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Resource Conservation and Waste Minimization for Property Networks

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Outline

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- **Introduction: why property-based design?**
- **Problem definition**
- **Optimality conditions**
- **Approach**
- **Case study**
- **Conclusions**

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Objective

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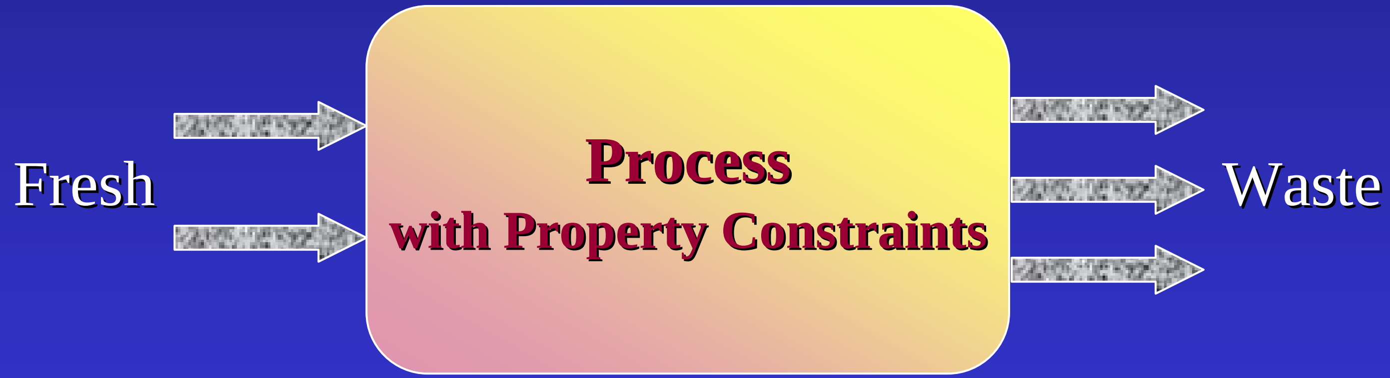
To develop an algebraic procedure to minimize fresh usage and waste discharge through recycle/reuse in a process with property-based constraints.



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Motivation

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- **Traditional recycle/reuse strategies in mass integration have been “chemo-centric,i.e. “component dependent”**
- **Many constraints on recycle are governed by properties and not only chemicals**
- **Process performance & product quality tied to properties**
- **Environmental performance is linked to properties**
  (e.g., pH, COD, BOD, color, toxicity, etc.)

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Need a new design paradigm:
based on properties and functionalities

Property Integration

Property-based holistic approach to the allocation and manipulation of streams and processing units, which is based on tracking, adjusting and matching functionalities throughout the process

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Previews Work on Property Integration

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- Shelley and El-Halwagi (2000)

  Componentless design and clustering concept

- Glasgow et al. (2002), Eden et al. (2003) and El-Halwagi et al. (2004)

  Cluster-based lever-arm optimization rules

- Qin et al. (2004)

  Algebraic techniques for property integration

- Gani and Pistikopoulos (2002) and Eden et al. (2004)

  Simultaneous process and product design

- Kazantzi et al. (2004)

  Incorporation of process modifications

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Objective of this Work

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For property-based direct recycle, can we identify rigorous targets for:

- Minimum fresh usage?
- Maximum recycle of process resources?
- Minimum discharge of waste?

Objectives:

- *Derivation of optimality criteria*
- *Non-iterative visualization and algebraic approaches*
- *A priori targets ahead of detailed design!*

Problem Statement

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Given is a process with:

- a number of process sources (streams), N_s
  Each source has a given flowrate, F_i and a given property p_i

- a number of process units, N_u, which accept streams with a given flowrate, G_j, and an inlet property p^{in}_j, that satisfies the following constraint:

$$p^{min}_j < p^{in}_j < p^{max}_j$$

Given is also:

- a fresh resource with known property value, p_{fr}

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Problem Representation

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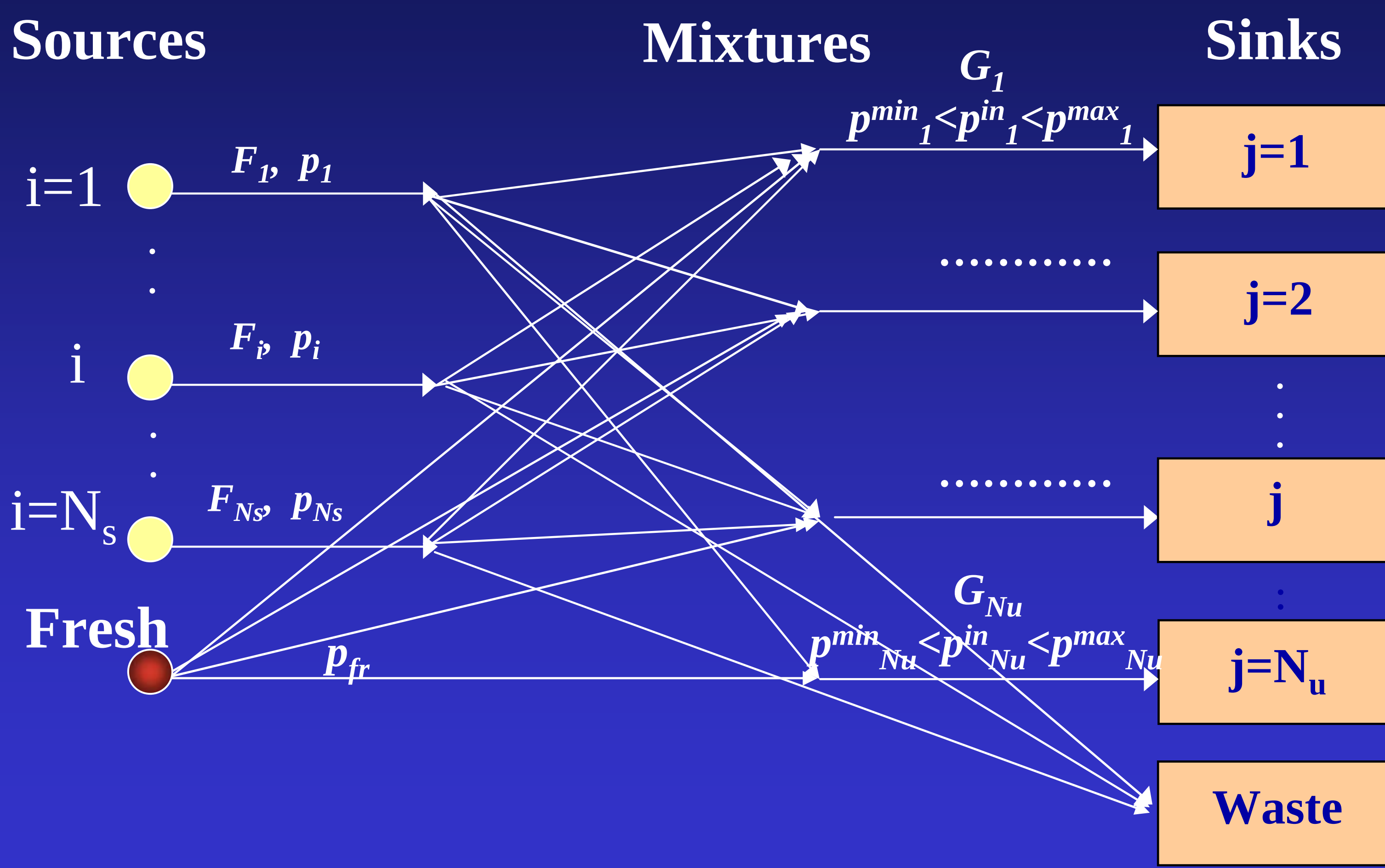

