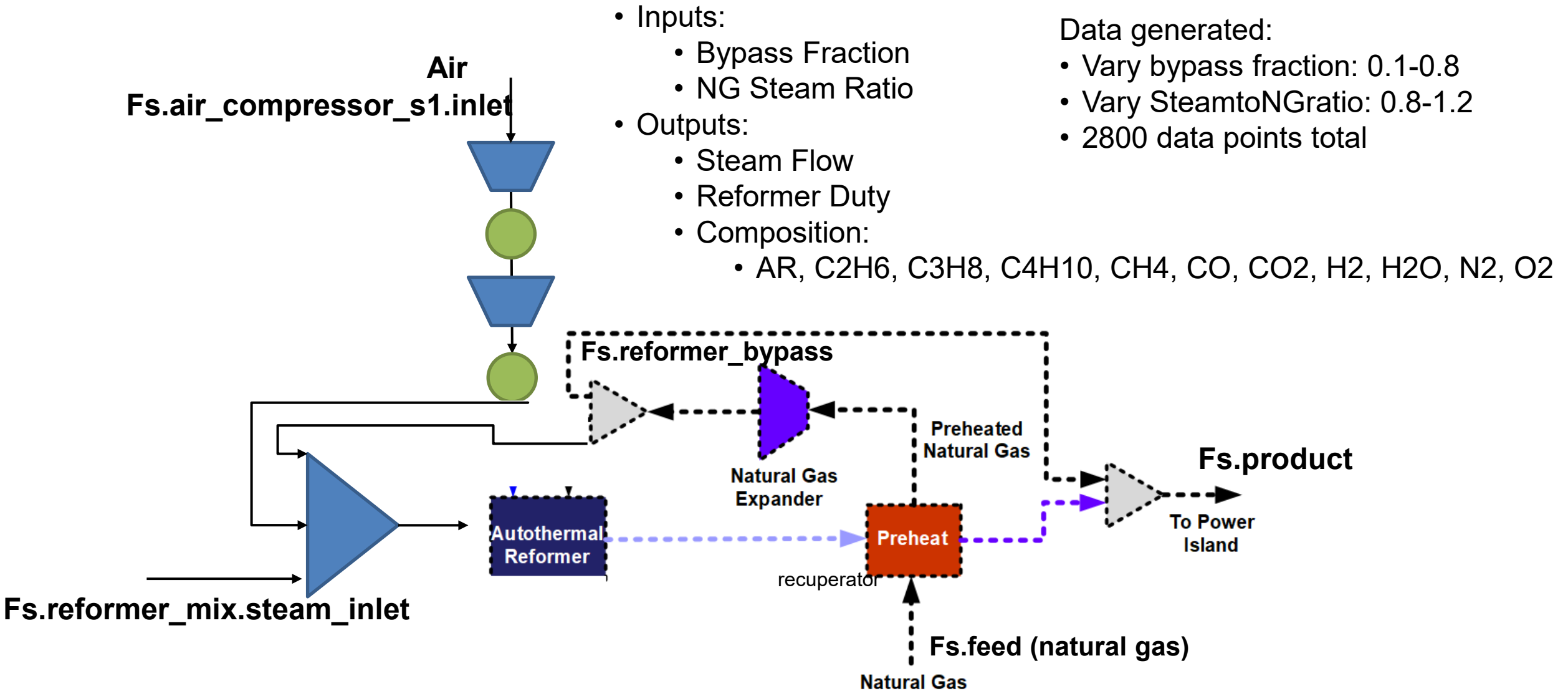
Conventional surrogate model implementation

```

import SRD

@self.Constraint(self.flowsheet().config.time,
                doc="Specific reboiler duty in GJ/t CO2")
def SRD_eqn(b, t):
    A2 = b.lean_loading[t]
    B2 = b.Pz_mol[t]
    return b.SRD[t] == (1297.92749665023 * A2 + 124.190464480941 * B2
                       - 1144.97804719883 * A2**2 - 14.8595802759414
                       * B2**2 + 553.845056558601 * A2**3
                       + 0.847572796795006 * B2**3 - 626.741015730156
                       * (A2*B2)**0.5 + 128.236265690663 * A2*B2
                       - 6.92413056110739 * (A2*B2)**2 + 0.3261654983218
                       * (A2*B2)**3 - 643.204744175051 * A2/B2
                       - 1.69063104541704 * B2/A2 + 698.322562008984
                       * (A2/B2)**2 + 0.00474692417757652 * (B2/A2)**2)
  
```

# End to End Demonstration: Autothermal Reformer Example



# Sampling “Best Practices”



IDAES Models and Properties



2800 samples (grid sampling method)

idaes.  
surrogate.sampling

## ALAMO Python Wrapper

- Highly tractable models (flexible, minimizes model size)
- Allows model validation, as well as multi-input/output

## PySMO (Polynomial, RBF, Kriging)

- Restrictive model forms, but highly accurate
- Allows model validation, as well as multi-input (single output)

## Tensorflow Keras (Sequential)

- Option-dependent accuracy, *a priori* knowledge is helpful
- Free of expression-driven modeling – models are complex
- Sequential limited to single input/output layer (see Functional API)

# Sampling “Best Practices”



IDAES Models and Properties



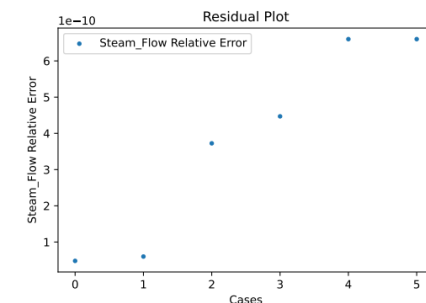
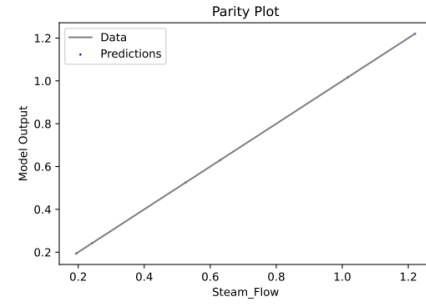
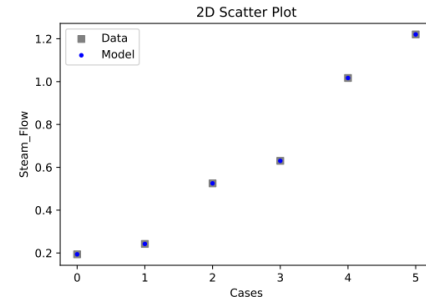
2800 samples (grid sampling method)

idaes.  
surrogate.sampling

ALAMO Python Wrapper

PySMO (Polynomial, RBF, Kriging)

