Property Integration for Simultaneous Process and Product Design

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Outline

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- Process Design vs. Molecular Design
- Simultaneous Process and Molecular Design
- Motivating Example
- Concepts of Property Clustering
- General Problem Statement
- General Problem Representation
- Minimum Flow Solution Methodology
- Case Study: VOC Recovery
- Conclusions

Introduction and Motivation

- Conventional Process Design Paradigm
  - Tracking individual chemical species through balances.
  - Nature and quantity of chemical constituents needed for characterization and design of chemical processes.
  - Requires enumeration of all constituents.

Properties given implicitly through components and energy

Introduction and Motivation 2:2

- New Design Paradigm of Property Integration
  - Many design problems are not component dependent.
  - Driven by properties or functionality of the streams and not their chemical constituency.
  - Only requires tracking of properties NOT chemical species.

Process Design vs. Molecular Design

Given set of molecular groups to be screened (building blocks)

Molecular Design

Discrete Decisions
(e.g. type of compound)

Continuous Decisions
(e.g. operating conditions)

Optimize molecular structures to meet given set of property values (e.g. physical, chemical)

How to identify candidate components ????

How to identify desired property values ?????

Given set of components to be screened (e.g. raw materials, MSA's)

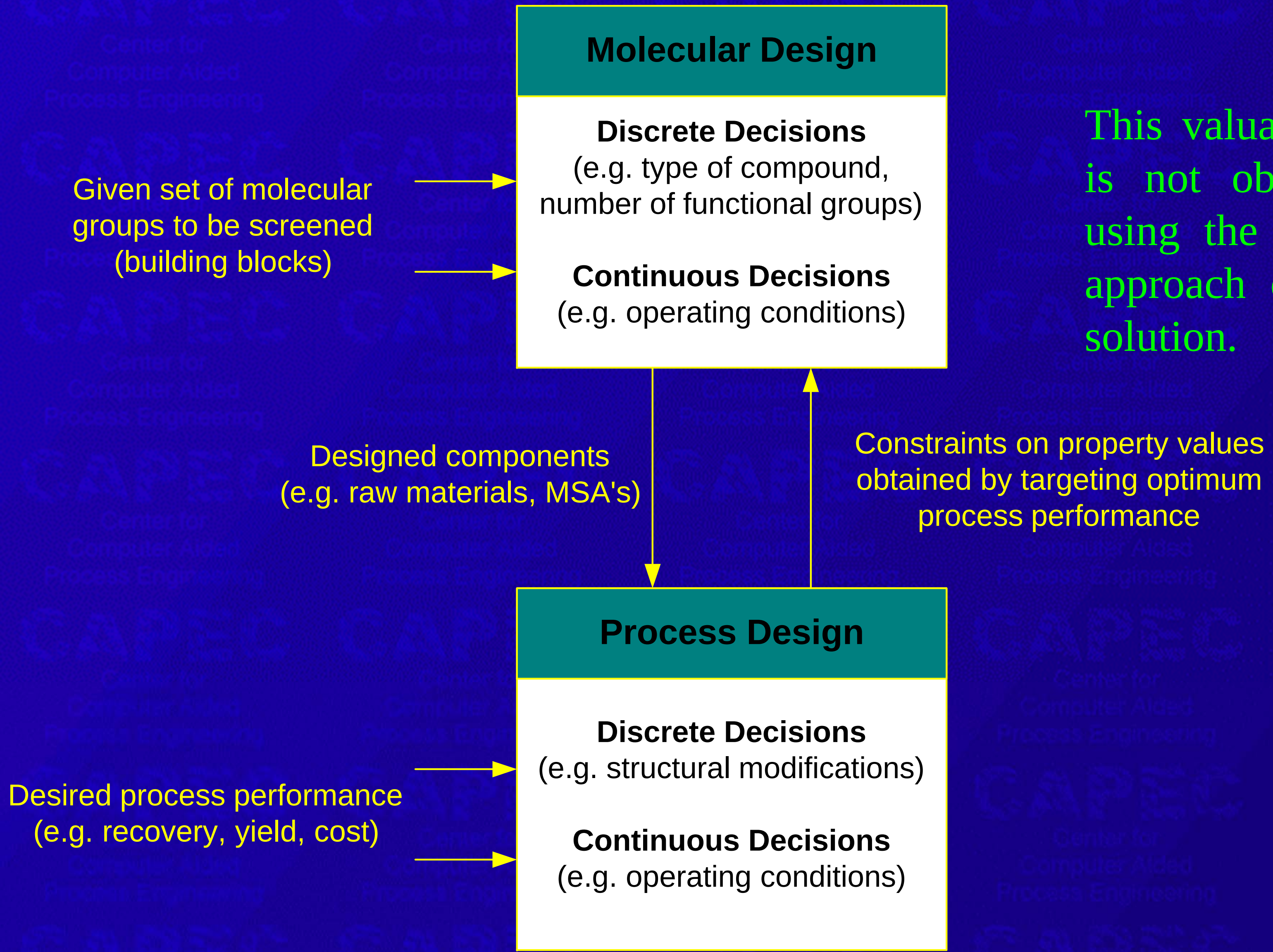
Process Design

Discrete Decisions
(e.g. structural modifications)

Continuous Decisions
(e.g. operating conditions)

Optimize process objectives to meet desired performance (e.g. recovery, yield, cost)

Simultaneous Process and Molecular Design



This valuable feedback is not obtained when using the conventional approach of sequential solution.

