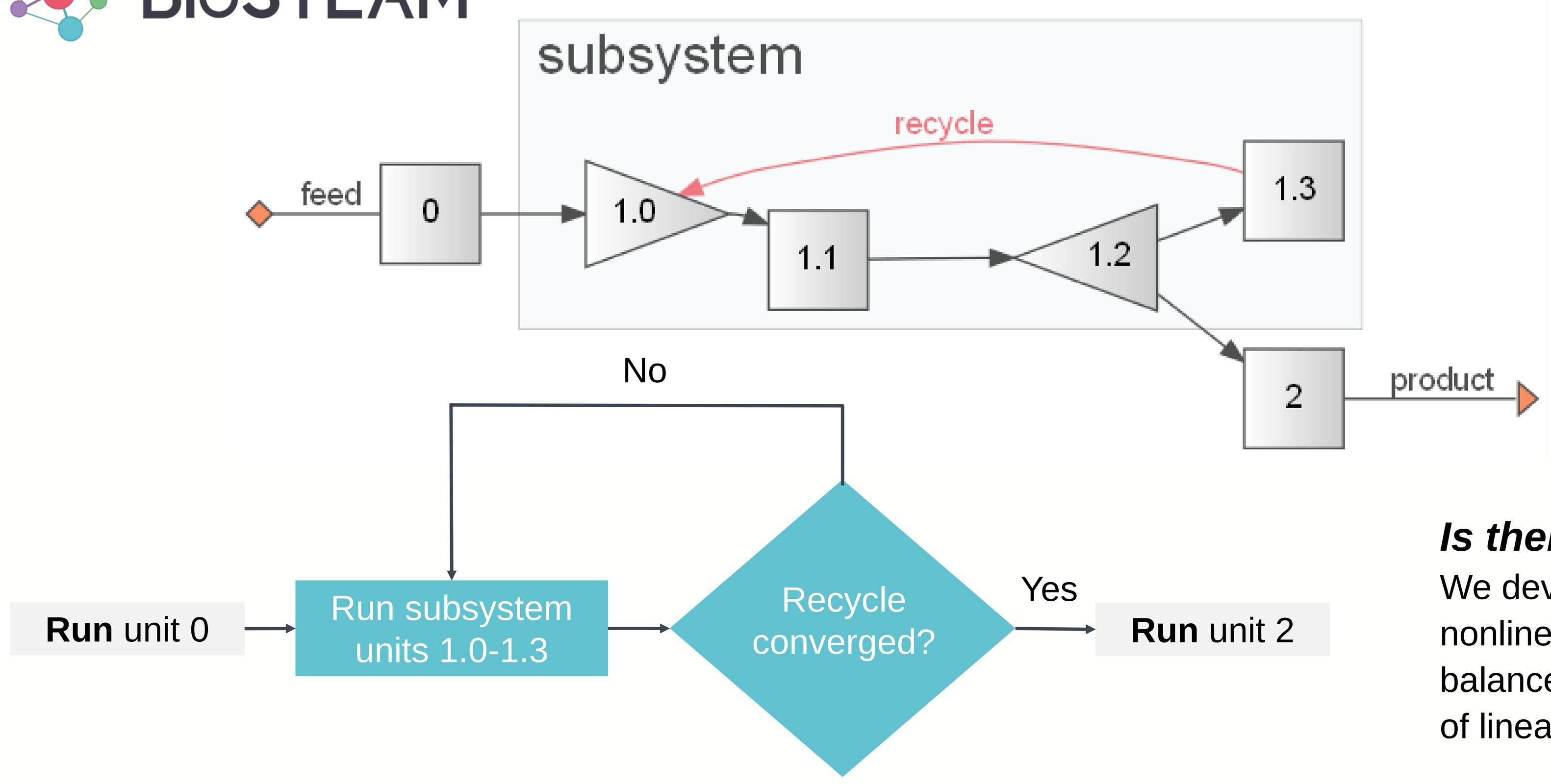
Graph-Based Representations and Applications to Process Simulation

