

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"

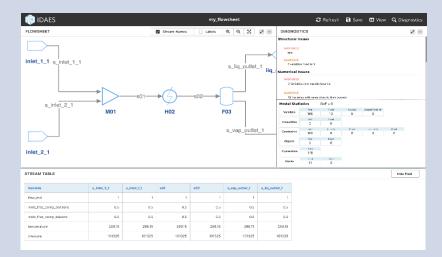
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With the addition of one line of code to your Jupyter Notebook or script..

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.



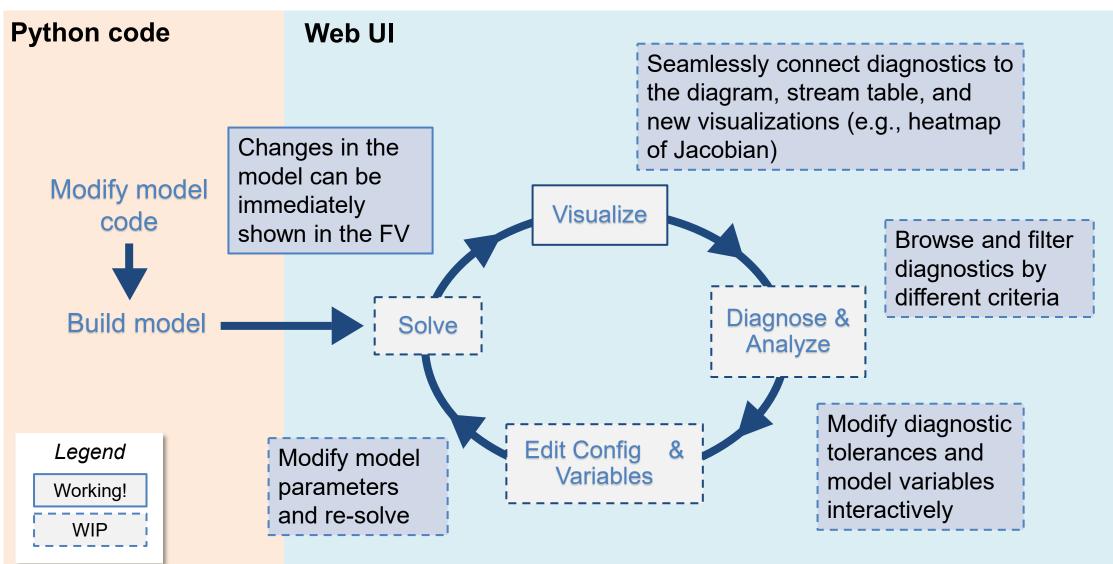
Latest changes for the FV

Important refactor to "normalize" the architecture ullet**IDAES Python** APIs **IDAES** model classes Re-do UI in ReactJS – layout improvements ulletPyomo and other libraries Solvers (ipopT, ETC) Model data & PARETC Aligns with metadata Network (local o Serialized model data & Wide-ARFA) Andrew Marketon Andrew Marketon Marketon Marketon Andrekton Andrekton Marketon Marke Reactjs other IDEAS And other iavascript fra **IDAES** core application javascript code **PSE UIs** Model data & metadat As application objects Rendered data **PYTHON UI** ΤΑΡ wrappers Python WEB APis UI actions / IDAE user input Process user input