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Property Mixing Rule

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$$\psi_j^{in} = \sum_{i=1}^{Ns} x_{i,j}\psi_i + x_{fr,j}\psi_{fr}$$

ψ^{in}_j is the property-mixing operator for mixture entering sink j

For a stream i and fresh entering sink j:

$$x_{i,j} = f_{i,j}/G_j \quad \text{and} \quad x_{fr,j} = f_{fr,j}/G_j$$

$$G_j\psi_j^{in} = \sum_{i=1}^{N_s} f_{i,j}\psi_i + f_{fr,j}\psi_{fr}$$

where $G_j = \sum_i f_{i,j} + f_{fr,j}$

Optimization Formulation

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$$\min = \sum_{j=1}^{N_u} f_{fr,j}$$

subject to :

$$F_i = \sum_{j=1}^{N_u} f_{i,j} + f_{i,waste} \quad for\ i = 1,2,\ldots,N_s$$

$$G_j = f_{fr,j} + \sum_{i=1}^{N_s} f_{i,j} \quad for\ j = 1,2,\ \ldots,\ N_\mathrm{u}$$

$$G_j \psi_j^{in} = \sum_{i=1}^{N_s} f_{i,j}\psi_i + f_{fr,j}\psi_{fr} \quad for\ j = 1,2,\ \ldots,\ N_\mathrm{u}$$

$$p_j^{\min} \le p_j^{in} \le p_j^{\max} \quad \text{or} \quad \psi_j^{\min} \le \psi_j^{in} \le \psi_j^{\max} \quad for\ j = 1,2,\ \ldots,\ N_\mathrm{u}$$

$$f_{i,j} \ge 0 \quad for\ i = 1,2,\ldots,N_s \quad j = 1,2,\ \ldots,\ N_\mathrm{u}$$

$$f_{fr,j} \ge 0 \quad for\ j = 1,2,\ \ldots,\ N_\mathrm{u}$$

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Derivation of Optimality Conditions

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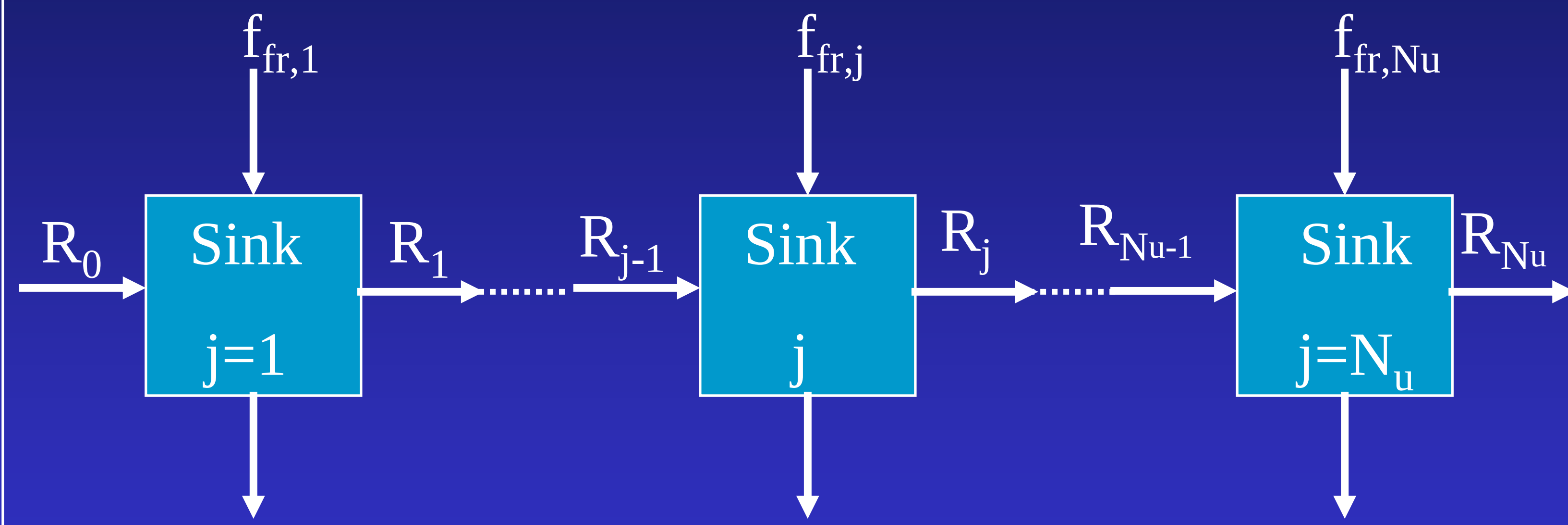
Parametric optimization through dynamic programming (Bellman's Principle)



$$R_j = \lfloor R_{1,j}, R_{2,j}, \ldots R_{i,j}, \ldots, R_{N_s,j} \rfloor$$

$$R_{i,j} = F_i - \sum_{j=1}^{j-1} f_{i,j} \quad for \;\; i = 1,\ 2, \ldots,\ N_s$$