Yoel R. Cortés-Peña and Victor Zavala
Department of Chemical and Biological Engineering, University of Wisconsin-Madison

Chemical Upcycling of Waste Plastics

Limitations to Classical Approaches to Flowsheet Convergence



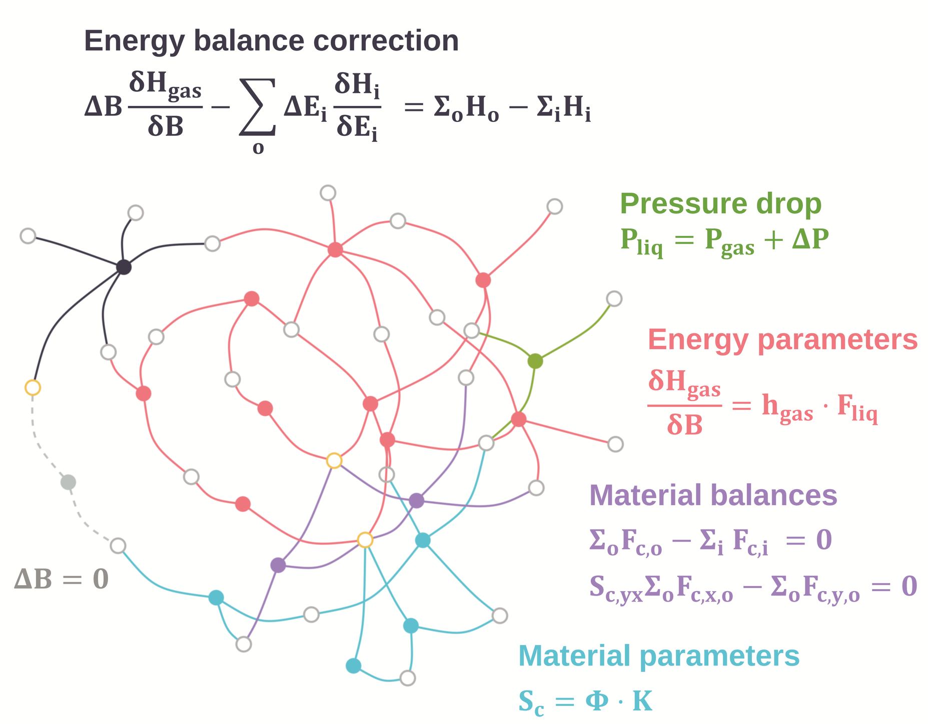
Sequential Modular Simulation
- Each unit is a separate model.
- Specialized methods converge individual units.
- Nonlinear coupling between units makes recycle systems challenging.

Equation Oriented Simulation
- All variables are simultaneously solved.
- Requires a good initial guess.
- Uses sequential modular simulation as a starting point.

Is there a better way to solve a flowsheet?
We developed a *graph-inspired* approach whereby nonlinear phenomena are decoupled from mass & energy balances, enabling key variables to be solved as systems of linear equations.

