Jacobian-based Model Diagnostics and Application to Equation Oriented Modeling of a Carbon Capture System

CCSI^2 Carbon Capture Simulation for Industry Impact

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Background

Equation-oriented (EO) models allow for efficient simulation and optimization of advanced energy systems. However, the large number of variables and equations (sometimes 10,000+) make them difficult to troubleshoot. Recently, IDAES has implemented a diagnostics toolbox[1] to consolidate the troubleshooting methods experienced users often relied upon to apply them automatically in a systematic manner.

Case Study: MEA carbon capture flowsheet

Variable and Constraint Scaling

- Example: two equations in process model

Mole Fraction → $y_{trace,in} - y_{trace,out} = f_1(\boldsymbol{x})$

Stream Enthalpy → $H_{in} + Q - H_{out} = f_2(\boldsymbol{x})$

↑ Heat Added

- When solving $f(\boldsymbol{x}) = 0$ using Newton's method, need equation residuals to be at same scale.
- Problem: enthalpy is $O(10^6)$ and trace component mole fraction is $O(10^{-6})$
- Solution: rescale equations:

$$10^6\left(y_{trace,in} - y_{trace,out}\right) = \tilde{f}_1(\boldsymbol{x})$$

$$10^{-6}\left(H_{in} + Q - H_{out}\right) = \tilde{f}_2(\boldsymbol{x})$$

- Problem: badly scaled Jacobian rows

$$J(\boldsymbol{x}) := \begin{bmatrix} 10^6 \frac{\partial f_1}{\partial x_1} & \cdots & 10^6 \frac{\partial f_1}{\partial x_n} \\ 10^{-6} \frac{\partial f_2}{\partial x_1} & \cdots & 10^{-6} \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \vdots \end{bmatrix}$$

- Solution: define scaled variables:

$$\tilde{y}_{trace,in} := 10^6 y_{trace,in} \qquad \tilde{y}_{trace,in} - \tilde{y}_{trace,out} = \tilde{f}_1(\tilde{\boldsymbol{x}})$$

$$\vdots$$

$$\tilde{H}_{out} := 10^{-6} H_{out} \qquad \tilde{H}_{in} + \tilde{Q} - \tilde{H}_{out} = \tilde{f}_2(\tilde{\boldsymbol{x}})$$

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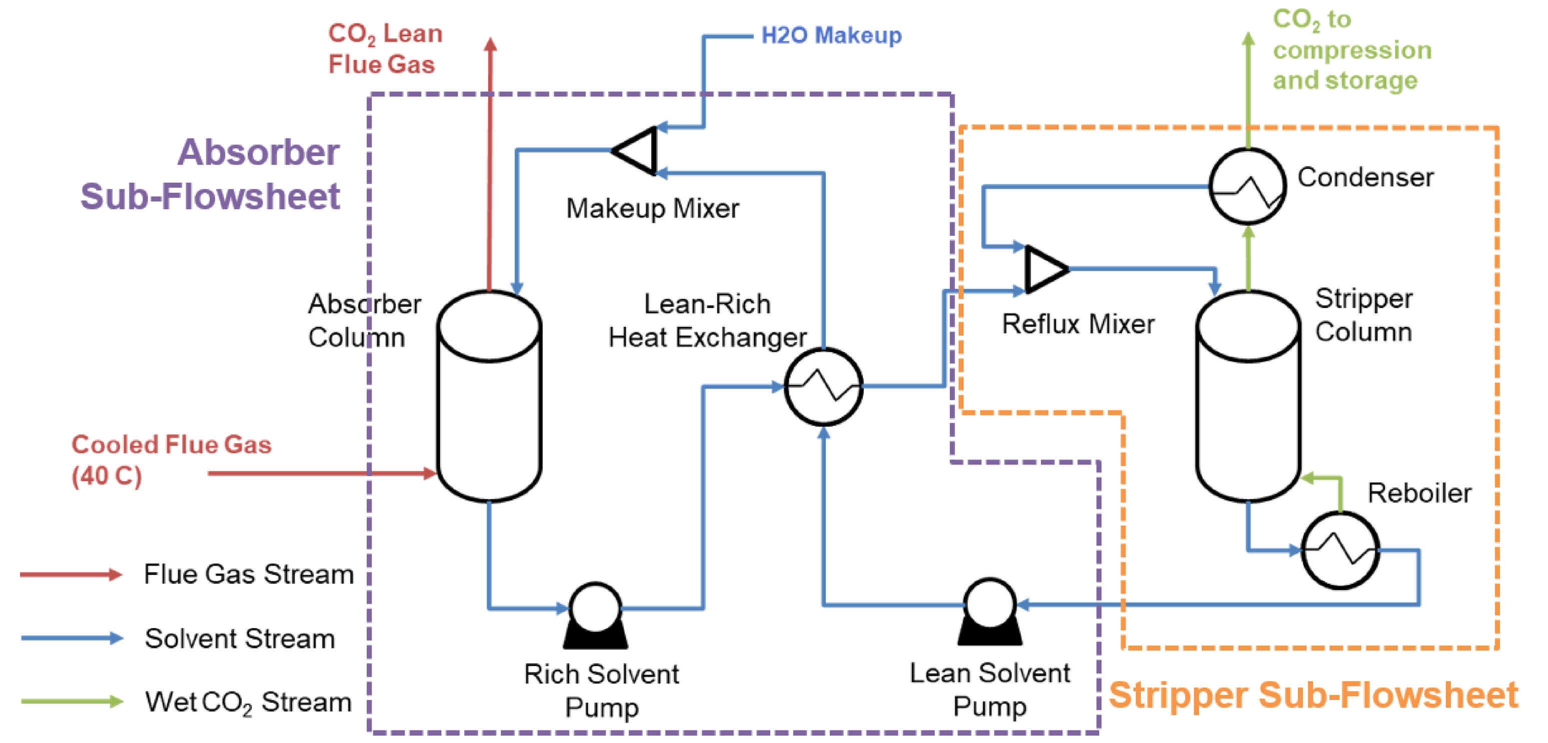
MEA Carbon Capture Flowsheet