Tensorflow Keras (Sequential)



```

19 # Import statements
20 import numpy as np
21 from idaes.surrogate.trainer import SurrogateBlock
22 from idaes.core import FlowSheetBlock
23 from idaes.core.util.convergence.convergence_base import run_ipopt_with_stats
24
25 # Import Pyomo libraries
26 from pyomo.environ import ConcreteModel, SolverFactory, Value, Var
27
28 def build_flowsheet(case="case_0", out_vars="Steam_Flow"):
29     # train and call the surrogate(s) we need from external module
30     surrogate = ARTrainer(trainer="ALAMO", out_vars=out_vars, case=case)
31
32     # create the IDAES model and flowsheet
33     m = ConcreteModel()
34     m.fs = FlowSheetBlock(defaults={"dynamic": False})
35
36     # create and fix flowsheet input variables
37     m.bypass_frac = Var(initialize=0.80, doc="natural gas bypass fraction")
38     m.ng_steam_ratio = Var(initialize=0.80, doc="natural gas to steam ratio")
39     m.reformer_duty = Var(initialize=10000, doc="reformer heat duty")
40
41     # create flowsheet output variables
42     m.steam_flowrate = Var(initialize=0.2, doc="steam flowrate")
43     m.reformer_duty = Var(initialize=10000, doc="reformer heat duty")
44
45     all_output_data = build_vars(m, case) # fixes inputs and retrieves
46     # output data (this is for all outputs from pre-defined dictionaries)
47     output_data = dict(zip(out_vars, [] * len(out_vars))) # pre-allocate
48     for var in out_vars: # we only need to return data for outputs of interest
49         output_data[var] = all_output_data[var]
50
51     inputs = [bypass_frac, m.ng_steam_ratio]
52     outputs = [m.steam_flowrate, m.reformer_duty]
53
54     # create the Pyomo/IDAES block that corresponds to the surrogate
55     m.surrogate = SurrogateBlock()
56     m.surrogate.build_model(surrogate, input_vars=inputs, output_vars=outputs)
57
58     return m, output_data
59
60 if __name__ == "__main__":
61     out_vars = ["Steam_Flow", "Reformer_Duty"]
62     cases = np.transpose(np.array([i for i in range(0)], ndmin=2))
63     idata = np.empty((len(cases), len(out_vars)))
64     zfit = np.empty((len(cases), len(out_vars)))
65     ipopt_status, ipopt_solved, ipopt_iter, ipopt_time = [], [], [], []
66     for i in range(len(cases)): # there are cases 0 through 5
67         case = "case_" + str(i)
68         m, output_data = build_flowsheet(case, trainer, basistype, out_vars)
69         solver = SolverFactory("ipopt")
70         [status_obj, solved, iters, time] = run_ipopt_with_stats(m, solver)
71         ipopt_iter.append(iters)
72         zfit[i, 0] = value(m.steam_flowrate)
73         zfit[i, 1] = value(m.reformer_duty)
74         zdata[i, 0] = output_data["Steam_Flow"]
75         zdata[i, 1] = output_data["Reformer_Duty"]

```

# Sampling “Best Practices”

Data Source



Sampling



Model Selection and Training

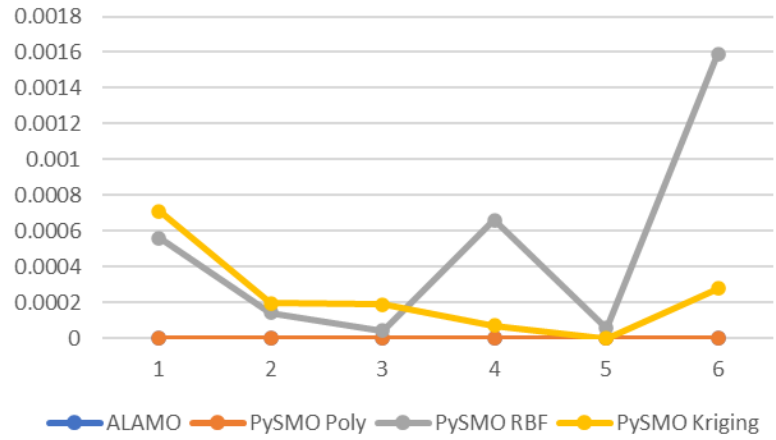


Visualization and Validation

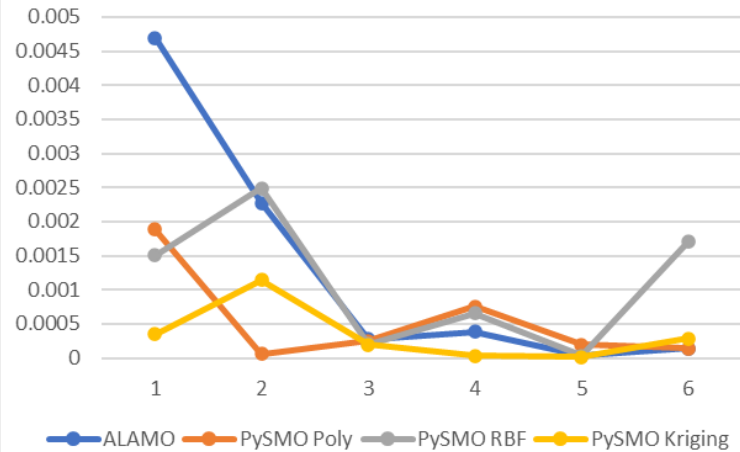


Integrated IDAES model

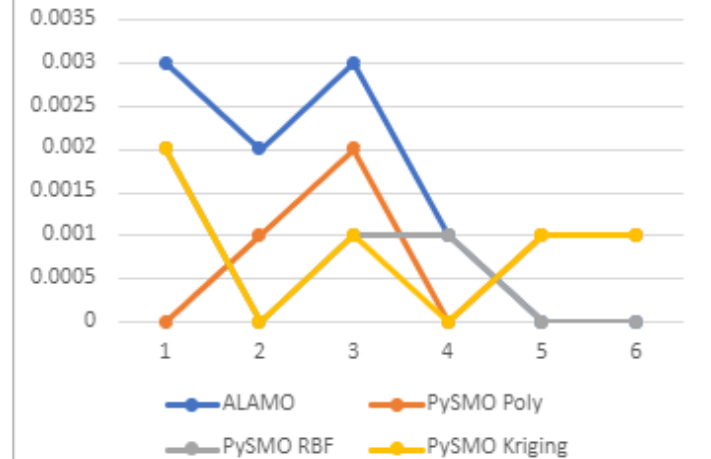
Steam Flow Error



Reformer Duty Error

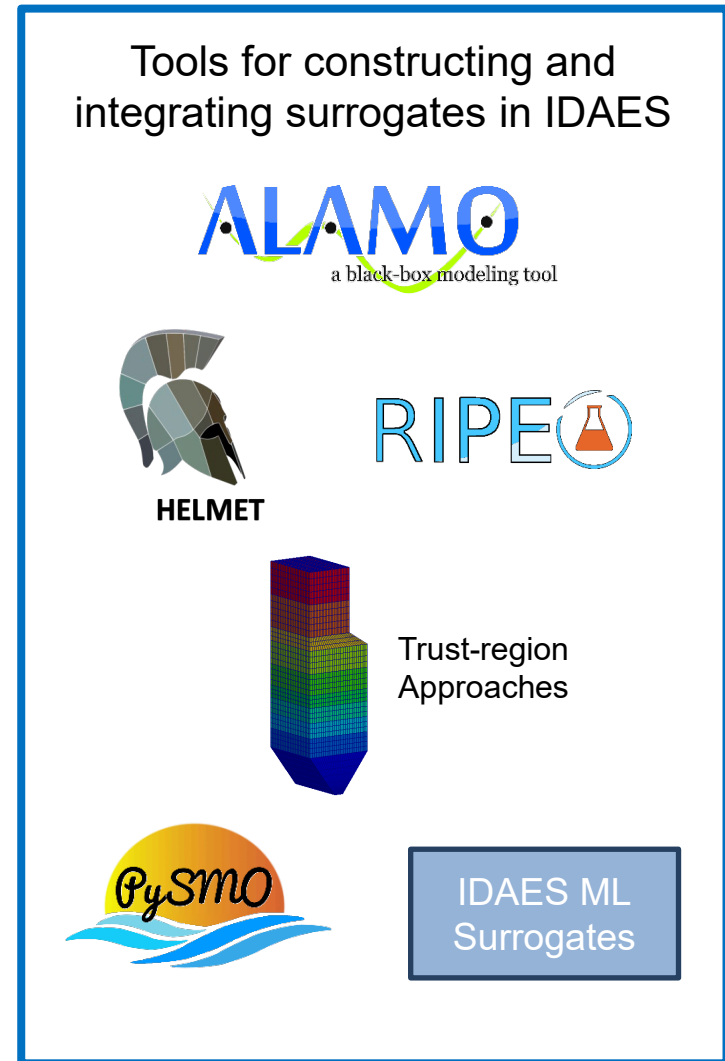


IPOPT Solver Time (s)