Phenomenological Relationships and Representation

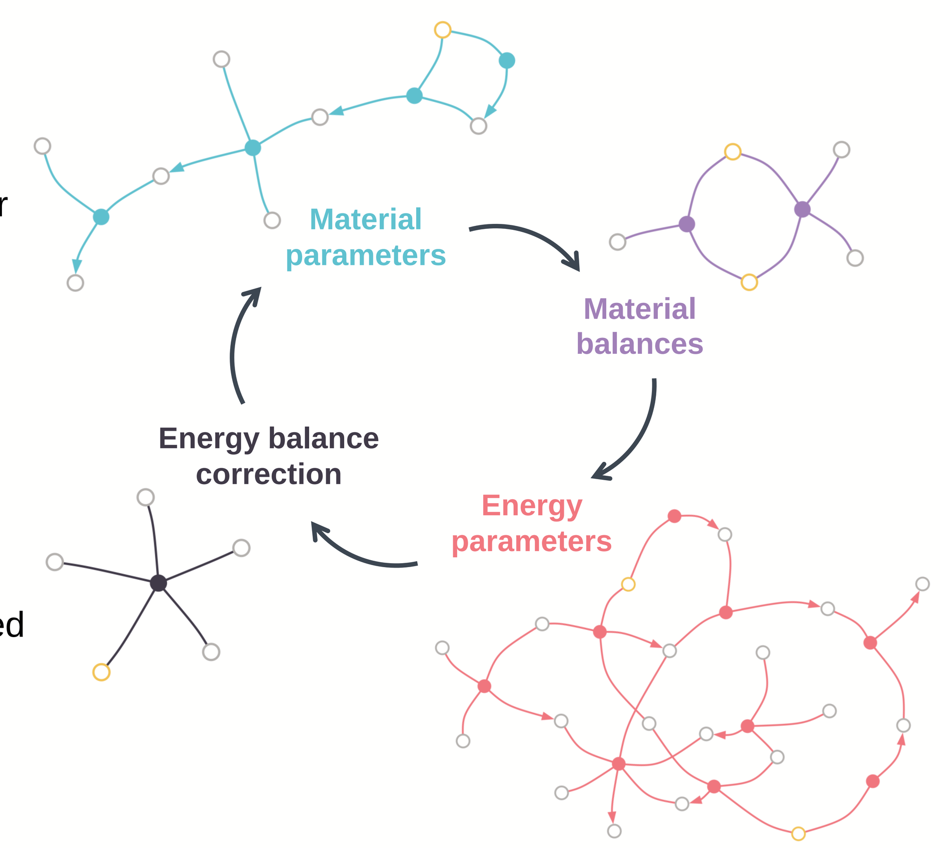
Vapor-liquid equilibrium



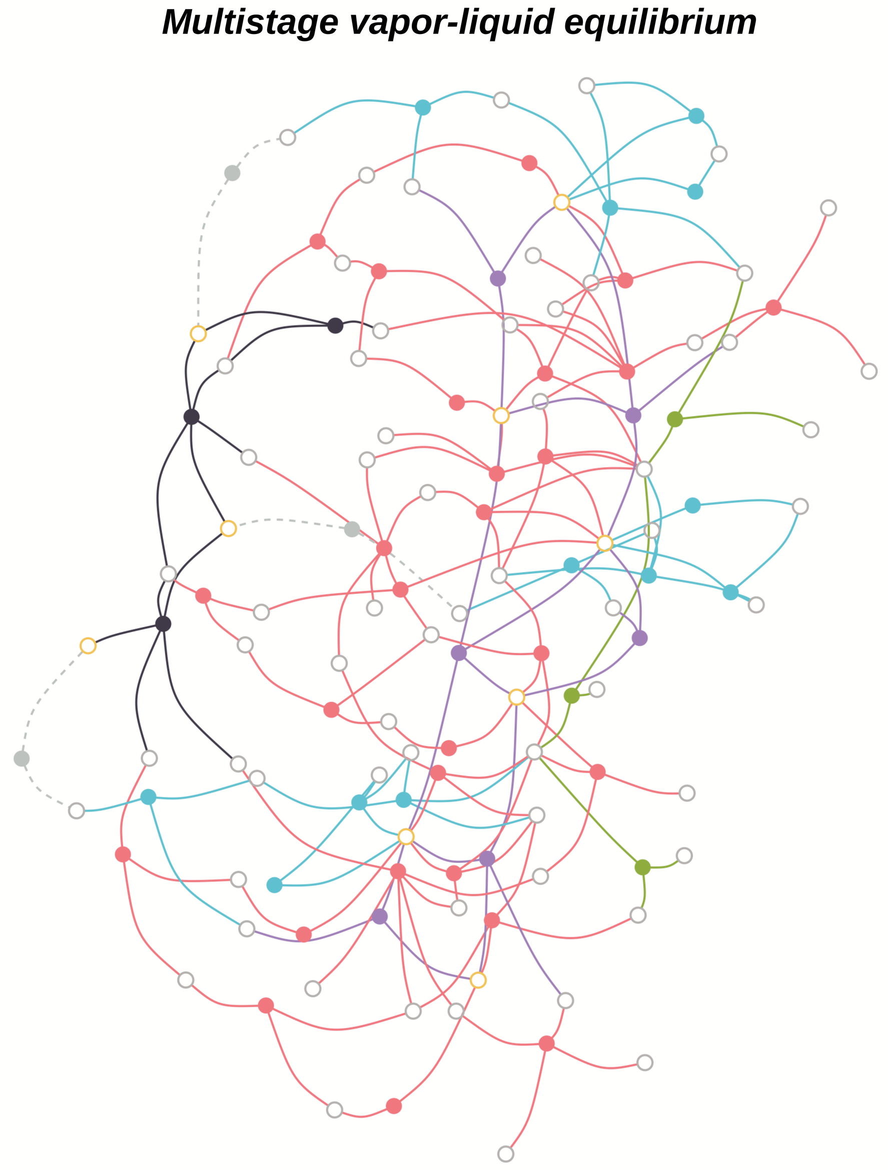
- Equations are nodes and variables are rings.
- Edges connect variables to their equations.
- Colors designate relationships to material & energy balances.