- Sized to capture CO_2 from a 690 MW NGCC plant.
- Difficult-to-solve rate-based column model that, despite effort[2], was not numerically robust enough for advanced analysis and optimization.

Diagnostic Toolbox for Scaling

- Display Jacobian columns (correspond to variables) with extremely large or small ℓ_2 norms:

```
from idaes.core.util.model_diagnostics import DiagnosticsToolbox
diag_tbx = DiagnosticsToolbox(model)
diag_tbx.display_variables_with_extreme_jacobians()
```

- Focus on debugging one variable in particular:

```
fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].temperature: 1.997E+08
```

- Find problematic constraints containing variable:

```
svd_tbx = diag_tbx.prepare_svd_toolbox()
svd_tbx.display_constraints_including_variable(
    model.fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].temperature
)
```

```
fs.stripper_section.reflux_mixer.enthalpy_mixing_equations[0.0]: 1.997e+08
fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].log_k_eq_constraint[bicarbonate]: 5.364e+00
fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].log_k_eq_constraint[carbamate]: 6.551e+00
fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].log_conc_mol_phase_comp_true_eq[Liq,MEACOO_-]: 1.514e+00
fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].log_conc_mol_phase_comp_true_eq[Liq,HCO3_-]: 2.333e-01
fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].log_conc_mol_phase_comp_true_eq[Liq,MEA_+]: 1.748e+00
fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].log_conc_mol_phase_comp_true_eq[Liq,H2O]: 3.183e+01
fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].log_conc_mol_phase_comp_true_eq[Liq,MEA]: 1.129e+00
fs.stripper_section.reflux_mixer.rich_solvent_state[0.0].log_conc_mol_phase_comp_true_eq[Liq,CO2]: 5.685e-03
```

- Enthalpy mixing equation is badly scaled because molar flow rate and enthalpy have not been scaled
- IDAES property packages allow for global default values for physical properties (for all unit models using package)
- Set scaling factors of 3×10^{-4} for both, problem solved

Singular Value Analysis

- Singular values close to zero indicate modeling issues.
- Use SVD Toolbox to find variables and constraints associated with such singular values to troubleshoot.

```
svd_tbx.display_underdetermined_variables_and_constraints()
```

- Smallest singular value: $\sigma_n = 3.1 \cdot 10^{-10}$
- Associated variables:

```
fs.stripper_section.reflux_mixer.reflux_state[0.0].log_conc_mol_phase_comp_true[Liq,HCO3_-]
fs.stripper_section.reflux_mixer.reflux_state[0.0].log_conc_mol_phase_comp_true[Liq,MEA_+]
fs.stripper_section.reflux_mixer.reflux_state[0.0].log_conc_mol_phase_comp_true[Liq,MEA]
fs.stripper_section.reflux_mixer.reflux_state[0.0].log_conc_mol_phase_comp_true[Liq,MEACOO_-]
```