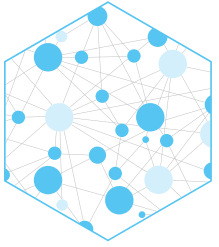


# Examples of when and why to use surrogates?

- Reducing model size, improve performance
  - Model more general than needed by a particular application (e.g., SOEC market analysis, auto-thermal reformer)
  - Opportunity to reduce model size and complexity
- Replacing “external” models (e.g., compiled code)
  - Convert external model to an EO model (e.g., fire side boiler, grid market surrogates)
  - Opportunity to obtain native EO model and improve performance
- Data-driven models
  - Data to replace missing first-principles model
- Improve convergence reliability
  - Push convergence challenges “offline” (controlled initialization)
  - Produce data from rigorous model – surrogate for application (e.g., auto-thermal reformer)
- Global optimization and MINLP (discrete + nonlinear)
  - Improve performance by replacing detailed nonlinear model
  - Surrogates may be lower order or piecewise linear







**IDAES**<sup>®</sup>  
Institute for the Design of  
Advanced Energy Systems

# IDAES Diagnostics Toolbox

Andrew Lee, Stakeholder Summit 2023





# Bad models are easy to write

- A model can only be valuable if you can solve it
- Good models take time and experience
  - We spend a significant amount of time debugging models
- One of the biggest limitations on the adoption of EO tools

# A Simple Example...

8 Variables:

v1: [m]

v2: [m]

v3:  $\in [0, 5]$

v4:

v5:  $\in [0, 1]$

v6:

v7: [m],  $\in [0, 1]$

v8:

4 Constraints:

c1:  $v_1 + v_2 = 10$

c2:  $v_3 = v_4 + v_5$

c3:  $2v_3 = 3v_4 + 4v_5 + v_6$

c4:  $v_7 = 1 \times 10^{-8} v_1$

```
import pyomo.environ as pyo
```

```
m = pyo.ConcreteModel()
```

```
m.v1 = pyo.Var(units=pyo.units.m)
```

Fix 3 Degrees of Freedom

```
v4 = 2 : m.v4.fix(2)
```

```
v5 = 2 : m.v5.fix(2)
```

```
v6 = 0 : m.v6.fix(0)
```

```
bounds=(0, 1))
```

```
m.v8 = pyo.Var()
```

```
m.c1 = pyo.Constraint(expr=m.v1 + m.v2 == 10)
```

```
m.c2 = pyo.Constraint(expr=m.v3 == m.v4 + m.v5)
```

```
m.c3 = pyo.Constraint(expr=2*m.v3 == 3*m.v4 + 4*m.v5 + m.v6)
```

```
m.c4 = pyo.Constraint(expr=m.v7 == 1e-8*m.v1)
```

## ...and a Common Outcome

```
EXIT: Converged to a point of local infeasibility. Problem may be infeasible.  
WARNING: Loading a SolverResults object with a warning status into  
model.name="unknown";
```

- termination condition: infeasible
- message from solver: Ipopt 3.13.2\x3a Converged to a locally infeasible point. Problem may be infeasible.

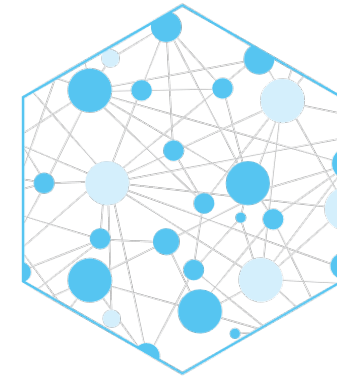
# If Only There Was A Tool To Help...

```
from idaes.core.util import DiagnosticsToolbox
```

```
dt = DiagnosticsToolbox(m)
```

```
dt.report_structural_issues()
```

**Now Available**



**v2.2.0**

```
=====  
Model Statistics
```

```
Activated Blocks: 1 (Deactivated: 0)
```

```
Free Variables in Activated Constraints: 4 (External: 0)
```

```
=====  
Model Statistics
```

```
Activated Blocks: 1 (Deactivated: 0)
```

```
Free Variables in Activated Constraints: 4 (External: 0)
```

```
Free Variables with only lower bounds: 0
```

```
Free Variables with only upper bounds: 0
```

```
Free Variables with upper and lower bounds: 2
```

```
Fixed Variables in Activated Constraints: 3 (External: 0)
```

```
Activated Equality Constraints: 4 (Deactivated: 0)
```

```
Activated Inequality Constraints: 0 (Deactivated: 0)
```

```
Activated Objectives: 0 (Deactivated: 0)
```

```
-----  
suggested next steps:
```

```
display_components_with_inconsistent_units()
```

```
display_underconstrained_set()
```

```
display_overconstrained_set()
```

```
=====
```

=====  
Model Statistics

Activated Blocks: 1 (Deactivated: 0)  
Free Variables in Activated Constraints: 4 (External: 0)  
    Free Variables with only lower bounds: 0  
    Free Variables with only upper bounds: 0  
    Free Variables with upper and lower bounds: 2  
Fixed Variables in Activated Constraints: 3 (External: 0)  
Activated Equality Constraints: 4 (Deactivated: 0)

-----  
2 WARNINGS

WARNING: 1 Component with inconsistent units

WARNING: Structural singularity found

    Under-Constrained Set: 3 variables, 2 constraints

    Over-Constrained Set: 1 variables, 2 constraints

-----  
Caution: 1 variable fixed to 0

Caution: 1 unused variable (0 fixed)

-----  
Suggested next steps:

display\_components\_with\_inconsistent\_units()

display\_underconstrained\_set()

display\_overconstrained\_set()

=====  
Model Statistics

```
Activated Blocks: 1 (Deactivated: 0)
Free Variables in Activated Constraints: 4 (External: 0)
  Free Variables with only lower bounds: 0
  Free Variables with only upper bounds: 0
  Free Variables with upper and lower bounds: 2
Fixed Variables in Activated Constraints: 3 (External: 0)
Activated Equality Constraints: 4 (Deactivated: 0)
Activated Inequality Constraints: 0 (Deactivated: 0)
```

-----  
2 Cautions

```
Caution: 1 variable fixed to 0
Caution: 1 unused variable (0 fixed)
```

-----  
Caution: 1 variable fixed to 0  
Caution: 1 unused variable (0 fixed)

Suggested next steps:

```
display_components_with_inconsistent_units()
display_underconstrained_set()
display_overconstrained_set()
```

=====  
Model Statistics

Activated Blocks: 1 (Deactivated: 0)  
Free Variables in Activated Constraints: 4 (External: 0)  
    Free Variables with only lower bounds: 0  
    Free Variables with only upper bounds: 0  
    Free Variables with upper and lower bounds: 2  
Fixed Variables in Activated Constraints: 3 (External: 0)  
Activated Equality Constraints: 4 (Deactivated: 0)