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

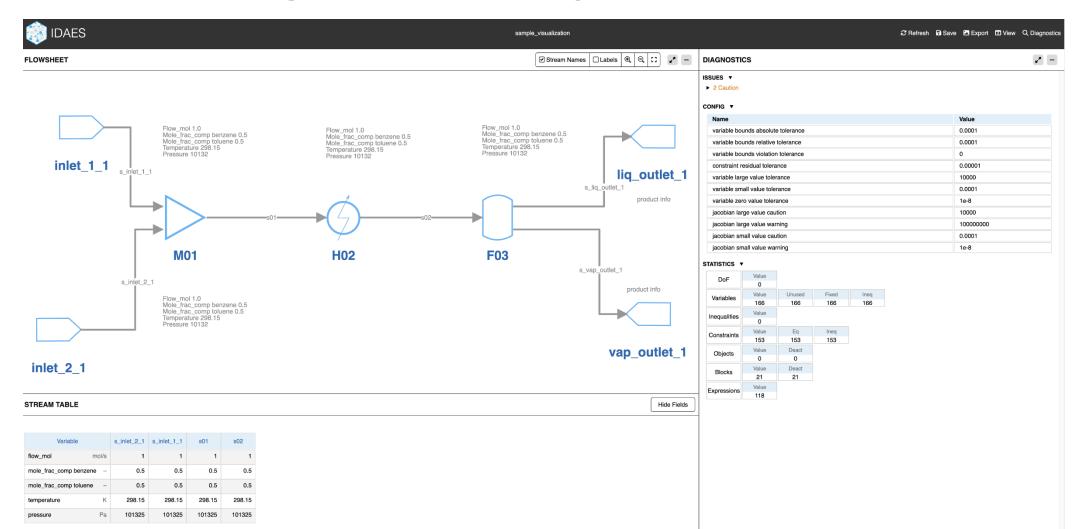


Plans for diagnostics (..and beyond!)





Diagnostics Prototype Screenshot





Diagnostics Prototype Screenshot Detail

IAGNOSTICS	<i>2</i> *
SUES 🔻	
2 Caution	
ONFIG 🔻	
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	10000000
jacobian small value caution	0.0001
jacobian small value warning	1e-8

STATISTICS **v**

DoF	Value			
201	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

DIAGNOSTIC	S							2. ²⁷
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CONFIG V								
Name						Va	lue	
variable bou	nds absolut	e tolerance				0.0	0001	
variable bou	nds relative	tolerance				0.0	0001	
variable bour	nds violation	n tolerance				0		
constraint residual tolerance			0.0	00001				
variable large value tolerance			10	000				
variable small value tolerance			0.0	0001				
variable zero value tolerance				1e	-8			
jacobian large value caution				10	000			
jacobian large value warning				10	0000000			
jacobian small value caution				0.0	0001			
jacobian small value warning				1e	-8			
STATISTICS V								
DoF	Value 0							
Variables	Value	Unused	Fixed	Ineq				
	166	166	166	166				
Inequalities	Value 0							
	Value	Eq	Ineq					
Constraints	153	153	153					
Objects	Value	Deact						
00,000	0	0						
Blocks Value De		Deact						

21 Value

118

Expressions



View variables with "extreme values"

▼	
aution	
aution 1: variables with extreme values ▼ extreme_values : 72	
𝕎 Search	
fs.M01.minimum_pressure[0.0,1]	101324.999999999999
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
fe M01 mixed_state(0.0) onth_mol_phase_comp[Vap.toluono]	58320 53040320868



Filter variables by name (etc.)