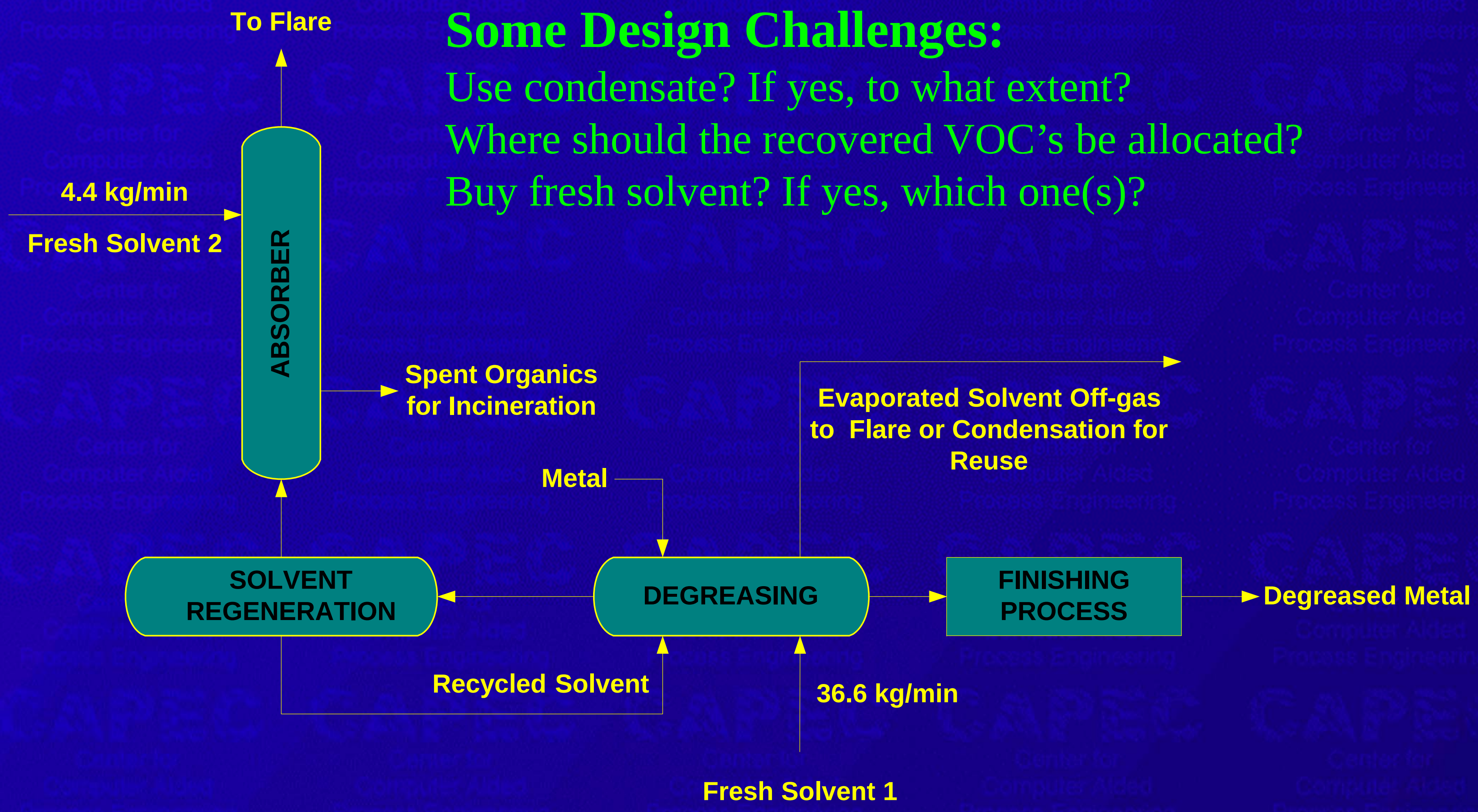
Motivating Example: VOC Recovery

Some Design Challenges:

Use condensate? If yes, to what extent?

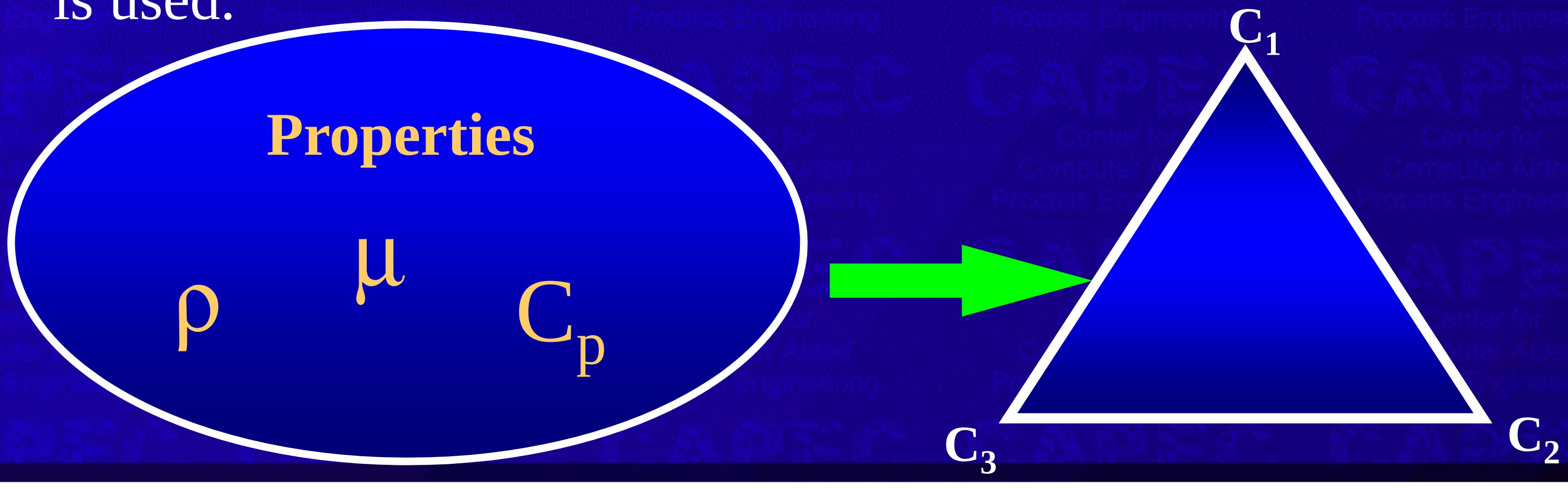
Where should the recovered VOC's be allocated?