Optimality Conditions

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Example: **Fresh has property operator less than process streams** $\psi_1 \geq \psi_{fr}$

Sink Optimality Conditions

When a fresh source is mixed with a process source, the inlet property operator to the sink should be assigned to its maximum feasible value, i.e. $\psi_{N_u}^{in} = \psi_{N_u}^{\max}$

Source Prioritization Optimality Conditions

$$f_{1,N_u}^{opt} = f_{1,N_u}^{\max} \qquad \psi_1 \leq \psi_2 \qquad R_{1,N_u} = F_1 - \sum_{j=1}^{N_u - 1} f_{1,j} \geq 0$$

Maximize use of process sources ranked in ascending order of their property operators

Use source and sink optimality conditions in graphical representation

Graphical Targeting Procedure

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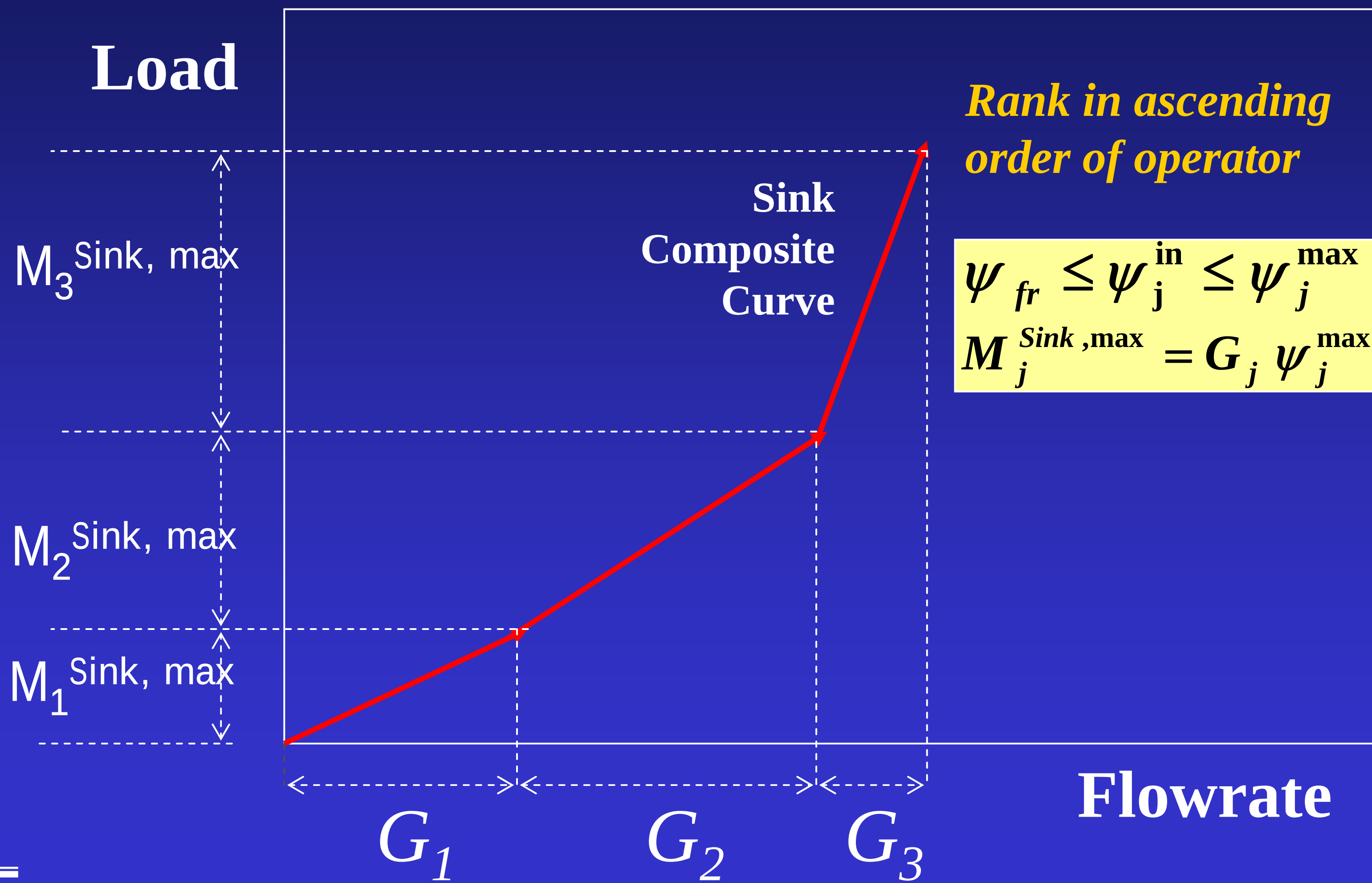
Sink Composite Diagram



