Goal-Oriented Process Synthesis Augmented with Constraint-Oriented Process Synthesis

Jeffrey J. Siirola
Purdue University
Carnegie Mellon University
## Process Innovation Sequence

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Each step involves generating alternatives
Design Paradigm

- **Formulation**
  - Needs, Objectives
  - Goals, Constraints, Specifications

- **Synthesis**
  - Structure, Parameters
  - Tactics, Reformulation

- **Analysis**
  - Internal Analysis
  - Analysis Methods
  - Optimization
  - Actual Behavior

- **Evaluation**
  - Satisfaction
  - Evaluation Methods
  - Evaluation

- **Acceptance**
  - Good Enough
  - Not Good Enough

Component Development
- Strategies, Representations, Synthesis Methods
Method Development
- Analysis Methods
Method Development
- Evaluation Methods
Abstraction, Learning
Process Synthesis

♦ The generation of process flowsheet alternatives

♦ Identification of...
  • *Phenomena to exploit*
  • *Equipment to implement*
  • *Interconnections*
Process Synthesis Approaches

♦ Evolutionary Modification
  • Traditional Method
  • Alter Existing Design

♦ Superstructure Optimization
  • Tear Down Redundant Design
  • Generalized Disjunctive Programming

♦ Systematic Generation
  • Build Up From Basic Components
  • Means-Ends Analysis
Means-Ends Analysis
Systematic Generation Approach

♦ Define initial and goal states in terms of physical properties
♦ Detect physical property differences
♦ Identify technologies to reduce differences
♦ Add unit operations to partial flowsheet
  • Retrosynthetically to goal state and specify inputs
  • Synthetically to present state and determine outputs
  • Strategically awaiting resolution of preconditions
♦ Recursively meet any technology preconditions
Chemical Process Physical Properties  
(Common resolution technologies)

- Component Identity  (Reaction)
- Amount or Flowrate  (Flow control)
- Concentration  (Mixing, separation)
- Phase  (Boiling, condensing, melting, solidification, etc.)
- Temperature, Pressure  (Heating, cooling, pumping, compressing, throttling, etc.)
- Size, Shape, Dispersion  (Various)
Task Orientation

- Address property differences in a hierarchical fashion
- Think specifically in terms of tasks to be accomplished and phenomena to be exploited, not equipment to be used
- Identify tasks not necessarily in the same direction as material flow
- Consider tasks at different levels in the design hierarchy in a coordinated manner
Hierarchical Systematic Generation

Process Synthesis Model

♦ Reaction Path Synthesis
♦ Species Allocation
♦ Task Identification
♦ Task Integration
♦ Utility Infrastructure
♦ Equipment Design

Onion Model, AIDES, BALTAZAR, PIP
Task Coordination and Integration

♦ Integrate complementary tasks in the same level for efficiency
  - *Heat exchanger networks*
  - *Power integration*

♦ Coordinate tasks at different levels to maximize efficiency-improving opportunities
  - *Heat-integrated distillation sequences*
  - *Multiple-effect distillation*
Task Coordination and Integration

♦ Integrate multiple technologies for enhanced performance or synergism
  • *Azeotropic and extractive distillation*
  • *Reactive separation*

♦ Integrate consecutive tasks for process intensification or simplification
  • *Design equipment to accomplish multiple tasks*
Task Coordination and Integration

Integrate complementary tasks in the same level for efficiency

- Heat exchanger networks
- Power integration
- Pinch Technology
Task Coordination and Integration

- Coordinate tasks at different levels to maximize efficiency-improving opportunities
  - Heat-integrated distillation sequences
  - Multiple-effect distillation
Pressure Optimized Distillation Sequence

0.3 Atm

2.4 Atm

1.1 Atm

D

A

B

C
Pressure Selection Anticipating Heat Integration

Typical 35-40% Net Present Cost Savings
Pressure Selection Anticipating Steam Generation

Low Pressure Steam Generator

High Pressure Steam

Medium Pressure Steam

Typical 35-40% Net Present Cost Savings
Multiple-Effect Distillation

Typical 40-50% Energy Savings
Task Coordination and Integration

♦ Integrate multiple technologies for enhanced performance or synergism

• *Azeotropic and extractive distillation*
  + Mass separation agents to alter activity coefficients