Buy fresh solvent? If yes, which one(s)?



Concepts of Property Clustering 1:3

- Definition of Property-based Clusters
  - Surrogate properties which allow the tracking of unconserved raw properties. They are obtained by mapping raw properties into an equi-dimensional domain. The clusters are tailored to have the attractive features of intra-stream and inter-stream (mixing/splitting) conservation. For visualization purposes a maximum of three property clusters is used.



Concepts of Property Clustering 2:3

- Property Operat

$$\frac{1}{\bar{\rho}} = \sum_{s=1}^{N_s} \frac{x_s}{\rho_s} \quad \text{thus} \quad \psi(\bar{\rho}) = \frac{1}{\bar{\rho}} \quad , \quad \psi(\rho_s) = \frac{1}{\rho_s}$$

  – It is assumed ... be described by a

$$\psi_i(\bar{p}_i) = \sum_{s=1}^{N_s} x_s \cdot \psi_i(p_{i,s}) \quad \text{, where} \quad x_s = \frac{F_s}{\sum_{s=1}^{N_s} F_s}$$

  – By dividing by an arbitrary reference value the operators are made dimensionless. The summation of the dimensionless operators define the AUgmented Property index.

$$\Omega_{i,s} = \frac{\psi_i(p_{i,s})}{\psi_i^{ref}} \quad \text{and} \quad AUP_s = \sum_{i=1}^{N_C} \Omega_{i,s}$$

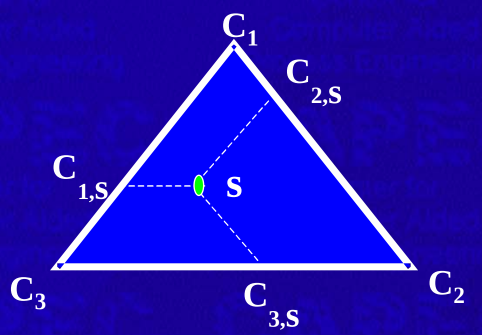
Concepts of Property Clustering

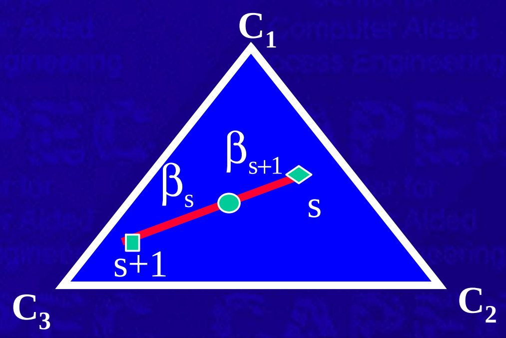
- Cluster Definition
  - Full derivation, Shelley & El-Halwagi (2000)

$$C_{i,s} = \frac{\Omega_{i,s}}{AUP_s}$$

  - Intra-stream and inter-stream conservation.

$$\sum_{i=1}^{N_C} C_{i,s} = 1 \qquad \bar{C}_i = \sum_{s=1}^{N_S} \beta_s C_{i,s}$$