-----  
Suggested next steps:

```
display_components_with_inconsistent_units()  
display_underconstrained_set()  
display_overconstrained_set()
```

=====

Caution: 1 variable fixed to 0  
Caution: 1 unused variable (0 fixed)

-----  
Suggested next steps:

```
display_components_with_inconsistent_units()  
display_underconstrained_set()  
display_overconstrained_set()
```



# Inconsistent Units

```
dt.display_components_with_inconsistent_units()
```

```
=====
```

The following component(s) have unit consistency issues:

```
    c1
```

For more details on unit inconsistencies, import the `assert_units_consistent` method from `pyomo.util.check_units`

```
=====
```

$$c1: v_1 + v_2 = 10$$

**Constant has no units!**

$$v_1 - [m]$$

$$v_2 - [m]$$

# Structural Singularities

```
dt.display_overconstrained_set()
```

---

Dulmage-Mendelsohn Over-Constrained Set

Independent Block 0:

Variables:

v3

Constraints:

c2

c3

**2 Constraints, 1 Variable  
-1 Degrees of Freedom!**

# Structural Singularities

```
dt.display_overconstrained_set()
```

---

Dulmage-Mendelsohn Over-Constrained Set

Independent Block 0:

Variables:

v3

Constraints:

c2

c3

$$\text{c2: } v_3 = v_4 + v_5$$

$$\text{c3: } 2v_3 = 3v_4 + 4v_5 + v_6$$

$$v_4 = 2, \quad v_5 = 2, \quad v_6 = 0$$

---

**Fixed 1 Variable I shouldn't have:** `m.v4.unfix()`

# Structural Singularities

```
dt.display_underconstrained_set()
```

---

```
Dulmage-Mendelsohn Under-Constrained Set
```

```
Independent Block 0:
```

```
Variables:
```

```
v2
```

```
v1
```

```
v7
```

```
Constraints:
```

```
c1
```

```
c4
```

**3 Variable, 2 Constraints  
1 Degrees of Freedom!**

**Shows which variables I can fix**

**Fix 1 of these Variables:  $v_2 = 5$  : `m.v2.fix(5)`**

---

# Lets Try Again...

=====  
Model Statistics

```
Activated Blocks: 1 (Deactivated: 0)
Free Variables in Activated Constraints: 4 (External: 0)
  Free Variables with only lower bounds: 0
  Free Variables with only upper bounds: 0
  Free Variables with upper and lower bounds: 2
Fixed Variables in Activated Constraints: 3 (External: 0)
```

-----  
Suggested next steps:

```
Try to initialize/solve your model and then call report_numerical_issues()
```

=====

2 Cautions

```
Caution: 1 variable fixed to 0
Caution: 1 unused variable (0 fixed)
```

-----  
Suggested next steps:

```
Try to initialize/solve your model and then call report_numerical_issues()
```

=====

# Still a Common Outcome...

```
EXIT: Converged to a point of local infeasibility. Problem may be infeasible.  
WARNING: Loading a SolverResults object with a warning status into  
model.name="unknown";
```

- termination condition: infeasible
- message from solver: Ipopt 3.13.2\x3a Converged to a locally infeasible point. Problem may be infeasible.

# Numerical Issues

```
=====  
Model Statistics
```

```
Jacobian Condition Number: 1.700E+01
```

```
-----  
2 WARNINGS
```

```
2 WARNINGS
```

```
WARNING: 1 Constraint with large residuals
```

```
WARNING: 2 Variables at or outside bounds
```

```
-----  
Caution: 1 extreme Jacobian Entry
```

```
-----  
Suggested next steps:
```

```
display_constraints_with_large_residuals()
```

```
display_variables_at_or_outside_bounds()
```

```
=====
```

# Numerical Issues

```
=====
Model Statistics
```

```
Jacobian Condition Number: 1.700E+01
-----
```

```
-----
Suggested next steps:
```

```
display_constraints_with_large_residuals()
display_variables_at_or_outside_bounds()
=====
```

```
Caution: 1 extreme Jacobian Entry
```

```
-----
Suggested next steps:
```

```
display_constraints_with_large_residuals()
display_variables_at_or_outside_bounds()
=====
```



# Possible Bounds Violations

```
dt.display_variables_at_or_outside_bounds()
```

```
=====
```

The following variable(s) have values at or outside their bounds:

```
v3 (free): value=0.0 bounds=(0, 5)  
v5 (fixed): value=2 bounds=(0, 1)
```

```
=====
```

## Two Issues

- v3 : might be limited by lower bound, possibly infeasible
- v5 : value and bounds were set to incompatible values

## Relax Bounds

- m.v3.setlb(-5)
- m.v5.setub(10)

# Try to Solve Again...

iter	objective	inf_pr	inf_du	lg(mu)	d	lg(rg)	alpha_du	alpha_pr	ls
0	0.0000000e+00	6.67e-01	0.00e+00	-1.0	0.00e+00	-	0.00e+00	0.00e+00	0
1	0.0000000e+00	6.66e-03	2.97e+00	-1.0	2.00e+00	-	7.17e-01	9.90e-01h	1
2	0.0000000e+00	6.27e-05	9.38e+00	-1.0	2.00e-02	-	1.00e+00	9.91e-01h	1
3	0.0000000e+00	8.88e-16	1.13e-12	-1.0	1.88e-04	-	1.00e+00	1.00e+00h	1

Number of Iterations.....: 3

EXIT: Optimal Solution Found.

An Optimal Solution does not mean the model is robust!

# Numerical Issues Again

=====  
Model Statistics

Jacobian Condition Number: 1.700E+01

0 WARNINGS

No warnings found!

No Warnings

5 Cautions

Caution: 1 Variable with value close to their bounds

Caution: 1 Variable with value close to zero

Caution: 1 Variable with extreme value

Caution: 1 Variable with None value

Caution: 1 extreme Jacobian Entry

-----  
Suggested next steps:

If you still have issues converging your model consider:

svd\_analysis(TBA)

degeneracy\_hunter (TBA)

=====

# Numerical Issues Again

=====  
Model Statistics

Jacobian Condition Number: 1.700E+01

---

## 5 Cautions

Caution: 1 Variable with value close to their bounds

Caution: 1 Variable with value close to zero

Caution: 1 Variable with extreme value

Caution: 1 Variable with None value

Caution: 1 extreme Jacobian Entry

---

Suggested next steps:

If you still have issues converging your model consider:

svd\_analysis(TBA)

degeneracy\_hunter (TBA)

=====

# Variables with Extreme Values

```
dt.display_variables_with_extreme_values()
```

=====

The following variable(s) have extreme values:

v7: 4.99999999999999945e-08

=====

**Scaling Issue:** v7 has very small value and is close to lower bound of 0

**Solution:** scale v7 and associated constraint c4

# Try to Solve Again...

iter	objective	inf_pr	inf_du	lg(mu)	d	lg(rg)	alpha_du	alpha_pr	ls
0	0.0000000e+00	1.40e+01	0.00e+00	-1.0	0.00e+00	-	0.00e+00	0.00e+00	0
1	0.0000000e+00	3.55e-15	4.88e+02	-1.0	6.00e+00	-	2.02e-03	1.00e+00	1

Number of Iterations.....: 1

EXIT: Optimal Solution Found.