Decomposition

- Arrows point to solved parameters.
- Yellow rings are variables solved as a linear system of equations.
- Nonlinearities are isolated from material & energy balances.



Multistage vapor-liquid equilibrium

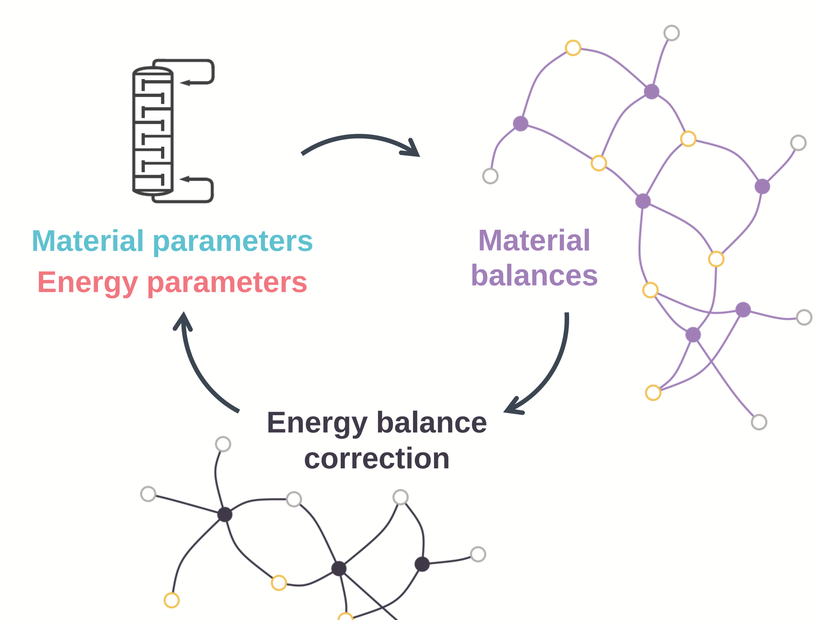


Aggregate stages

- Phenomenodes can be aggregated through the overall material & energy balance.
- Advanced methods can be used to solve a unit's overall material & energy parameters.
- This allows for hierarchical simulation.

Aggregate parameters

- Advanced methods can be used to solve all material & energy parameters.
- The material & energy balances can then be solved at the flowsheet level.
- This allows for consolidated material & energy balances during convergence.



This is the **first time** a **phenomenological decomposition scheme** has been **generalized to solve flowsheets**.

These **graph-theoretic** decomposition and aggregation **approaches** are **broadly applicable to any flowsheet**;.