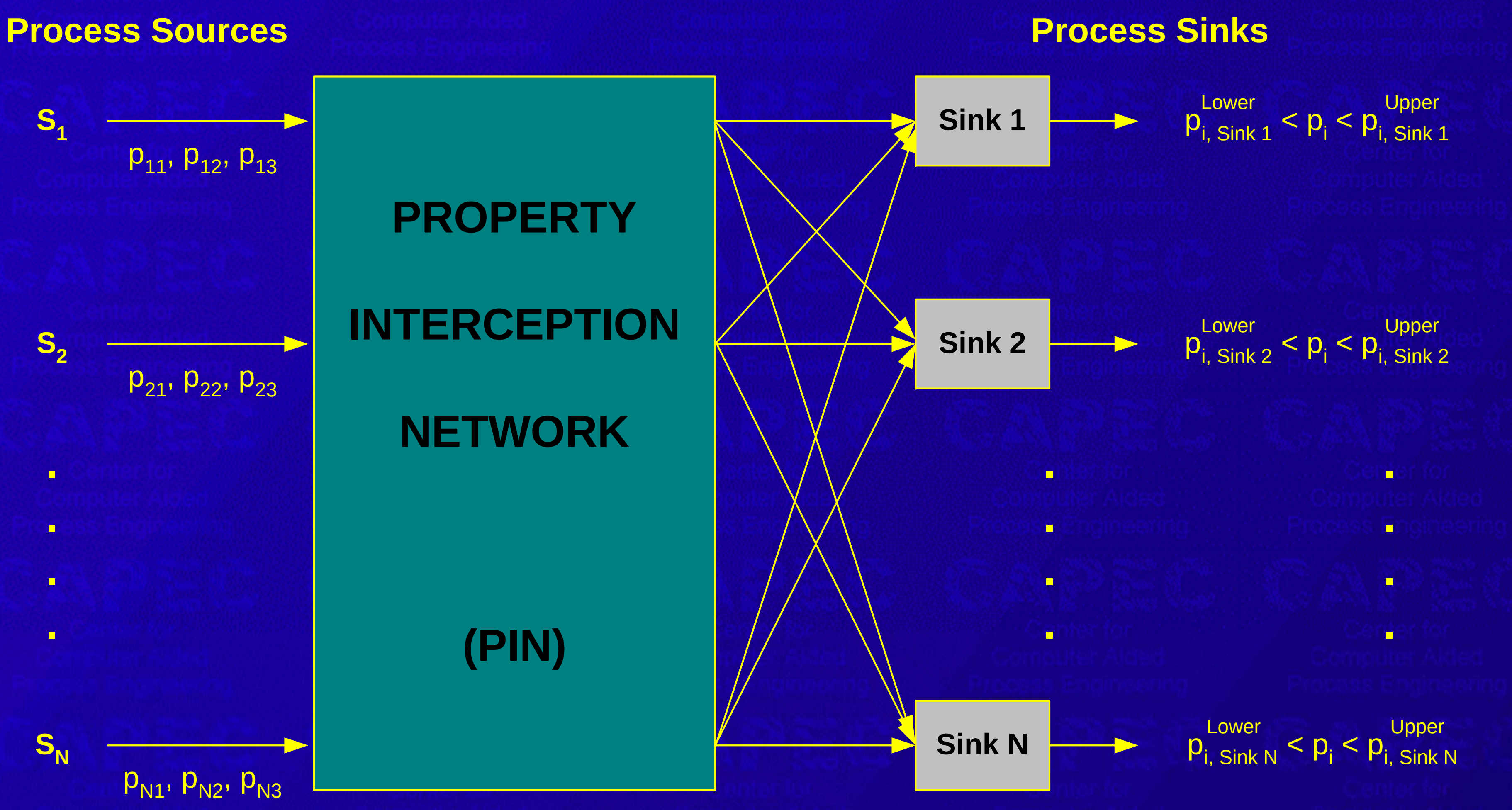




General Problem Statement

- Given
  - Process sources with known **properties**.
  - Process sinks with constraints on their feed **properties**.
  - Interception techniques, which can alter property values.
- Desired
  - Process objectives of optimum allocation, recovery, and interception.

General Problem Representation



Minimum Flow Solution Methodology

Given
Data for process sources
Process sink constraints
Performance objectives

Calculate and plot cluster values, flowrate and AUP for
Process sources
Process sinks

Identify all feasible mixing paths
Feasible mixing paths satisfy inter-stream conservation and sink constraints

Identify the minimum fresh flow cluster for each mixing path
Lever-arm approach for minimum arm β results in minimum fractional flow contribution x for the fresh process fluid

Calculate x_{fresh} for each minimum flow solution using

$$\beta_{fresh} = x_{fresh} \cdot \frac{AUP_{source}}{AUP_{sink}}$$

Calculate AUP_{fresh} for each minimum flow solution using

$$AUP_{Sink} = x_{fresh} \cdot AUP_{fresh} + x_{source} \cdot AUP_{source}$$

Convert the cluster solutions to property values using

$$C_{i,fresh} = \frac{\Omega_{i,fresh}}{AUP_{fresh}} \quad , \quad \Omega_{i,fresh} = \frac{\psi_i(p_{i,fresh})}{\psi_i^{ref}}$$

Identify and screen candidate fresh fluids using
Molecular design methods and/or databases
Environmental, health and/or safety concerns

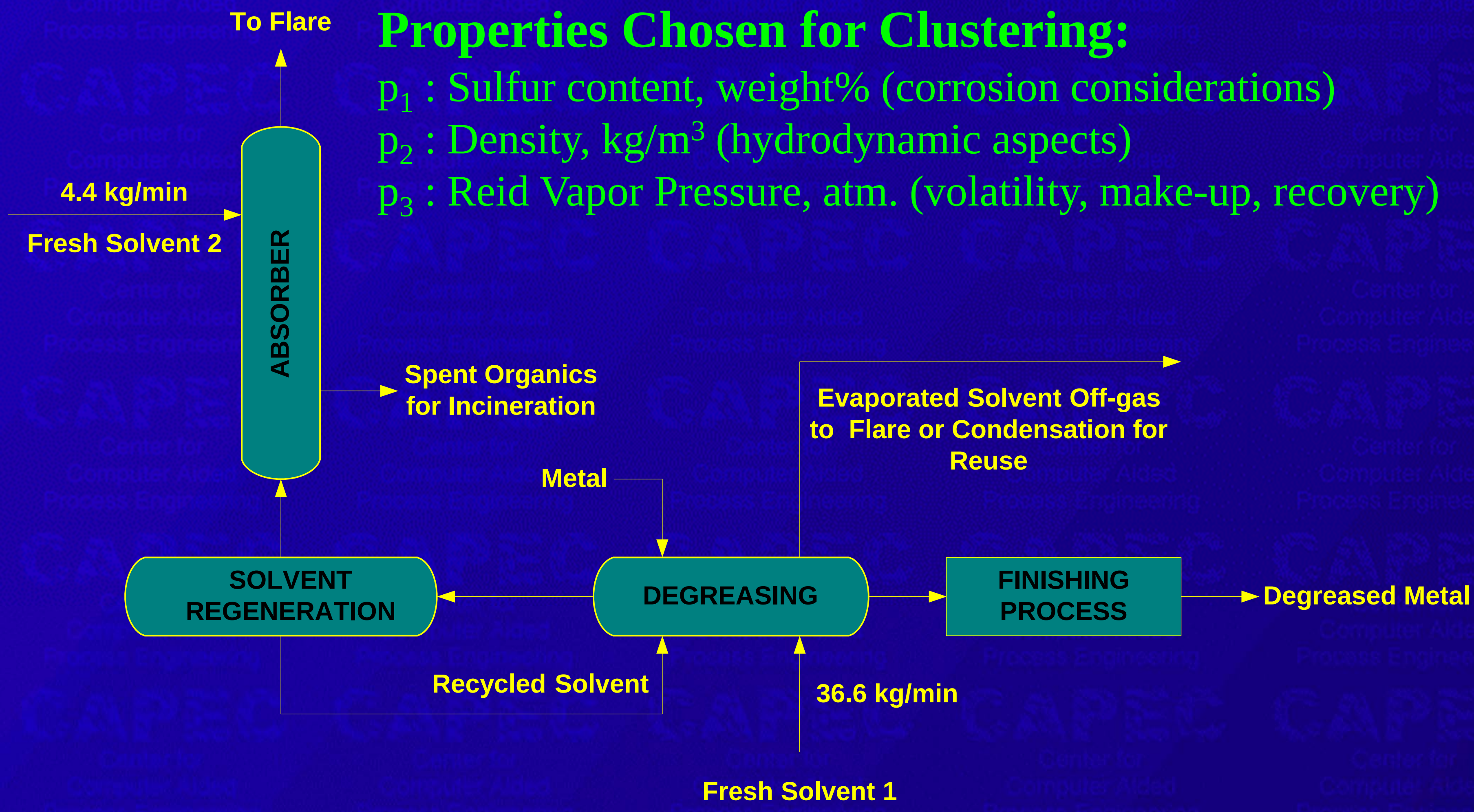
Case Study: VOC Recovery

Properties Chosen for Clustering:

p_1 : Sulfur content, weight% (corrosion considerations)