# Conclusions

- Writing good models is still hard, but...
- Diagnostics Toolbox helps you find issues
  - Expert help at your fingertips
  - Reduces time, effort and expertise required to debug models
- For more information, see the poster

# All You Need to Remember...

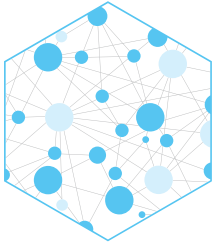
```
from idaes.core.util import DiagnosticsToolbox
```

```
dt = DiagnosticsToolbox(m)
```

```
dt.report_structural_issues()
```

[https://idaes-pse.readthedocs.io/en/stable/explanations/model\\_diagnostics/index.html](https://idaes-pse.readthedocs.io/en/stable/explanations/model_diagnostics/index.html)





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Advanced Energy Systems

# IDAES Visualization

**Dan Gunter**, Sheng Pang, Sarah Poon, Cody O'Donnell  
Stakeholder Summit 2023



# Visualization is important

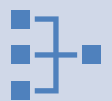


IDAES models are built in Python code, but..



Complex models are routinely diagrammed

Validation: are the connections correct  
Communication to others (and yourself)



Diagrams provide context for model properties

Stream values, unit values, constraints, structure



Visualization is much more than diagrams (of course)

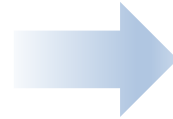
Plots of results, visual diagnostics, etc.

# IDAES has a visualization tool “built in”

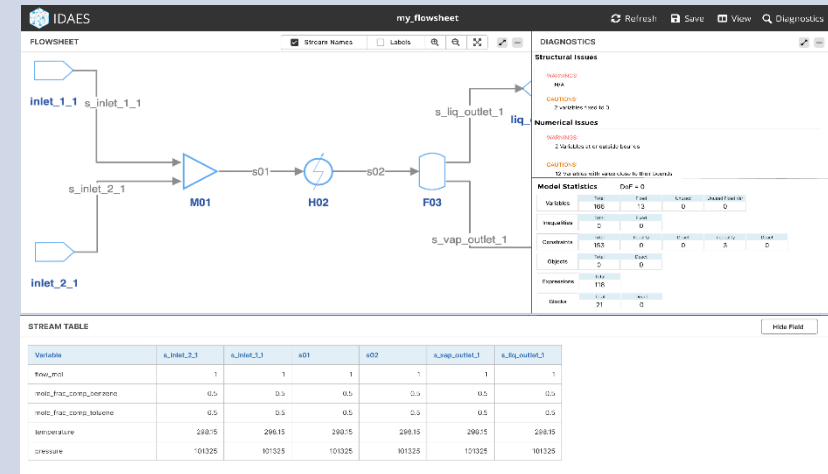
With the addition of one line of code to your Jupyter Notebook or script..



```
model = build_model()
model.visualize("my_flowsheet")
```



..you get a web-based UI that automatically displays a model diagram and a stream table..



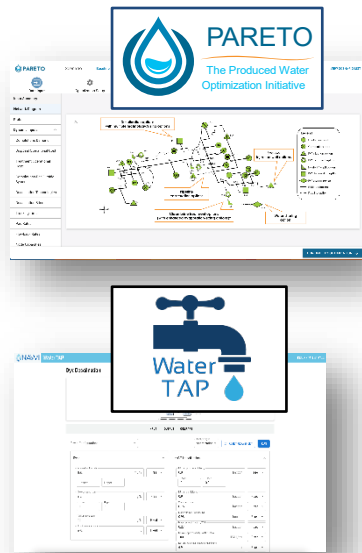
..and retains a connection to the model so you can interact with it.



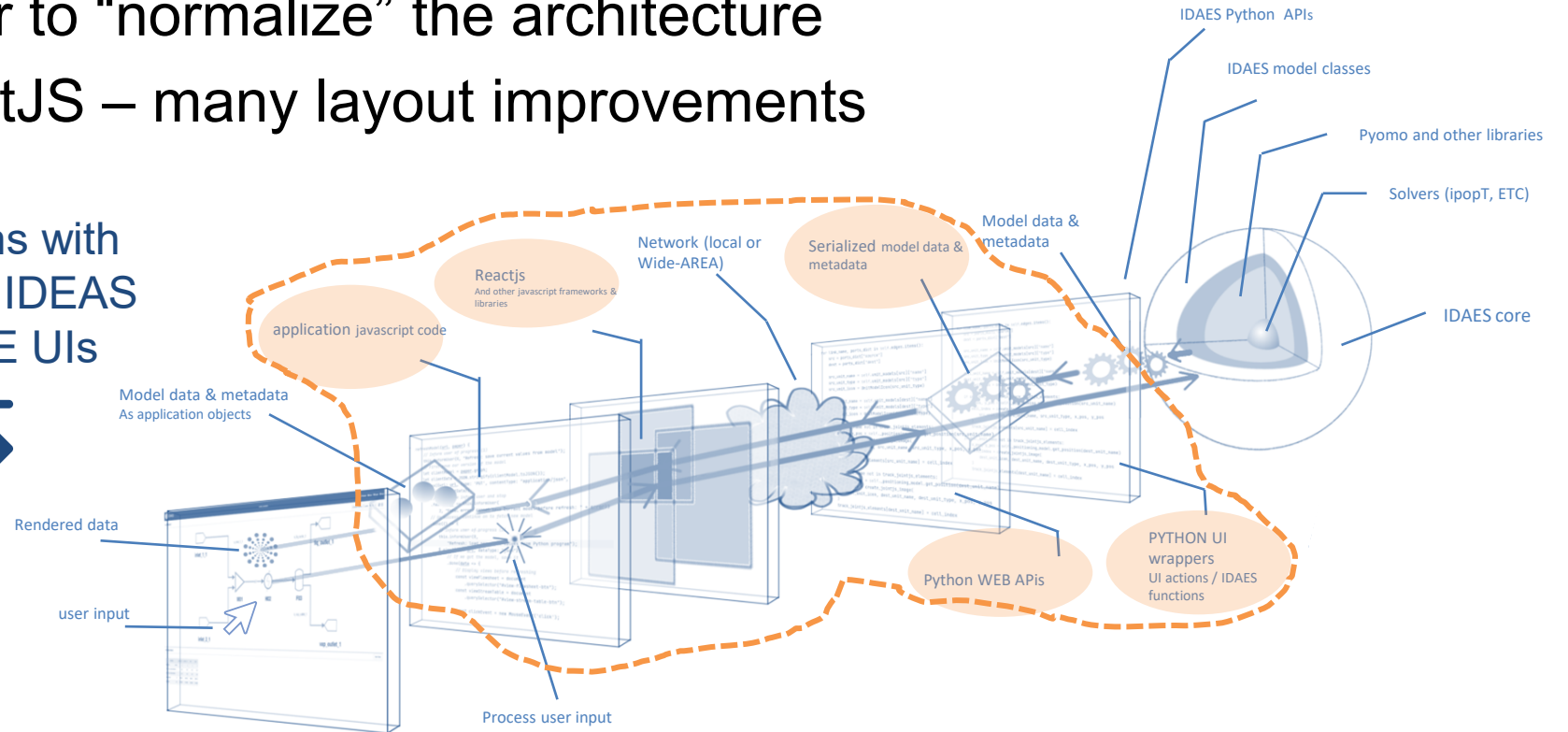
We call this tool the **Flowsheet Visualizer (FV)**

# Latest changes for the FV

- Important refactor to “normalize” the architecture
- Re-do UI in ReactJS – many layout improvements