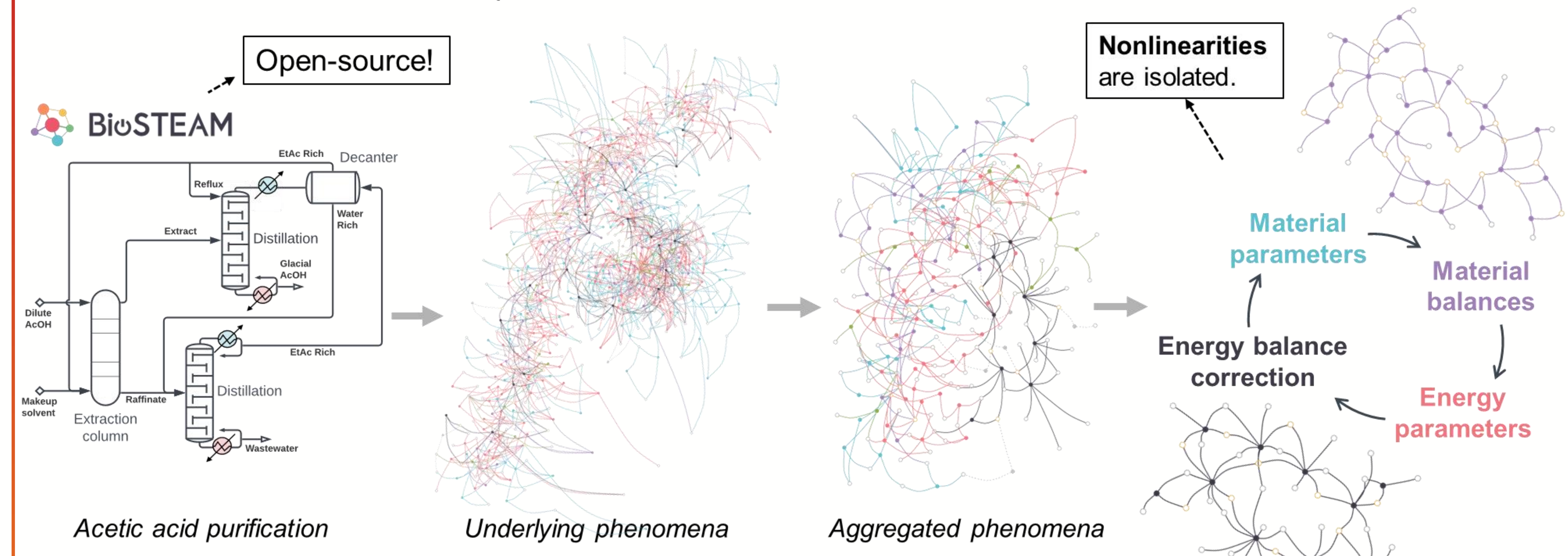
Phenomena-Oriented Approach

Step 0: User creates and connects unit operations.

Step 1: Software unfolds all equations and variables.

Step 2: *Aggregate* highly coupled equations.

Step 3: *Decompose* and solve sequentially.



$$\begin{bmatrix} b_1 & c_1 & & & 0 \\ a_2 & b_2 & c_2 & & \\ & a_3 & b_3 & \ddots & \\ & & \ddots & \ddots & c_{n-1} \\ 0 & & & a_n & b_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \\ d_n \end{bmatrix}.$$

Material & **energy** balances are solved as a *system of linear equations.*

Material balance equations:

$$\Sigma_o F_{c,o} - \Sigma_i F_{c,i} = 0 \quad (1)$$

$$\Phi K_c \Sigma_o F_{c,top,o} - \Sigma_o F_{c,bottom,o} = 0 \quad (2)$$

Energy balance correction equations:

VLE stage: $$\Delta\Phi h_{gas} \Sigma_o F_{liq,o} - \Sigma_i C_{liq,i} \Delta T_i - \Sigma_i \Delta\Phi_i h_{gas,i} F_{liq,i} = \Sigma_o H_o - \Sigma_i H_i \quad (3)$$