Rank in ascending order of operator

$$\psi_{fr} \leq \psi_j^{\text{in}} \leq \psi_j^{\max}$$

$$M_j^{Sink,\max} = G_j \, \psi_j^{\max}$$

Graphical Targeting Procedure

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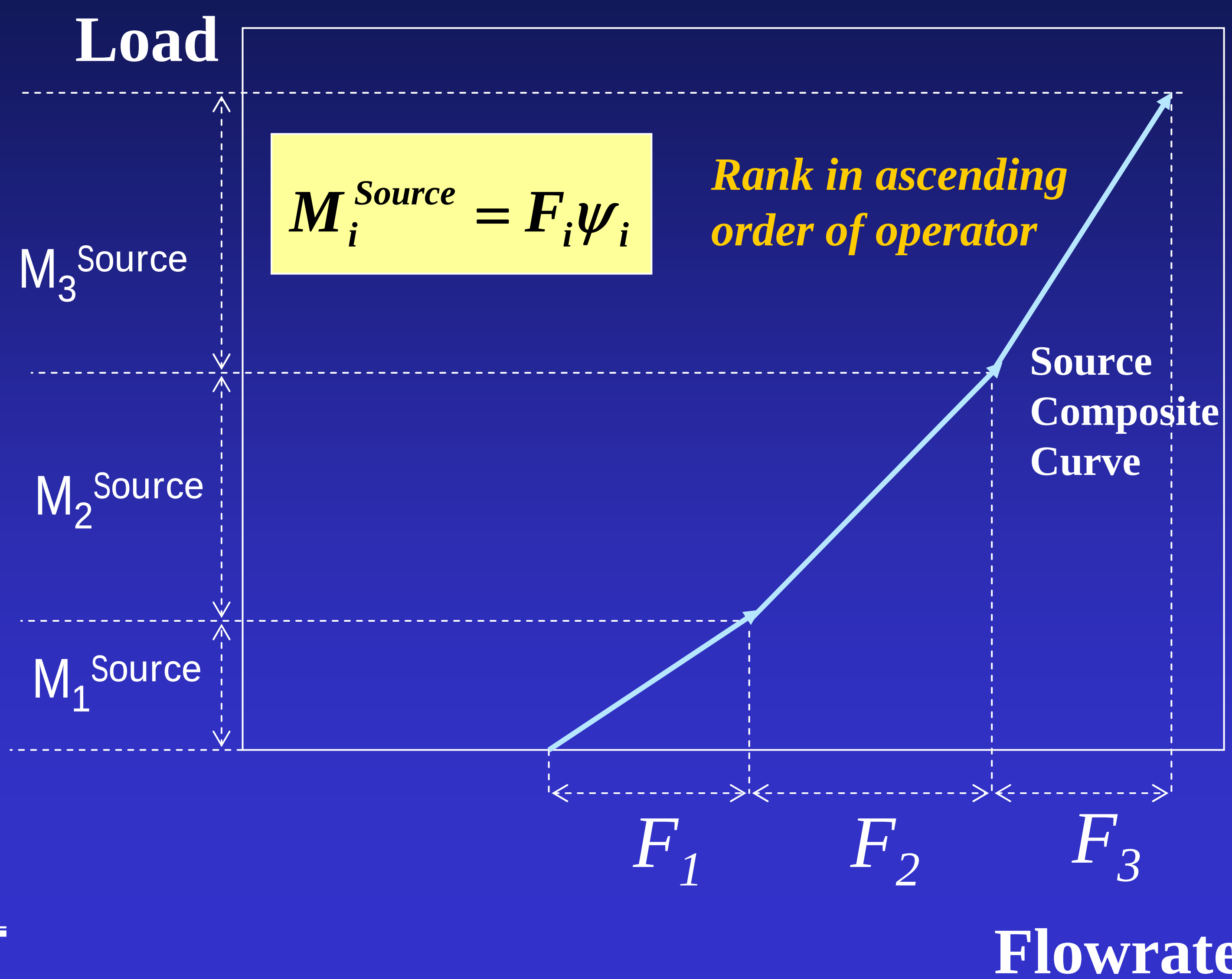
Source Composite Diagram



Property-based Material Recycle Pinch Diagram

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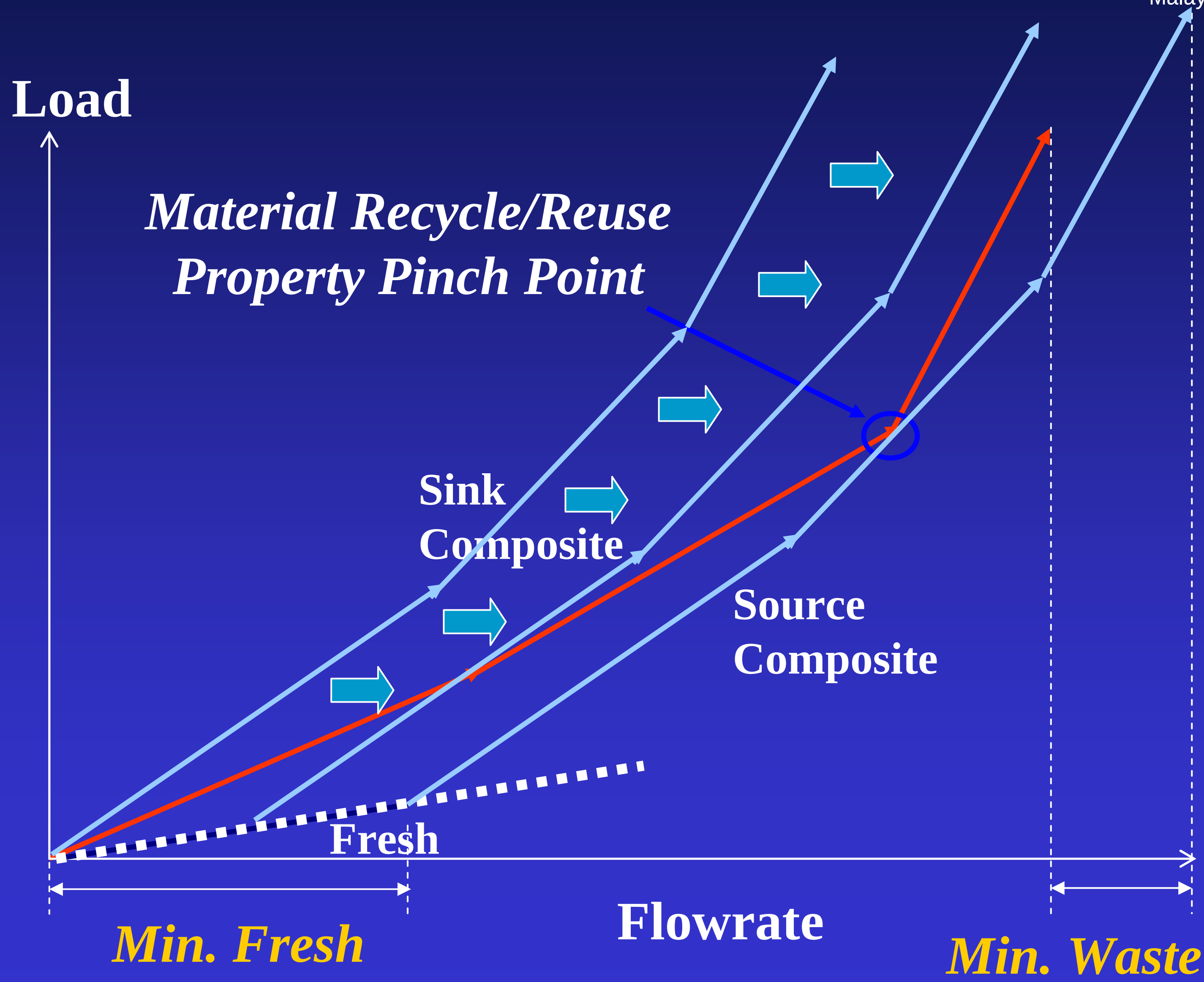