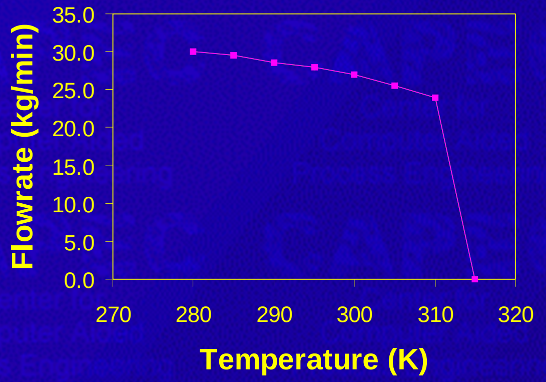
p_2 : Density, kg/m^3 (hydrodynamic aspects)

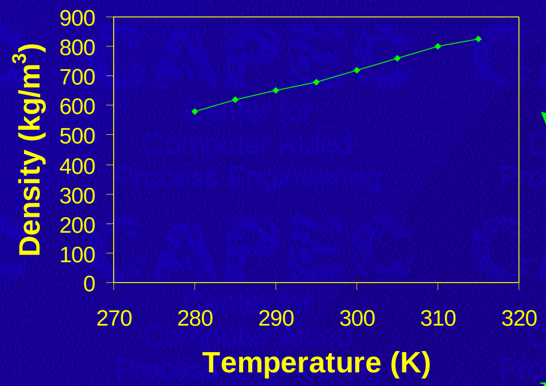
p_3 : Reid Vapor Pressure, atm. (volatility, make-up, recovery)



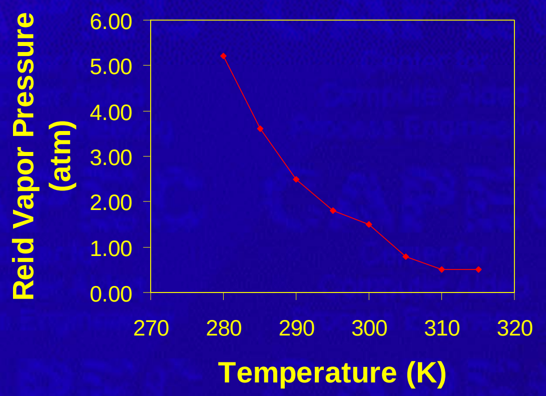
Case Study: VOC Recovery

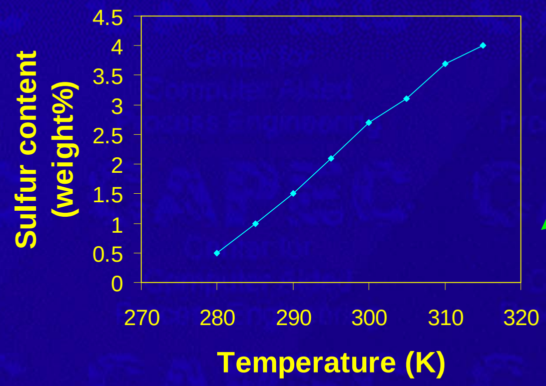
- Experimental Data
  - Property values are available for the off-gas condensate as a function of condensation temperature at 2 atm.