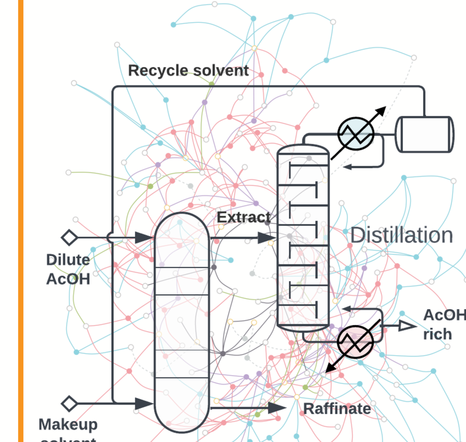
LLE stage: $$\Delta T \Sigma_o C_{liq,o} - \Sigma_i C_{liq,i} \Delta T_i - \Sigma_i \Delta\Phi_i h_{gas,i} F_{liq,i} = \Sigma_o H_o - \Sigma_i H_i \quad (4)$$

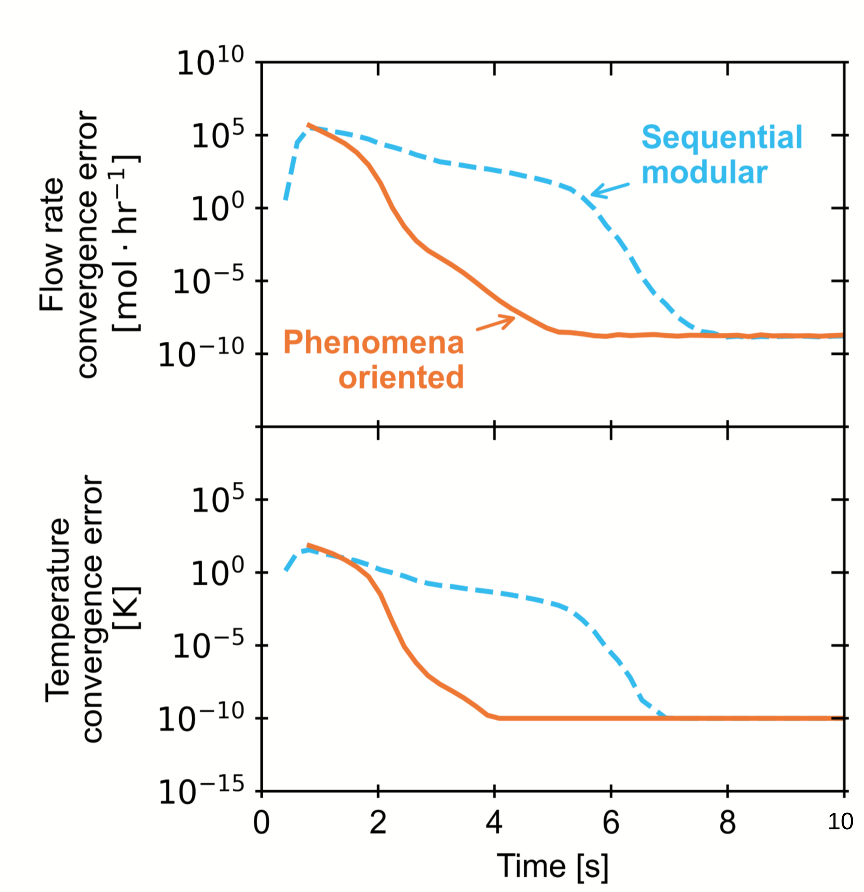
Preliminary Phenomena-Oriented Algorithm