• *Reactive separation*
  + Simultaneous separation to enhance reaction
  + Reaction to lessen separation difficulty
Synergistic Technology Integration
Reactive Separation

♦ Use of Separation to enhance Reaction
  • Remove product to shift equilibrium
  • Remove catalyst inhibitor
  • Improve reaction selectivity

♦ Use of Reaction to enhance Separation
  • Combine reaction equilibria and phase equilibria to alter azeotrope formation
  • React to completion to eliminate a subsequent composition-adjusting (separation) task
Task Coordination and Integration

♦ Integrate consecutive tasks for process simplification
  - Design equipment to accomplish multiple tasks

♦ Equipment design for process intensification
  - Manipulate areas, gradients, and fields for faster transport and kinetics and smaller equipment
Methyl Acetate Process

Methanol + Acetic Acid $\rightleftharpoons$ Methyl Acetate + Water
Task Approach to Methyl Acetate Process Synthesis

Acetic Acid → Catalyst → Methanol

Equilibrium Reaction Task

Distillative Separation Task

Methyl Acetate-Water Azeo Methanol

Solvent-Enhanced Distillative Separation Task

(Methyl Acetate and Water)

Methanol Water Acetic Acid

Recycle to Somewhere

(Methyl Acetate)

Distillative Separation Task

Water Acetic Acid

Water

Acetic Acid

Recycle to Somewhere
Synergistic Task Integration
Reaction to Alter Separation Problems

Acetic Acid
Catalyst
Methanol

Equilibrium Reaction Task A
(Eliminates Methanol)

Separative Reaction Task B
(Eliminates Acetic Acid)

Separative Reaction Task E

Solvent-Enhanced Distillative Separation Task F
(Removes Water)

(Methyl Acetate)

Distillative Separation Task C
(Removes Methyl Acetate)

Recycle to Somewhere

Distillative Separation Task D
(Removes Methanol)

Acetic Acid
Water

Recycle to Somewhere

Distillative Separation Task G
(Removes Acetic Acid)
Synergistic Task Integration
Routing Task Coproduct Streams

Acetic Acid
Catalyst
Methanol

Equilibrium Reaction Task A

Separative Reaction Task B

Separative Reaction Task E

Solvent-Enhanced Distillative Separation Task F

Distillative Separation Task G

Distillative Separation Task C

Distillative Separation Task D

Methyl Acetate
Acetic Acid
Water

Methanol
Wter
Consecutive Task Integration for Process Intensification
Single Column Methyl Acetate Process

- Distillation Task G
- Extractive Distillation Task F
- Reactive Distillation Task E
- Reaction Task A
- Reactive Distillation Task B
- Distillation Tasks C and D

Inputs:
- Acetic Acid
- Catalyst
- Methanol

Outputs:
- Methyl Acetate
- Water
Goal-Oriented Process Synthesis

- Systematic process synthesis methods have reached the point of industrial applicability
- Means-ends analysis is a useful paradigm for the systematic generation approach
- Tasks to be accomplished are considered separately from equipment to be employed
- Process integration and intensification enhancements
  - Complementary tasks for operating efficiency
  - Coordinated tasks for maximizing opportunity
  - Combined phenomena for enhanced performance
  - Consecutive tasks for process simplification
  - Manipulated areas and gradients for higher rates
Synthesis of Separation Schemes for Nonideal Mixtures

an example of

Constraint-Oriented Process Synthesis
Three-Column System for Ethanol Dehydration

Feed → Ethanol → Water
Two-Column System for Ethanol Dehydration
Conventional Methyl Acetate Flowsheet

Acetic Acid
Methanol
Catalyst

Methyl Acetate
Solvent

Solvent/Entrainer

Water
Heavies

Water
Reactive-Extractive Distillation Process for Methyl Acetate

Methyl Acetate

Acetic Acid

Catalyst

Methanol

Water
Single Column for Acetic Acid Dehydration

Feed

Water

Acetic Acid
Detailed Acetic Acid Dehydration Flowsheet

Extractor

Acid Boiler

Low Pressure Azeo

High Pressure Azeo

Flash

Feed

HOAc

H₂O

Spg

Stm

Med

Stm

Ethyl Acetate

H₂O
Early Process Synthesis for Separation Schemes

- Enumerative and heuristic goal-oriented opportunistic approaches for nearly ideal systems
  - *Phenomena to exploit*
  - *Equipment to implement*
  - *Interconnections*
- Heat-integrated distillation scheme synthesis
- Multiple-effect distillation
Nonideal Separation System Synthesis