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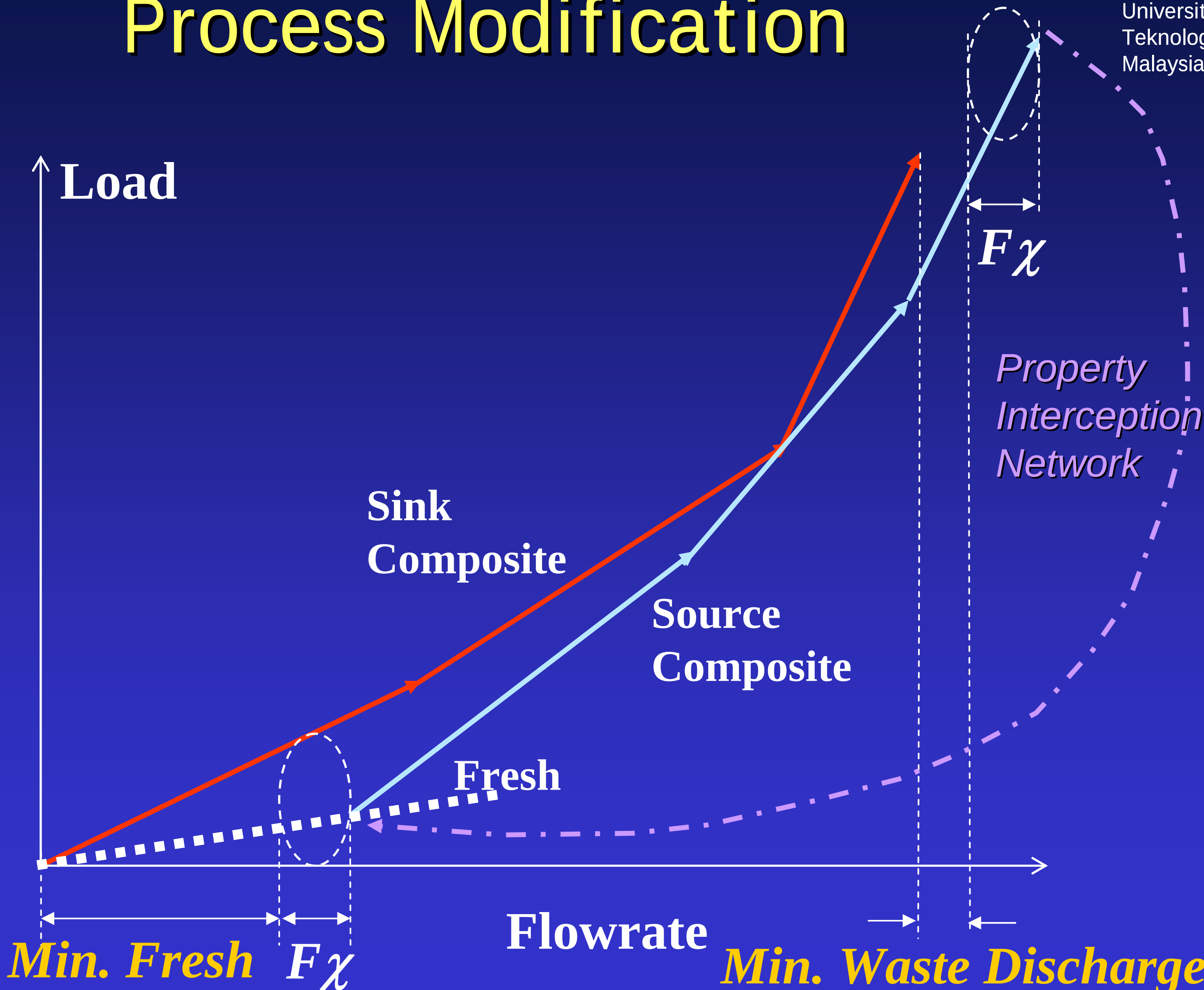
Implementing Process Modification