Aligns with  
other IDEAS  
PSE UIs

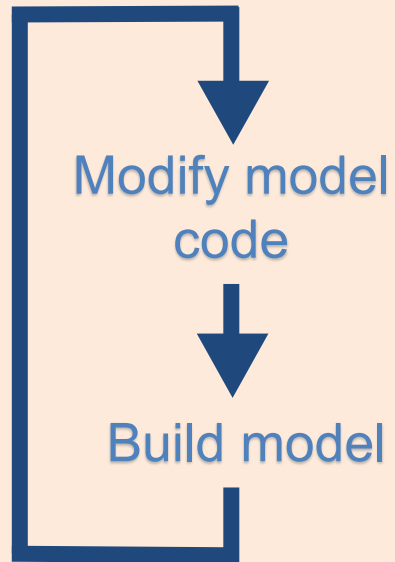


We are preparing the way for incorporating new, interactive elements, starting with: IDAES Diagnostics

# Diagnostics and Plan/Do/Evaluate Cycle

Python code

Flowsheet Visualizer



Changes in the model can be immediately shown in the FV

Seamlessly connect diagnostics to the diagram, stream table, and new visualizations (e.g., heatmap of Jacobian)

Solve

Visualize

Diagnose & Analyze

Browse and filter diagnostics by different criteria

Edit Config & Variables

Modify diagnostic tolerances and model variables interactively

**Legend**

- Working! (solid blue border)
- Proposed (dashed blue border)

# Diagnostics Prototype Screenshot



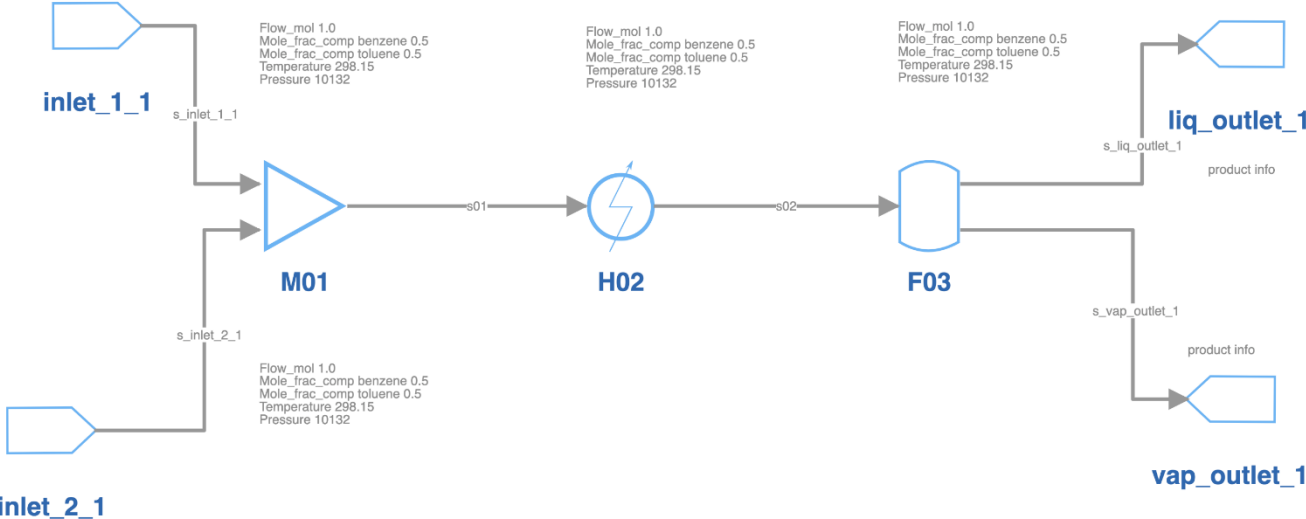
sample\_visualization

Refresh Save Export View Diagnostics

FLWSHEET

Stream Names Labels

DIAGNOSTICS



STREAM TABLE

Hide Fields

Variable		s_inlet_2_1	s_inlet_1_1	s01	s02
flow_mol	mol/s	1	1	1	1
mole_frac_comp benzene	-	0.5	0.5	0.5	0.5
mole_frac_comp toluene	-	0.5	0.5	0.5	0.5
temperature	K	298.15	298.15	298.15	298.15
pressure	Pa	101325	101325	101325	101325

ISSUES

2 Caution

CONFIG

Name	Value
variable bounds absolute tolerance	0.0001
variable bounds relative tolerance	0.0001
variable bounds violation tolerance	0
constraint residual tolerance	0.00001
variable large value tolerance	10000
variable small value tolerance	0.0001
variable zero value tolerance	1e-8
jacobian large value caution	10000
jacobian large value warning	100000000
jacobian small value caution	0.0001
jacobian small value warning	1e-8

STATISTICS

DoF	Value			
	0			
Variables	Value	Unused	Fixed	Ineq
	166	166	166	166
Inequalities	Value			
	0			
Constraints	Value	Eq	Ineq	
	153	153	153	
Objects	Value	Deact		
	0	0		
Blocks	Value	Deact		
	21	21		
Expressions	Value			
	118			

# Diagnostics Prototype Screenshot Detail

### DIAGNOSTICS

ISSUES ▾  
▶ 2 Caution

CONFIG ▾

Name	Value
variable bounds absolute tolerance	0.0001
variable bounds relative tolerance	0.0001
variable bounds violation tolerance	0
constraint residual tolerance	0.00001
variable large value tolerance	10000
variable small value tolerance	0.0001
variable zero value tolerance	1e-8
jacobian large value caution	10000
jacobian large value warning	100000000
jacobian small value caution	0.0001
jacobian small value warning	1e-8

STATISTICS ▾

DoF	Value	0		
Variables	Value	Unused	Fixed	Ineq
	166	166	166	166
Inequalities	Value	0		
Constraints	Value	Eq	Ineq	
	153	153	153	
Objects	Value	Deact		
	0	0		
Blocks	Value	Deact		
	21	21		
Expressions	Value	118		

# Browse to view cautions

**DIAGNOSTICS**

**ISSUES** ▾

- ▾ 2 Caution
  - ▾ Caution 1: variables with extreme values
    - ▶ extreme\_values : 72
  - ▾ Caution 2: variables close to their bounds
    - ▶ var\_near\_bounds : 12

**CONFIG** ▾

Name	Value
variable bounds absolute tolerance	0.0001
variable bounds relative tolerance	0.0001
variable bounds violation tolerance	0
constraint residual tolerance	0.00001
variable large value tolerance	10000
variable small value tolerance	0.0001
variable zero value tolerance	1e-8
jacobian large value caution	10000
jacobian large value warning	100000000
jacobian small value caution	0.0001
jacobian small value warning	1e-8

**STATISTICS** ▾

DoF	Value	0		
Variables	Value	Unused	Fixed	Ineq
	166	166	166	166
Inequalities	Value	0		
Constraints	Value	Eq	Ineq	
	153	153	153	
Objects	Value	Deact		
	0	0		
Blocks	Value	Deact		
	21	21		
Expressions	Value	118		