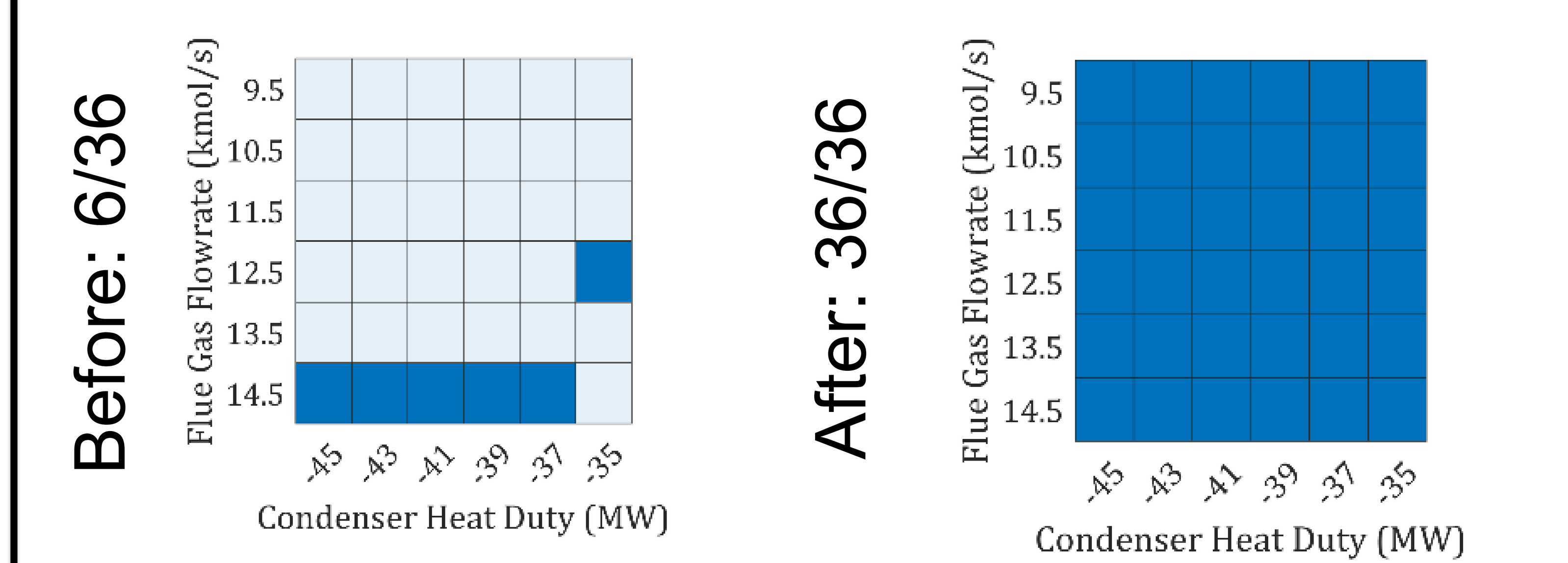
- Associated constraints:

```
fs.stripper_section.condenser.liquid_phase[0.0].appr_to_true_species[Liq,MEA]
fs.stripper_section.condenser.liquid_phase[0.0].true_mole_frac_constraint[Liq,HCO3_-]
fs.stripper_section.condenser.liquid_phase[0.0].true_mole_frac_constraint[Liq,MEA_+]
fs.stripper_section.condenser.liquid_phase[0.0].true_mole_frac_constraint[Liq,MEA]
fs.stripper_section.condenser.liquid_phase[0.0].log_conc_mol_phase_comp_true_eq[Liq,HCO3_-]
fs.stripper_section.condenser.liquid_phase[0.0].log_conc_mol_phase_comp_true_eq[Liq,MEA_+]
fs.stripper_section.condenser.liquid_phase[0.0].log_conc_mol_phase_comp_true_eq[Liq,MEA]
fs.stripper_section.condenser.liquid_phase[0.0].appr_to_true_species[Liq,HCO3_-]
fs.stripper_section.condenser.liquid_phase[0.0].appr_to_true_species[Liq,MEA_+]
```

- Variables and constraints for MEA speciation in mixer with nearly zero MEA concentration.
- Solution: remove apparent species for that mixer.

Convergence Analysis

- After model scaling and reformulation, the MEA flowsheet converges in all scenarios of a parameter sweep.



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[1] Lee, A., Dowling, A. W., Parker, R., Poon, S., Gunter, D., Nicholson, B. Model Diagnostics for Equation Oriented Models: Roadblocks and the Path Forward. *Proc of FOCAPD*. (2024)

[2] Akula, P., Eslick, J., Bhattacharyya, D., Miller, D.C. Model Development, Validation, and Optimization of an MEA-Based Post-Combustion CO_2 Capture Process under Part-Load and Variable Capture Operations. *Ind Eng Chem Res* 60:5176–5193 (2021)

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