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Extension to Other Cases

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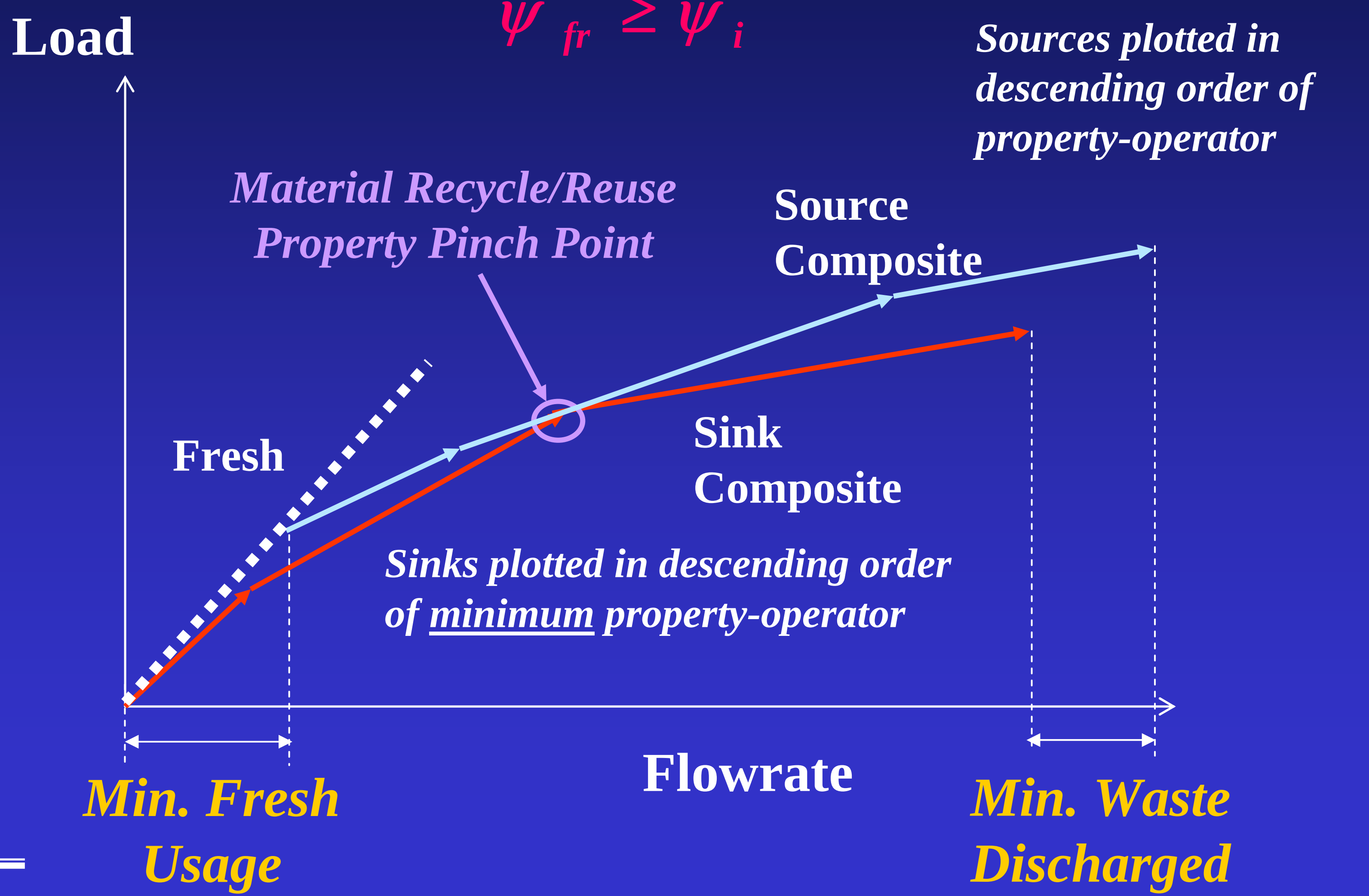
Fresh has property operator greater than process streams

$$\psi_{fr} \geq \psi_i$$



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Transformation to Algebraic Procedure

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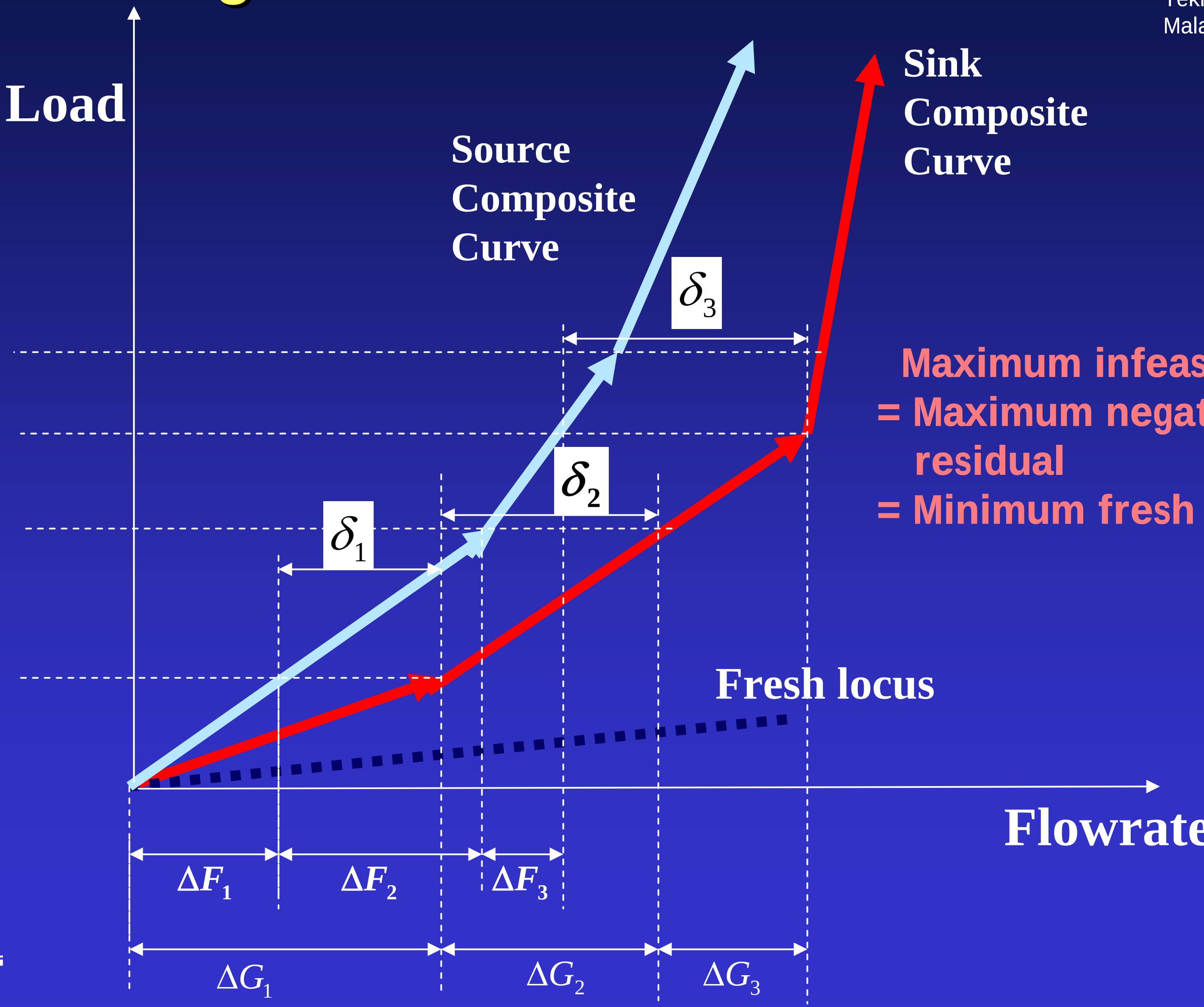