# View variables with “extreme values”

**DIAGNOSTICS**

ISSUES ▾

▼ 2 Caution

▼ Caution 1: variables with extreme values

▼ extreme\_values : 72

Search

fs.M01.minimum_pressure[0.0,1]	101324.99999999999
fs.M01.minimum_pressure[0.0,2]	101324.99999999997
fs.M01.inlet_1_state[0.0].mole_frac_comp[toluene]	0.00001
fs.M01.inlet_1_state[0.0].pressure	101325
fs.M01.inlet_2_state[0.0].mole_frac_comp[benzene]	0.00001
fs.M01.inlet_2_state[0.0].pressure	130000
fs.M01.mixed_state[0.0].pressure	101324.99999999997
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Liq,toluene]	0.00004226501650736347
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Vap,toluene]	0.000016239937390247786
fs.M01.inlet_1_state[0.0].pressure_sat_comp[benzene]	101327.63707622685
fs.M01.inlet_1_state[0.0].pressure_sat_comp[toluene]	38933.18380178968
fs.M01.inlet_1_state[0.0].enth_mol_phase[Liq]	59403.464839923574
fs.M01.inlet_1_state[0.0].enth_mol_phase[Vap]	89602.98646808404
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Liq,benzene]	59404.366946131
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Liq,toluene]	24005.117152243132
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Vap,benzene]	89602.59458088383
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Vap,toluene]	58559.44869427196
fs.M01.inlet_2_state[0.0].mole_frac_phase_comp[Liq,benzene]	0.000018948688821340677
fs.M01.inlet_2_state[0.0].mole_frac_phase_comp[Vap,benzene]	0.00004334161298390463
fs.M01.inlet_2_state[0.0].pressure_sat_comp[benzene]	297350.9006893184
fs.M01.inlet_2_state[0.0].pressure_sat_comp[toluene]	129996.82889148161
fs.M01.inlet_2_state[0.0].enth_mol_phase[Liq]	25813.44309761046
fs.M01.inlet_2_state[0.0].enth_mol_phase[Vap]	59876.807741757904
fs.M01.inlet_2_state[0.0].enth_mol_phase_comp[Liq,benzene]	60968.170946131
fs.M01.inlet_2_state[0.0].enth_mol_phase_comp[Liq,toluene]	25812.518818909797
fs.M01.inlet_2_state[0.0].enth_mol_phase_comp[Vap,benzene]	90653.83510796717
fs.M01.inlet_2_state[0.0].enth_mol_phase_comp[Vap,toluene]	59874.87498323029
fs.M01.mixed_state[0.0].pressure_sat_comp[benzene]	156860.8353206145
fs.M01.mixed_state[0.0].pressure_sat_comp[toluene]	63534.71863733716
fs.M01.mixed_state[0.0].enth_mol_phase[Liq]	38039.7329520597
fs.M01.mixed_state[0.0].enth_mol_phase[Vap]	77818.48958992377
fs.M01.mixed_state[0.0].enth_mol_phase_comp[Liq,benzene]	59130.24754889732
fs.M01.mixed_state[0.0].enth_mol_phase_comp[Liq,toluene]	23688.342072640477
fs.M01.mixed_state[0.0].enth_mol_phase_comp[Vap,benzene]	89419.03516967919
fs.M01.mixed_state[0.0].enth_mol_phase_comp[Vap,toluene]	58229.53049239868

# Filter variables by name (etc.)

**DIAGNOSTICS** ↗ -

**ISSUES** ▼

▼ 2 Caution

▼ Caution 1: variables with extreme values

▼ extreme\_values : 72

🔍 fs.M01.inlet\_1\_state[0.0]

fs.M01.inlet_1_state[0.0].mole_frac_comp[toluene]	0.00001
fs.M01.inlet_1_state[0.0].pressure	101325
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Liq,toluene]	0.00004226501650736347
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Vap,toluene]	0.000016239937390247786
fs.M01.inlet_1_state[0.0].pressure_sat_comp[benzene]	101327.63707622685
fs.M01.inlet_1_state[0.0].pressure_sat_comp[toluene]	38933.18380178968
fs.M01.inlet_1_state[0.0].enth_mol_phase[Liq]	59403.464839923574
fs.M01.inlet_1_state[0.0].enth_mol_phase[Vap]	89602.98646808404
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Liq,benzene]	59404.366946131
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Liq,toluene]	24005.117152243132
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Vap,benzene]	89602.59458088383
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Vap,toluene]	58559.44869427196

▼ Caution 2: variables close to their bounds

▶ var\_near\_bounds : 12

🔍 Search

fs.M01.inlet_1_state[0.0].mole_frac_comp[benzene]	1
fs.M01.inlet_1_state[0.0].mole_frac_comp[toluene]	0.00001
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Liq,benzene]	0.9999677349834927
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Liq,toluene]	0.00004226501650736347
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Vap,benzene]	0.9999937600626098
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Vap,toluene]	0.000016239937390247786

**CONFIG** ▼

Name	Value
variable bounds absolute tolerance	0.0001
variable bounds relative tolerance	0.0001

# Advanced interactive explorations

IDAES

sample\_visualization

Refresh Save Export View Diagnostics

**FLWSHEET**

Stream Names
Labels
🔍
🔍
🔍

1a. Highlight on diagram

**DIAGNOSTICS**

**ISSUES**

- ▼ 2 Caution
- ▼ Caution 1: variables with extreme values
- ▼ extreme\_values : 72

1. Select variable in caution

fs.M01.inlet_1_state[0].u.j.pressure	101325
fs.M01.inlet_1_state[0].mole_frac_phase_comp[Liq,toluene]	0.00004226501650736347
fs.M01.inlet_1_state[0].mole_frac_phase_comp[Vap,toluene]	0.000016239937390247786
fs.M01.inlet_1_state[0].pressure_sat_comp[benzene]	101327.63707622685
fs.M01.inlet_1_state[0].pressure_sat_comp[toluene]	38933.18380178968
fs.M01.inlet_1_state[0].enth_mol_phase[Liq]	59403.464839923574
fs.M01.inlet_1_state[0].enth_mol_phase[Vap]	89602.98646808404
fs.M01.inlet_1_state[0].enth_mol_phase_comp[Liq,benzene]	59404.366946131
fs.M01.inlet_1_state[0].enth_mol_phase_comp[Liq,toluene]	24005.117152243132
fs.M01.inlet_1_state[0].enth_mol_phase_comp[Vap,benzene]	89602.59458088383
fs.M01.inlet_1_state[0].enth_mol_phase_comp[Vap,toluene]	58559.44869427196

- ▼ Caution 2: variables close to their bounds
- ▶ var\_near\_bounds : 12

2a. Filter variables shown in issues

Search

fs.M01.inlet_1_state[0].mole_frac_comp[benzene]	1
fs.M01.inlet_1_state[0].mole_frac_comp[toluene]	0.00001
fs.M01.inlet_1_state[0].mole_frac_phase_comp[Liq,benzene]	0.9999677349834927
fs.M01.inlet_1_state[0].mole_frac_phase_comp[Liq,toluene]	0.00004226501650736347
fs.M01.inlet_1_state[0].mole_frac_phase_comp[Vap,benzene]	0.9999937600626098
fs.M01.inlet_1_state[0].mole_frac_phase_comp[Vap,toluene]	0.000016239937390247786

**STREAM TABLE**

Variable	s_inlet_2_1	s_inlet_1_1	s01	s02
flow_mol	mol/s	1	1	1
mole_frac_comp benzene	-	0.5	0.5	0.5
mole_frac_comp toluene	-	0.5	0.5	0.5
temperature	K	298.15	298.15	298.15
pressure	Pa	101325	101325	101325

1b. Highlight in stream table

2. Select in diagram or stream table

# Advanced interactive explorations (more..)

IDAES
sample\_visualization
Refresh Save Export View Diagnostics

**FLWSHEET**

Select unit

→

**DIAGNOSTICS**

**ISSUES**

- 2 Caution
  - Caution 1: variables with extreme values
    - extreme\_values : 72
      - fs.M01.inlet\_1\_state[0.0]
- Caution 2: variables close to their bounds
  - var\_near\_bounds : 12