Near linearity is of no significance





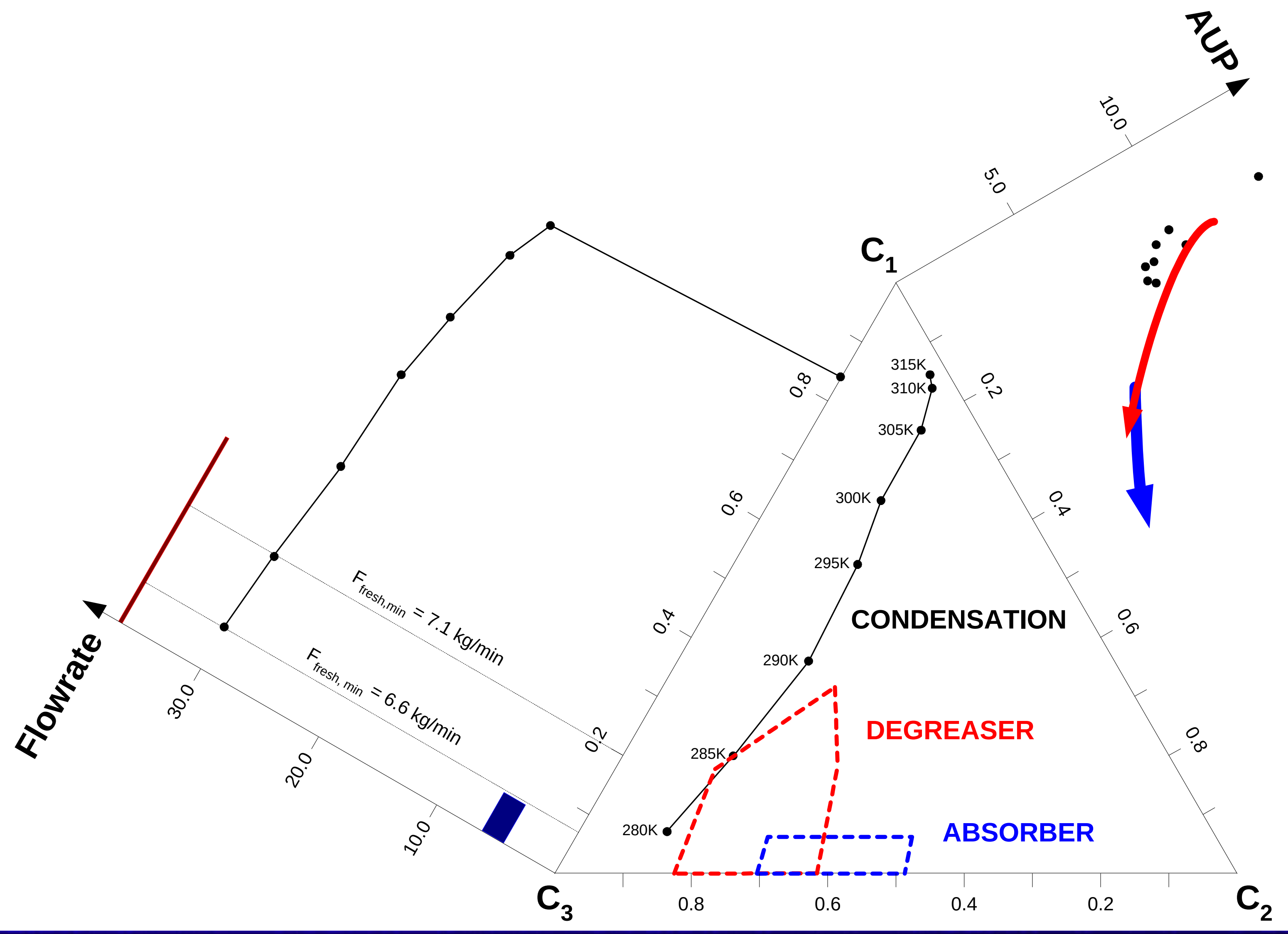
Case Study: VOC Recovery

- Sink Constraints

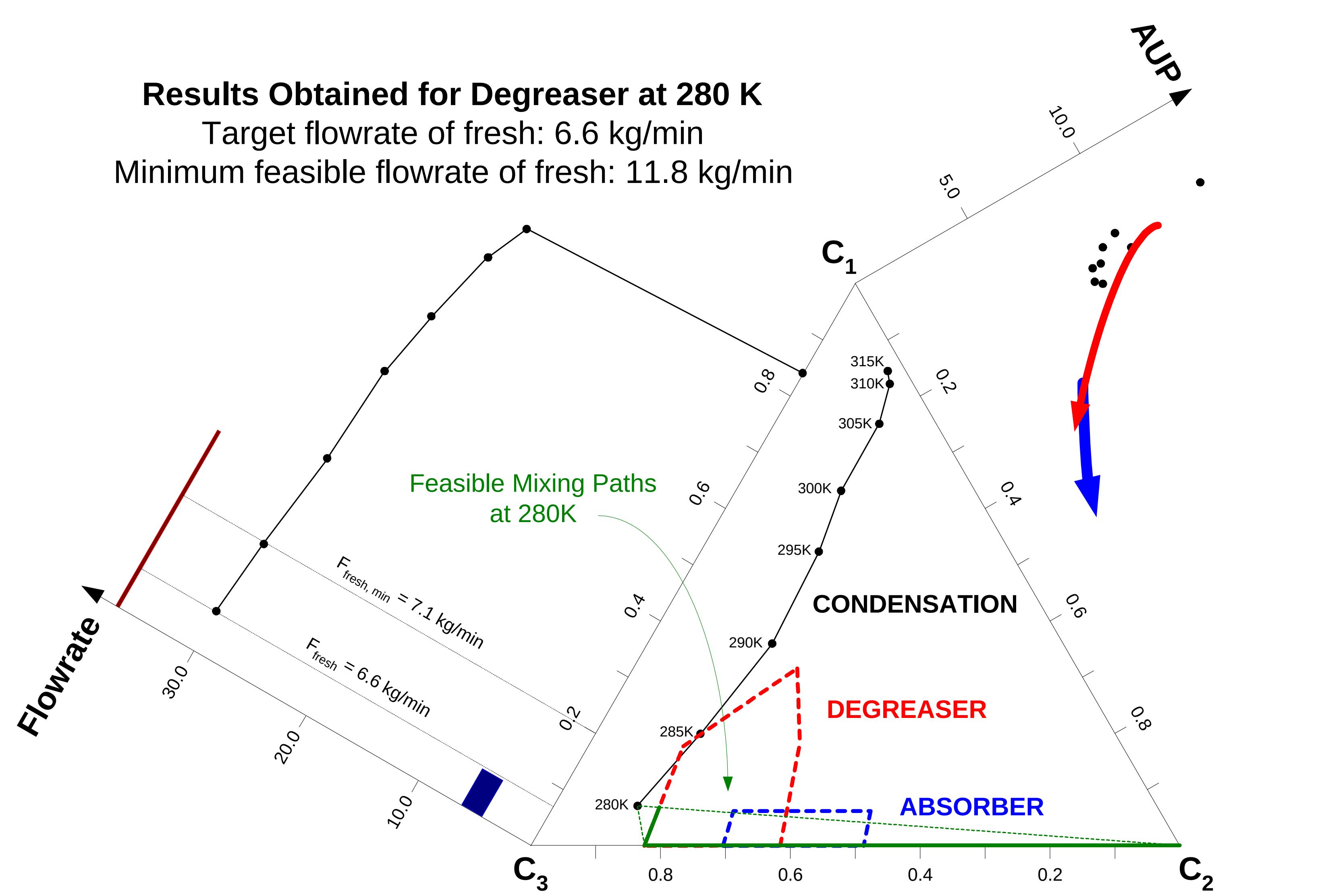
Sink	Absorber	Degreaser
Sulfur content (weight%)	$0.0 < p_1 < 0.1$	$0.0 < p_1 < 1.0$
Density (kg/m^3)	$530 < p_2 < 610$	$555 < p_2 < 615$
Reid Vapor Pressure (atm)	$1.5 < p_3 < 2.5$	$2.1 < p_3 < 4.0$
Flowrate (kg/min)	$4.4 < F < 6.2$	$36.6 < F < 36.8$