Maximum infeasibility
= Maximum negative residual
= Minimum fresh target

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Property-Load Interval Diagram

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Interval	Load	Interval Load (ΔM_k)	Sources	Source Flow per Interval (ΔF_k)	Sinks	Sink Flow Per Interval (ΔG_k)
1	M_1	ΔM_1	Source 1	$\frac{\Delta M_1}{\psi_{s,1} - \psi_{fr}}$	**Sink 1** $\psi_{u,1}^{max}$	$\frac{\Delta M_1}{\psi_{u,1}^{max} - \psi_{fr}}$
2	M_2	ΔM_2		$\frac{\Delta M_2}{\psi_{s,1} - \psi_{fr}}$	**Sink 2** $\psi_{u,2}^{max}$	$\frac{\Delta M_2}{\psi_{u,2}^{max} - \psi_{fr}}$
			Source 2	$\frac{\Delta M_3}{\psi_{s,2} - \psi_{fr}}$		$\frac{\Delta M_3}{\psi_{u,2}^{max} - \psi_{fr}}$
	M_{k-1}					
k	M_k	ΔM_k	Source 3	$\frac{\Delta M_k}{\psi_{\text{s in interval k}} - \psi_{fr}}$	**Sink 3**	$\frac{\Delta M_k}{\psi_{\text{u in interval k}}^{max} - \psi_{fr}}$
	M_{n-1}		Source N_s			
n	M_n	ΔM_n		$\frac{\Delta M_n}{\psi_{\text{s in interval n}} - \psi_{fr}}$	**Sink N_u**	$\frac{\Delta M_n}{\psi_{\text{u in interval n}}^{max} - \psi_{fr}}$

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Cascade Diagram

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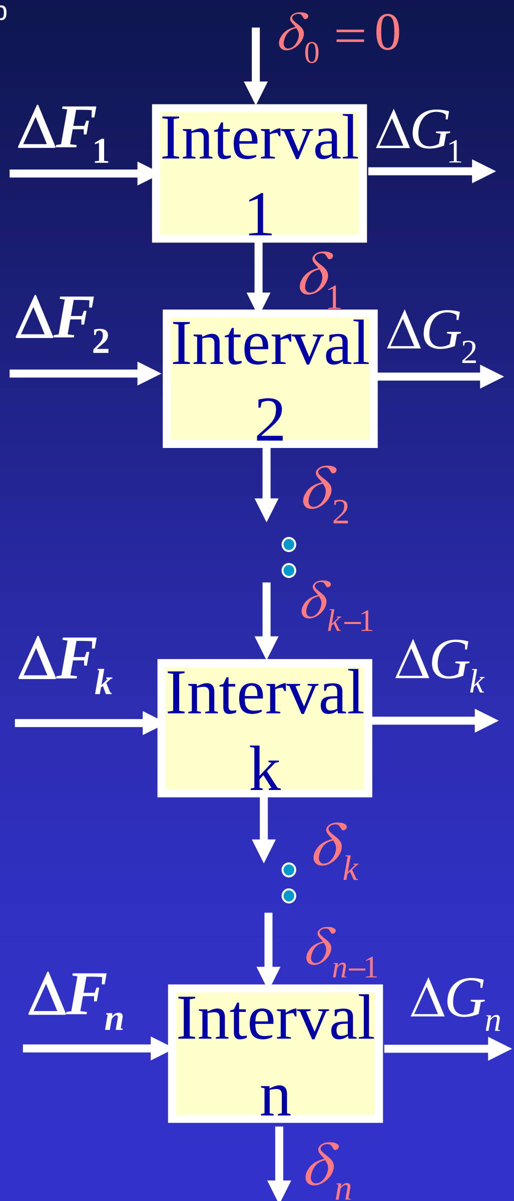

