**Abstract**

Rapid and robust simulation of a chemical production process is critical to address core scientific questions related to process design, optimization, and sustainability. However, efficiently solving a chemical process remains a challenge due to their highly coupled and nonlinear nature. Decoupling of phenomenological nonlinearities is widely used to linearize material and energy balances within multistage equilibrium columns and enable more robust simulation. In this work, we developed a phenomena-oriented simulation algorithm for the convergence of the complete flowsheet that expands and generalizes classical decomposition strategies for multistage unit operations. We implemented this new simulation algorithm in BioSTEAM —an open-source process simulation platform implemented in Python— and show how this phenomena-oriented algorithm enables more rapid and robust simulation of large, highly-coupled systems than classical sequential modular approaches. The production of glacial acetic acid (99.9% purity) from a dilute mixture of water and acetic acid is used as a representative complex system to benchmark the convergence profile of the phenomena-oriented algorithm against the sequential modular.

**Introduction**

Key ideas:

1. Phenomenological decomposition is not new; it is used to solve distillation and liquid-liquid extraction columns by decoupling material, equilibrium, summation, and enthalpy (MESH) equations.
2. It has not been extended to solve the complete flowsheet (until now).
3. We generalized the phenomenological decomposition approach to work for any unit operation.
4. The decomposition approach for the different phenomena is based on expert chemical engineering knowledge that is largely adapted from classical approaches.

**Materials and Methods**

**Results and Discussion**

**Unused**

used to reformulate the network of equations within

The governing material, energy, and phenomena equations are decomposed such that the material and energy balances are linearized. S

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To this end, we developed graph abstractions of the governing equations of separation equipment.

The graph abstraction consists of a mesh of interconnected variable nodes and equation nodes.

We demonstrate that partitioning the graph into separate material, enthalpy, and phenomenological subgraphs decouples nonlinearities and guide decomposition algorithms.

towards the convergence of the complete flowsheet

Decomposition of material, equilibrium, summation and enthalpy (MESH) equations is widely used to reformulate the network of equations within multistage unit operations and enable convergence through sequential substitution.

generalizable to any flowsheet and leverage

In this work, we show that graph representations of the underlying physical phenomena may help identify potential avenues to systematically reformulate the network of equations and enable more robust topology-aware simulation.

To this end, we developed graph abstractions of the governing equations of separation equipment.

The graph abstraction consists of a mesh of interconnected variable nodes and equation nodes.

We show that partitioning the graph into separate mass, energy, and phenomenological subgraphs can help decouple nonlinearities and guide decomposition algorithms.

We implemented this new simulation algorithm in BioSTEAM —an open-source process simulation platform implemented in Python— and show how this phenomena-oriented decomposition algorithm enables more rapid and robust simulation than classical sequential modular approaches.