Search

fs.M01.inlet_1_state[0.0].mole_frac_comp[toluene]	0.00001
fs.M01.inlet_1_state[0.0].pressure	101325
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Liq,toluene]	0.00004226501650736347
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Vap,toluene]	0.000016239937390247786
fs.M01.inlet_1_state[0.0].pressure_sat_comp[benzene]	101327.63707622685
fs.M01.inlet_1_state[0.0].pressure_sat_comp[toluene]	38933.18380178968
fs.M01.inlet_1_state[0.0].enth_mol_phase[Liq]	59403.464839923574
fs.M01.inlet_1_state[0.0].enth_mol_phase[Vap]	89602.98646808404
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Liq,benzene]	59404.366946131
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Liq,toluene]	24005.117152243132
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Vap,benzene]	89602.59458088383
fs.M01.inlet_1_state[0.0].enth_mol_phase_comp[Vap,toluene]	58559.44869427196

**CONFIG**

Name	Value
variable bounds absolute tolerance	0.0001
variable bounds relative tolerance	0.0001
variable bounds violation tolerance	0
constraint residual tolerance	0.00001
variable large value tolerance	10000
variable small value tolerance	0.0001
variable zero value tolerance	1e-8
jacobian large value caution	10000
jacobian large value warning	100000000
jacobian small value caution	0.0001
jacobian small value warning	1e-8

**STATISTICS**

DoF	Value
	0
Variables	Value Unused Fixed Ineq

**STREAM TABLE** Hide Fields

Variable	s_inlet_2_1	s_inlet_1_1	s01	s02
flow_mol	mol/s	1	1	1
mole_frac_comp benzene	-	0.5	0.5	0.5
mole_frac_comp toluene	-	0.5	0.5	0.5
temperature	K	298.15	298.15	298.15
pressure	Pa	101325	101325	101325

Calculate and display diagnostics for that unit

Select unit

# Integration with other PSE projects

- All the capabilities of the Flowsheet Visualizer can be potentially embedded into other Web UIs
- Capabilities being developed in e.g. WaterTAP can be “ported” to the FV
- Beginnings of a PSE UI “ecosystem”..?

**WaterTAP**

Dye Desalination

DEGREES OF FREEDOM: 3

RETURN TO LIST PAGE

INPUT OUTPUT COMPARE

Analysis Type: optimization

RESET FLOWSHEET RUN

Feed

Volometric flow rate: 120 m<sup>3</sup>/h

Dye concentration: 2.5 g/L

TDS concentration: 50 g/L

Solution temperature: 298 K

RHGO Nanofiltration

NF pump motor efficiency: 0.9

Water recovery: 0.75

Mass removal fraction, dye: 0.98

Mass removal fraction, TDS: 0.27

NF Water permeability Coefficient, A: 100 LMH/bar

Net driving pressure across membrane: 6.9 bar

Embed diagram and tools

Set variables and solve models

**IDAES**

Flowsheet Visualizer

inlet\_1\_1

M01

H02

F03

liq\_outlet\_1

vap\_outlet\_1

inlet\_2\_1

STREAM TABLE

Variable	inlet_1_1	inlet_2_1	M01	H02
flow_rate	1	1	1	1
rich_flow_comp_benzene	0.5	0.5	0.5	0.5
rich_flow_comp_toluene	0.5	0.5	0.5	0.5
temperature	298.15	298.15	298.15	298.15
pressure	101325	101325	101325	101325

DIAGNOSTICS

CONFIG

Name	Value
variable bounds absolute tolerance	0.0001
variable bounds relative tolerance	0.0001
variable bounds rotation tolerance	0
constraint residual tolerance	0.000001
variable large value tolerance	10000
variable small value tolerance	0.0001
variable zero value tolerance	1e-8
jacobian large value caution	10000
jacobian large value warning	100000000
jacobian small value caution	0.0001
jacobian small value warning	1e-8

STATISTICS

DoF	Value
Variables	100
Unavailable	166
Fixed	150
Free	166

Variables

Variable	Value
inlet_1_1	120
inlet_2_1	120
M01	120
H02	120
F03	120
liq_outlet_1	120
vap_outlet_1	120

# Summary



The Flowsheet Visualizer (FV) can easily visualize IDAES models today



Interactive access to IDAES Diagnostics Toolkit is being actively added

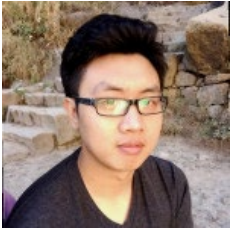


This will make the FV a more useful tool across IDAES PSE

# Please come talk to us! We want your feedback



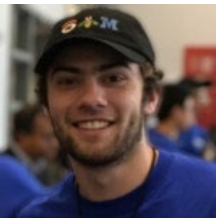
Dan Gunter, team lead



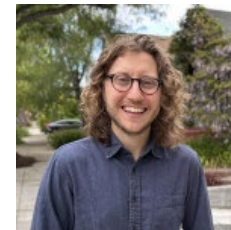
Sheng Pang, IDAES UI developer



Sarah Poon, User Experience (UX)



Mike Pesce, UI developer  
WaterTAP, PARETO



*Cody O'Donnell,  
IDAS UI designer  
(emeritus)*



# Acknowledgements

The IDAES team gratefully acknowledges support from the U.S. DOE's **Office of Fossil Energy and Carbon Management** through the **Simulation-Based Engineering/Crosscutting Research Program**.

**National Energy Technology Laboratory:** David Miller, Tony Burgard, John Eslick, **Andrew Lee**, **Miguel Zamarripa**, Jinliang Ma, Dale Keairns, Jaffer Ghouse, Ben Omell, Chinedu Okoli, Richard Newby, Arun Iyengar, Anca Ostace, Steve Zitney, Anuja Deshpande, Alex Noring, Naresh Susarla, Radhakrishna Gooty, **Doug Allen**, Ryan Hughes, Andres Calderon, **Brandon Paul**, Adam Atia, John Brewer, Nadejda Victor, Maojian Wang, Peng Liu

**Sandia National Laboratories:** **John Sirola**, **Bethany Nicholson**, **Michael Bynum**, Jordan Jalving, Emma Johnson, Katherine Klise, Shawn Martin, **Miranda Mundt**, **Edna Soraya Rawlings**, Kyle Skolfield

**Lawrence Berkeley National Laboratory:** Deb Agarwal, **Dan Gunter**, Keith Beattie, John Shinn, Hamdy Elgammal, Joshua Boverhof, Karen Whitenack, Oluwamayowa Amusat, **Sarah Poon**

**Carnegie Mellon University:** Larry Biegler, Chrysanthos Gounaris, Ignacio Grossmann, Carl Laird, John Eason, Owais Sarwar, Natalie Isenberg, Chris Hanselman, Marissa Engle, Qi Chen, Cristiana Lara, **Robert Parker**, Ben Sauk, Vibhav Dabadghao, Can Li, David Molina Thierry, Mingrui Li, Seolhee Cho, Georgia Stinchfield, Jason Sherman

**West Virginia University:** Debangsu Bhattacharyya, Paul Akula, Quang-Minh Le, Nishant Giridhar, Matthew Alastanos

**University of Notre Dame:** **Alexander Dowling**, Xian Gao, Nicole Cortes

**Georgia Tech:** Nick Sahinidis, Yijiang Li, Selin Bayramoglu

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