Amgen Seminar Series in Chemical Engineering

in

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"How Classical Field Theory Can Help in Process Flowsheet and Equipment Modeling: General Principles and Practical Reductions"

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Chemical process and equipment modeling is central to chemical engineering, comprising much of textbook content and providing the basis for much of engineering practice. This body of knowledge is traditionally learned as an extensive family of equations. The unifying principles behind them are not always evident.

The models most widely employed actually derive from integrations of the diffusion-convection-reaction PDEs. While detailed 3-D integrations are seldom practical for modeling of equipment performance or flowsheets, the usual practical models are still in fact approximate integrations of the continuum model. Because of this, classical field theory may be applied to reveal useful properties present in the physics but not evident from the familiar equations.

The underlying continuum PDEs are shown to be derived from a unified variational principle with convexity properties provided by the underlying physics. Behavior is represented with a set of primal fields (generalized densities) and dual fields (potentials). Applying geometries, these fields are integrated (in principal) over submodel volumes to obtain compact algebraic descriptions. Important solution existence and uniqueness properties are obtained.

This canonical primal-dual approach to modeling offers several advantages. Larger systems may be assembled from sets of submodels by connections at interfaces, analogous to components in an electrical circuit. Numerical convergence via homotopy can be guaranteed. The goal is to enable software that can automatically generate models that solve robustly.

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