♦ Azeotropes, pinches, multiple liquid phases
♦ More complex representations of underlying phenomena
  • Phase diagrams
  • Residue curve maps
♦ Mass separating agents
  • Intentional introduction of new components
♦ Critical Features and Strategic Approaches
Elements of Residue Curve Theory

♦ Residue curve families
♦ Node and saddle stationary points
♦ Distillation regions
♦ Reachable compositions
♦ Direct and indirect splits
Simple Open Still Liquid Compositions

Diagram showing a ternary system with points labeled as follows:
- **Ethanol**
- **Water**
- **Azeo**
- **Ternary**
- **Entrainer**

The diagram depicts the relationships between these components in a ternary system.
Residue Curve Map
Ternary system

Entrainer

Azeo

Azeo

Ternary

Ethanol Azeo Water
Rules:

1. Distillate, Bottoms, and net Feed Collinear

2. Distillate and Bottoms on same Residue Curve

Reachable Compositions
Single Feed Distillation

- Reachable Distillates
- Low-boiling Node Overhead (Direct Split)
- High-boiling Node Underflow (Indirect Split)

Entrainer

Ethanol

Water
Etnanol-Water System
Residue Curve Map
Ethanol-Intermediate-Water System
Reachable Compositions
Ethanol-Intermediate-Water System

Intermediate Boiler

Distillates

Mix

Bottoms

Ethanol  Azeo  Feed  Water
Ethanol Dehydration with Intermediate Boiler
Residue Curve Map
Ethanol-Entrainer-Water System
Overlaid VLE and LLE Representations

- Entrainer
- VLE Distillation Boundaries
- LLE Tie Lines
- Ethanol
- Water
Ethanol Dehydration with Entrainer Azeotropic Distillation

Diagram showing the process flow for ethanol dehydration using entrainer in an azeotropic distillation setup. The diagram illustrates the condensation and distillation steps involving ethanol, feed, and water components.
Distillation Pinch
Acetic Acid-Water System
Residue Curve Map
Acetic Acid-Water-Ethyl Acetate System
Liquid-Liquid Overlay
Acetic Acid-Water-Ethyl Acetate System

Diagram showing the liquid-liquid overlay for the Acetic Acid-Water-Ethyl Acetate system with the points labeled Acetic Acid, Feed, Ethyl Acetate, and Water.
Extractor
Acetic Acid-Water-Ethyl Acetate System
Reachable Compositions from Extract Acetic Acid-Water-Ethyl Acetate System
Easiest Azeotropic Distillation
Acetic Acid-Water-Ethyl Acetate System
Acetic Acid Dehydration
Extraction and Azeotropic Distillation
Detailed Acetic Acid Dehydration Flowsheet

Extractor

Low Pressure Azeo

High Pressure Azeo

Flash

Feed

Acid Boiler

HOAc

H₂O

Stm

Med

Spg

Ethyl Acetate

H₂O
Other Synthesis Considerations

♦ When are intentional excursions advantageous?
  • *Process costs are path dependent*

♦ When is it not most appropriate to drive blindly toward a goal?
  • *What triggers assessment that a segment cost may be too high?*

♦ Hierarchical property difference consideration
  • "*Strategic* units placed conditionally on flowsheet awaiting resolution of preconditions or lower-hierarchy property differences*
  • *Uninstantiated states resulted in some freedom to generate alternative paths*
Critical Features (Constraints)

♦ Distillation Boundaries
♦ Saddle Products
♦ Pinched or Close-boiling Regions
♦ Overlapping Melting/Boiling Points
♦ Temperature Sensitive Components
Overcoming Distillation Boundaries

- Exploit non-VLE behavior to cross boundary
- Mix with another stream to cross boundary
- Add new component such that boundary does not extend into new dimension
- Change pressure to shift boundary position
- Exploit extreme boundary curvature
- Redefine problem so boundary need not be crossed
Separations Synthesis for Non-ideal Mixtures