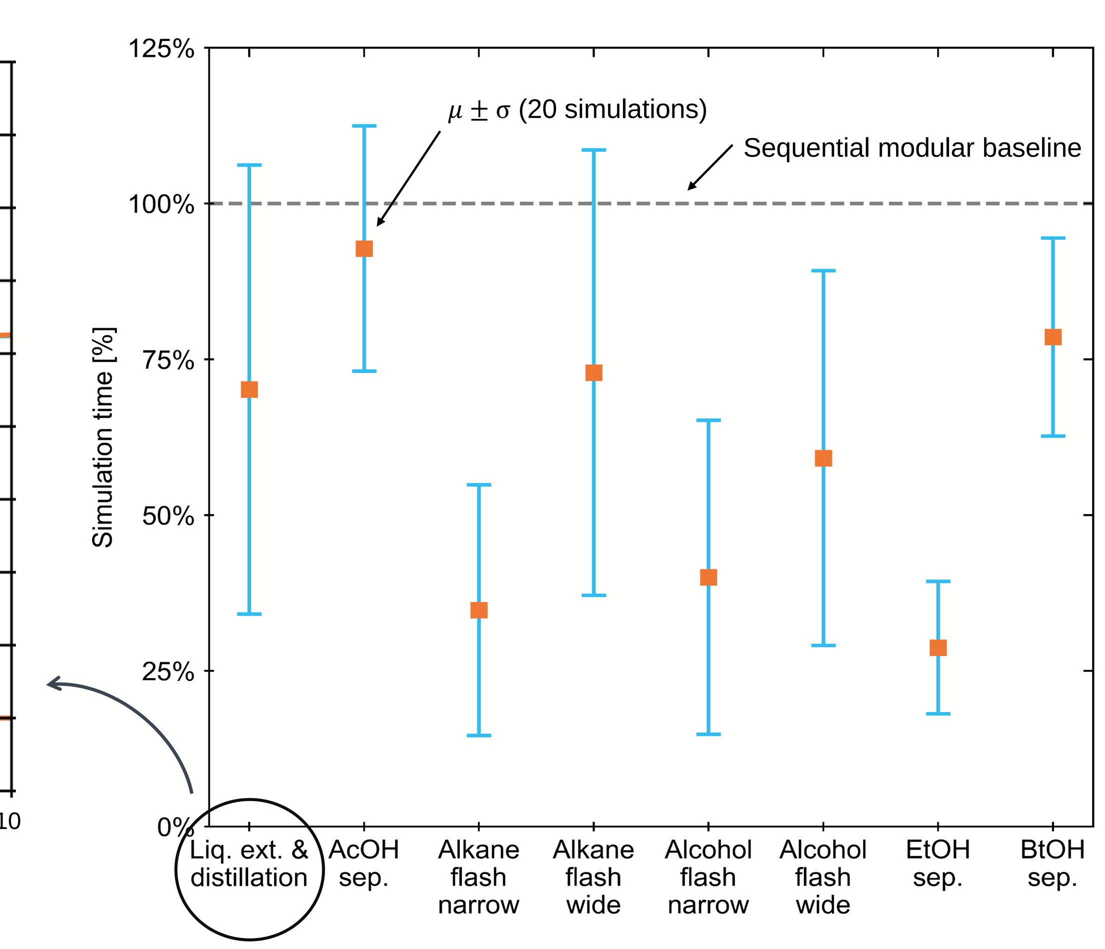
1. In the absence of an initial guess for all parameters, run each unit operation sequentially.
2. For each unit operation:
    1. Solve the unit operation and update material & energy parameters.
    2. Solve for material balance across all unit operations as a system of linear equations (eqs 1–2) and update.
    3. Solve for ΔE (e.g., ΔΦ for VLE stages, ΔT for LLE stages) as a system of linear equations (eqs 3–4) and update E.
3. Solve for material and energy parameters. For multistage LLE, solve for all stages simultaneously using the pseudo equilibrium approach.
4. Run steps 2.2 and 2.3.
5. If all parameters have not converged under a specified tolerance, repeat steps 2–4.

Sequential Modular vs. Phenomena-Oriented

Liquid extraction & distillation system







Advantages of phenomena-oriented approach
- Material & energy balances are consolidated in each iteration.
- Can be faster than sequential modular simulation.
- By decreasing computation time, we enable robust optimization and rigorous uncertainty and sensitivity analyses.

Future work
- Test a wider set of cases, including bigger systems with reactive distillation.
- Elucidate the relationship between convergence speed and the complexity of a flowsheet.

This material is based upon work supported by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Bioenergy Technologies Office under Award Number DE-EE0009285.