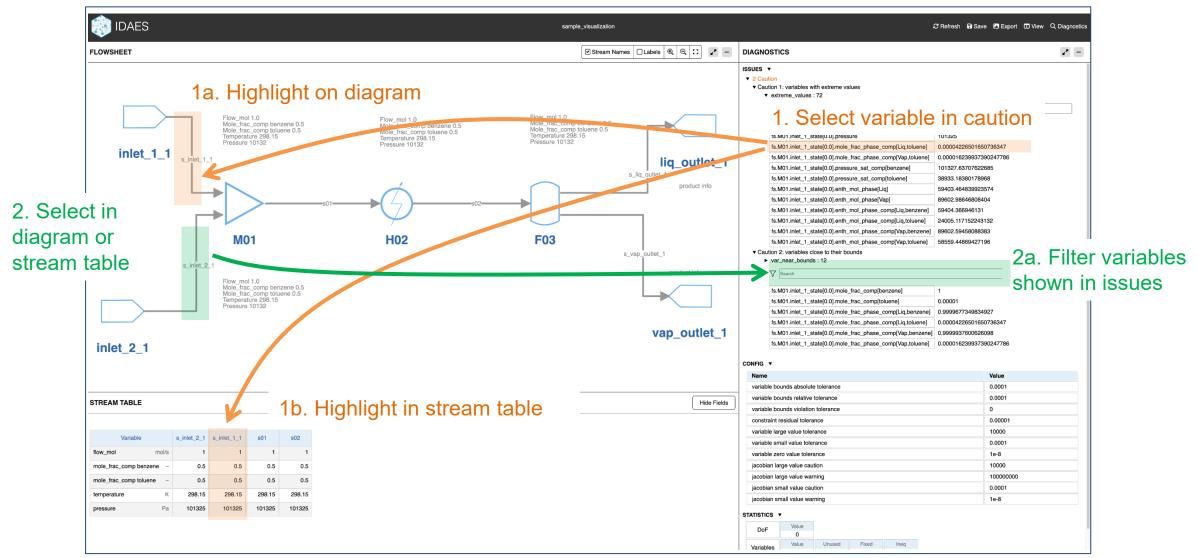
DIAGNOSTICS	x* -			
SSUES ▼				
▼ 2 Caution				
Caution 1: variables with extreme values				
▼ extreme_values : 72				
fs.M01.inlet_1_state[0.0]				
fs.M01.inlet_1_state[0.0].mole_frac_comp[toluene]	0.00001			
fs.M01.inlet_1_state[0.0].pressure	101325			
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Liq,toluene]	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				
γ 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	Vap,benzene] 0.9999937600626098			
fs.M01.inlet_1_state[0.0].mole_frac_phase_comp[Vap,toluene]	0.000016239937390247786			
CONFIG V				
Name	Value			
variable bounds absolute tolerance	0.0001			

variable bounds relative tolerance

0.0001



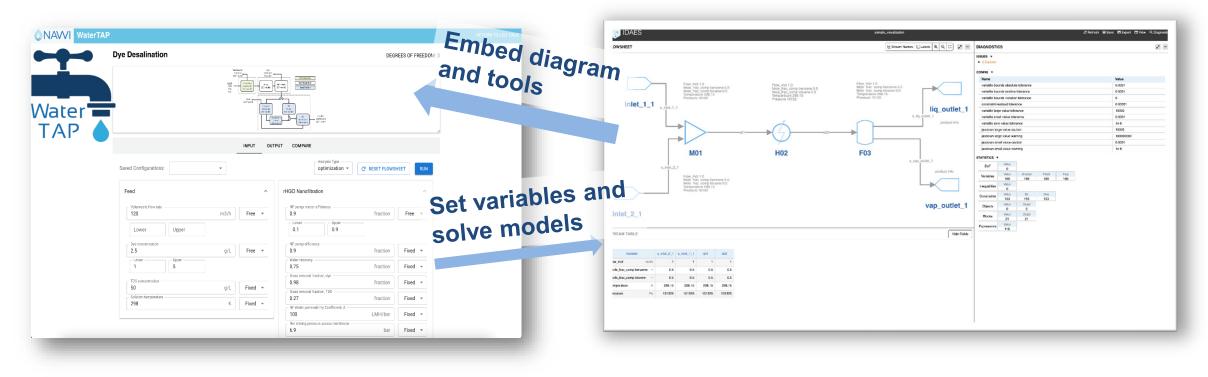
Advanced interactive explorations





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
- Towards an open (and open-source) UI "ecosystem"...





Visualization Summary



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



Interactive access to IDAES Diagnostics Toolkit is being actively added

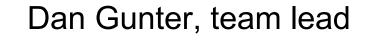


This will make the FV a more useful tool across IDAES PSE



Please come talk to us! We want your feedback







Sheng Pang, primary UI developer



Sarah Poon, User Experience (UX)



Cody O'Donnell, UI developer (emeritus, not attending)

UI-related Sessions

- Posters
 - IDAES Visualizer
 - WaterTAP
- Talks: WaterTAP UI
- Demos:
 - WaterTAP UI
 - PARETO UI



Mike Pesce, UI developer [WaterTAP, PARETO]