- Solution Objectives
  - Minimize flowrate of fresh organic solvent
  - Synthesize single component solvent for each unit

Case Study: VOC Recovery



Case Study: VOC Recovery 5:9

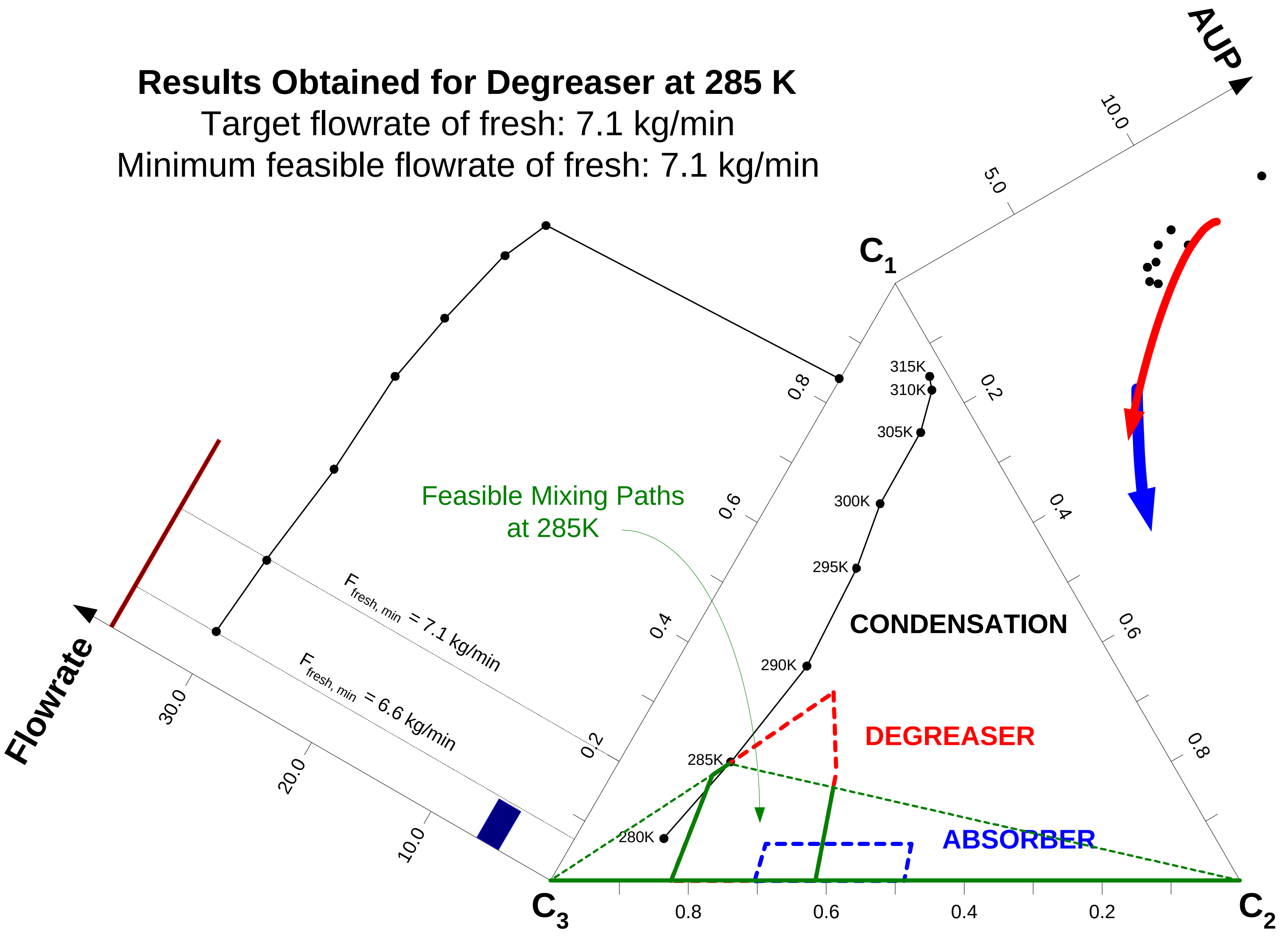


Case Study: VOC Recovery

Results Obtained for Degreaser at 285 K

Target flowrate of fresh: 7.1 kg/min

Minimum feasible flowrate of fresh: 7.1 kg/min



Case Study: VOC Recovery

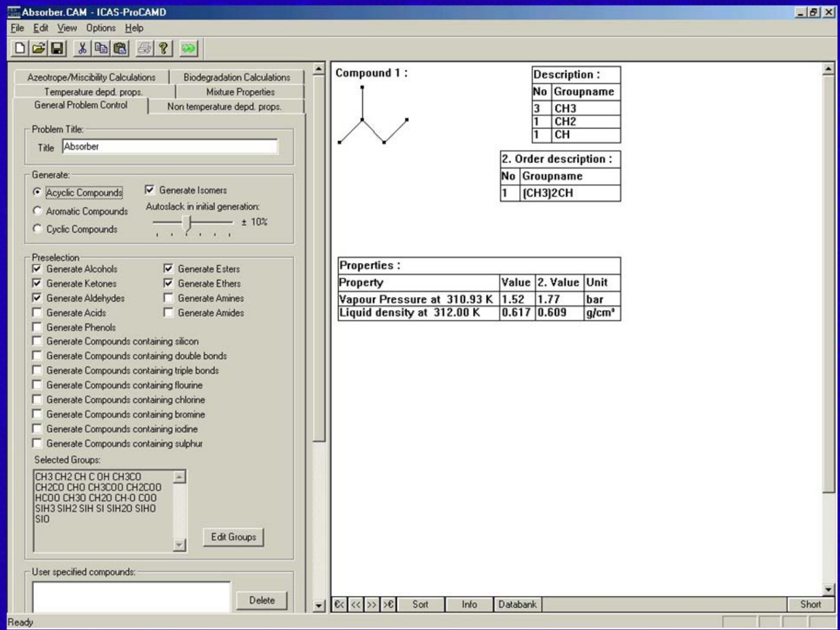
- Reducing the Solution Space of the CAMD Problems
  - No phenols, amines, amides or polyfunctional compounds.
  - No compounds containing double/triple bonds.
  - No compounds containing silicon, fluorine, chlorine, bromine, iodine and sulfur.