♦ Strategic Operations
  - Identification of tasks for *avoiding, overcoming, or exploiting* Critical Features (Constraints)
  - Aided by Residue Curve Map and other thermodynamic representations

♦ Opportunistic Operations
  - *Distill low-boiling node overhead* (direct split)
  - *Distill high-boiling node as bottoms* (indirect split)
  - Decant two-phase liquid mixture
Separation Synthesis Algorithm

♦ Define Problem
  - *Determine feed compositions; construct Source list*
  - *Determine goal compositions; construct Destination list*
  - *Identify additional mass separation agents*

♦ Thermodynamics
  - *Examine VLE, LLE, SLE; determine variation with temperature and pressure*
  - *Construct Residue Curve Map; overlay LLE, SLE phase diagrams*
  - *List Compositions of Interest (potential internal mass separation agent compositions)*
Separation Synthesis Algorithm

♦ Choose Stream to Process
  • Choose stream from Source list
  • List Critical Features pertinent to all remaining goals

♦ Process Stream
  • Label as Destination (goal), or
  • Recycle to previous part of flowsheet and update, or
  • Specify Composition-changing Operation
    + List Strategic Operations for Critical Features
    + List Opportunistic Operations
    + Choose a Strategic or Opportunistic Operation
Separation Synthesis Algorithm

♦ Update Flowsheet
  • Place Operation on flowsheet
  • Connect streams anchored to previous parts of flowsheet and update
  • Place unanchored feed streams on Destination list (new subgoals)
  • Place remaining outputs on Source list (may not be completely defined)

♦ Continue Processing
  • Repeat until Source list is empty and all goals are satisfied and all assumed mass separating agent compositions have been regenerated

♦ Generate Flowsheet Alternatives
  • Integrate operations into complex equipment
  • Choose alternative decisions
Diethoxymethane Purification

Diethoxymethane
Product

Water
Coproduct

Reactant
Effluent

Ethanol
Reactant
Ethanol
Reactant
Water
Coproduct
Diethoxymethane
Product
Reactor
Effluent
Strategic Decanter
Opportunistic Direct Distillation
Water Coproduct
Ethanol Reactant
Reactor Effluent
{(N), (S), (N), (N), (N), (N), (N), (N), (S), (S), (N), (S)}
Diethoxymethane

Product

Ethanol
Reactant

Water
Coproduct

Reactor
Effluent

H₂O

Strategic
Decanter

Opportunistic
Direct Distillation

Reactor
Effluent
Strategic Process Synthesis

Summary

♦ Critical feature (constraint) orientation
  - Critical features arise from complicated physical molecular interactions
  - Likely to generate tangential subgoals in addition to property resolution goals

♦ Greater reliance on strategy
  - Based on recognizing complex physical property relationships
  - Assumed existence of useful compositions (compositions of interest) resulting in subsequent recycle

♦ Unanchored (strategic) as well as forward-chained (opportunistic) operations
Complex Property Representations

- The present algorithm involves extensive graphical processing
  - Detecting region boundaries, pinched areas, and other critical features
  - Detecting overlapping regions and other relationships among different property representations
  - Estimating "closeness" (i.e., for opportunistic recycle)
  - Flowrate-composition (lever arm) relationships
  - Determining appropriate goals for each stream
Strategic Process Synthesis

- We have a verbal synthesis algorithm
- Designers readily exploit complex graphical representations (at least for limited number of components)
- Designers rarely go back to explore alternative choices
- We have been unsuccessful in developing a formal explicit computer implementation
Design Agent Challenge

♦ Why is it that designers so readily process complex graphical interrelationships?
  • Parallel processing?
  • Some other kind of geometrical reasoning?

♦ Can large collections of simultaneous autonomous entities be exploited to extract features from graphical relationships (or other complex or higher dimensional representations)?

♦ Can an agent-based architecture be designed to excel at strategic planning, constraint avoidance, and goal achievement?

♦ Can an agent distinguish between a sufficient flowsheet and a redundant superstructure? Detect degenerate structures?

♦ Can an agent understand process intent?