- Property Constraints

Sink	Absorber	Degreaser
Density (kg/m^3)	$530 < p_2 < 610$	$555 < p_2 < 615$
Reid Vapor Pressure (atm)	$1.5 < p_3 < 2.5$	$2.1 < p_3 < 4.0$

Case Study: VOC Recovery

- Solving CAMD Problem

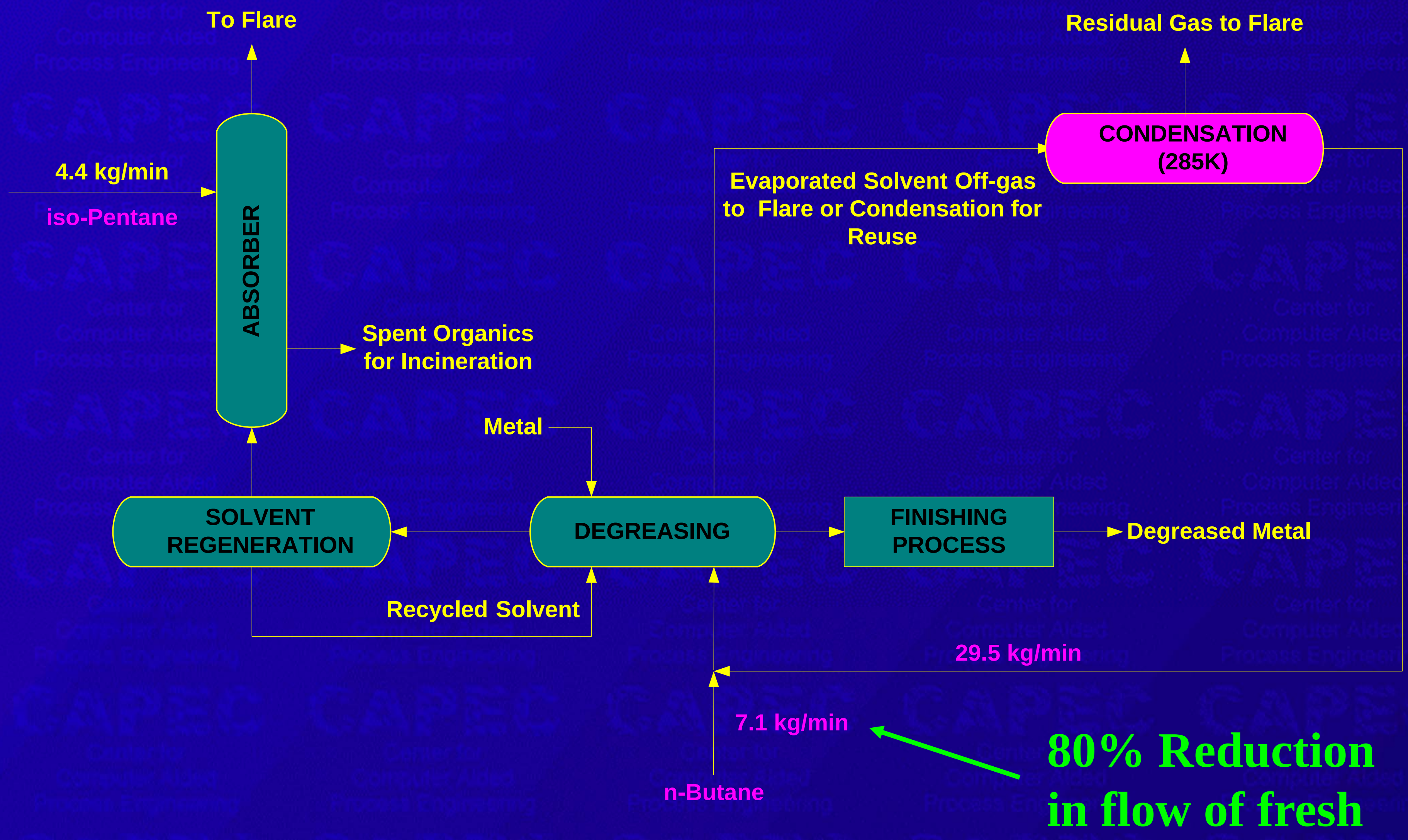


- **ProCAMD, CAPEC (2001)**
- **Algorithm, Harper (2000)**

Sink	Component
Absorber	iso-Pentane
Degreaser	n-Butane

Component	n-Butane	iso-Pentane
Density (kg/m^3)	614 @ 284K	609 @ 312K
Reid Vapor Pressure (atm)	3.80	1.75

Case Study: VOC Recovery



Conclusions

- Property Integration
  - New paradigm for integrated design of processes.
  - Property Interception Network provides property-based representation of the system.
  - Visualization provides insights to solving overall problem.
- Simultaneous Process and Molecular Design
  - Identifies property values corresponding to optimum process performance without committing to components.
  - Property values are then used for molecular design yielding the corresponding components.
  - Usefulness demonstrated by case study.

Further Information

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