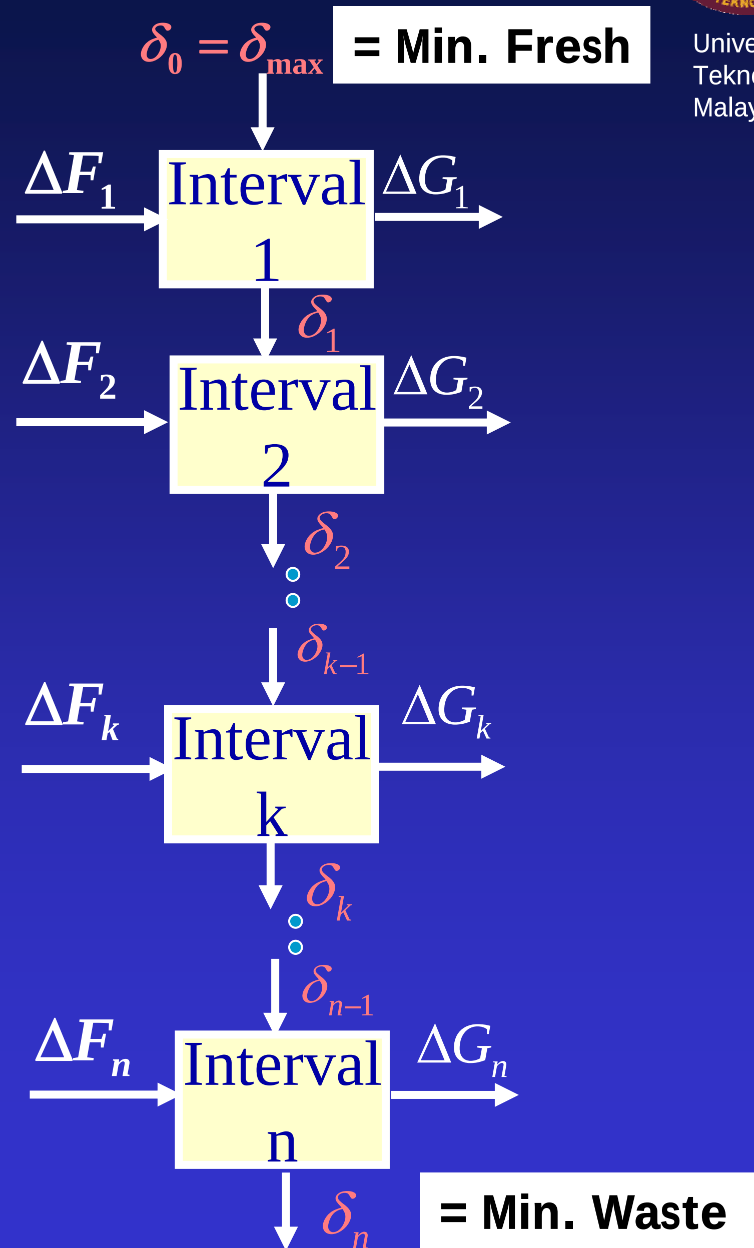

Case Study

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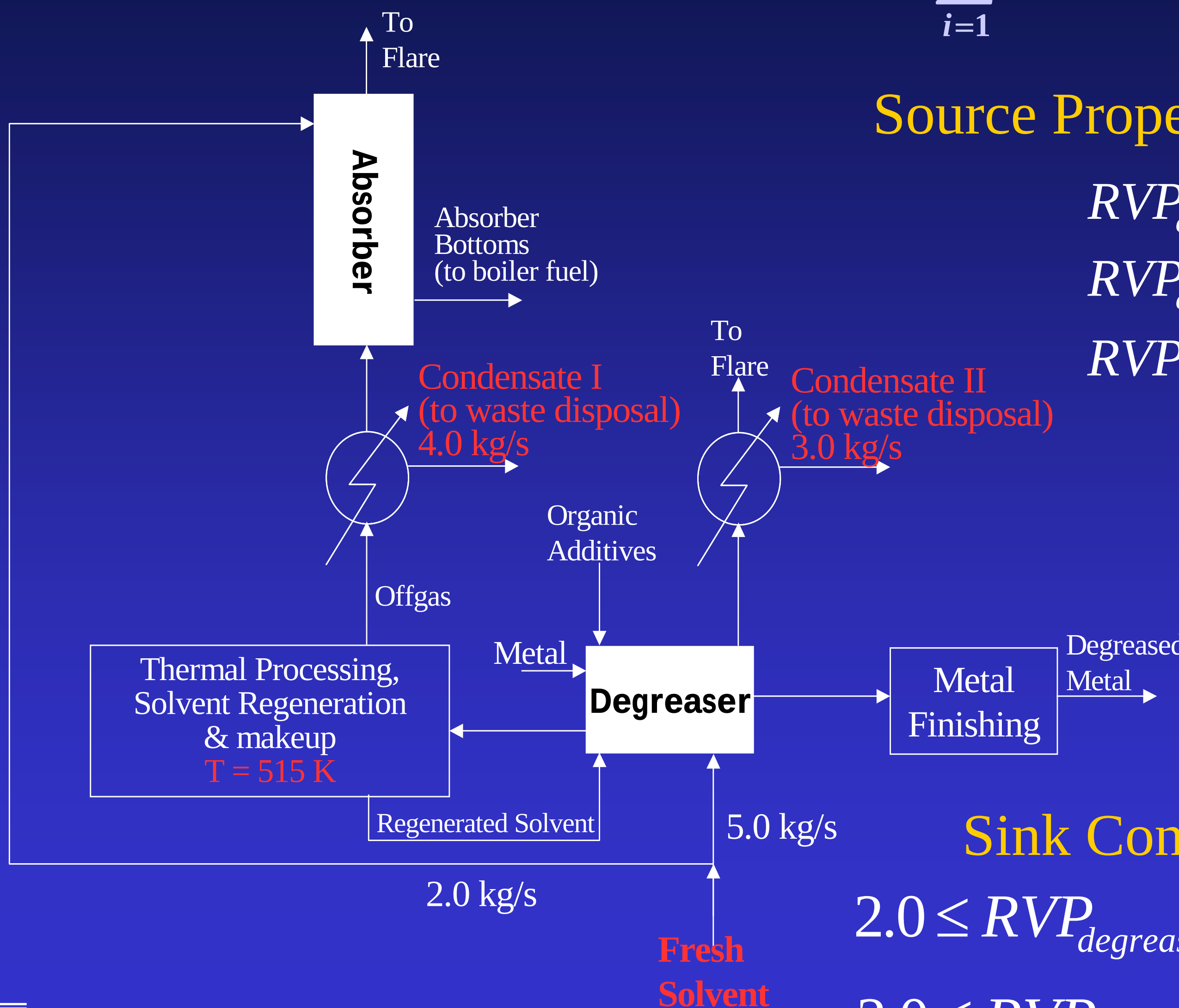
Property Mixing Rule

$$\overline{RVP}^{1.44} = \sum_{i=1}^{N_s} x_i RVP_i^{1.44}$$



Source Property Values

$$RVP_{cond.II} = 2.5 atm$$

$$RVP_{cond.I} = 6.0 atm$$

$$RVP_{fresh} = 2.0 atm$$

Sink Constraints

$$2.0 \le RVP_{degreaser}(atm) \le 3.0$$

$$2.0 \le RVP_{absorber}(atm) \le 4.0$$

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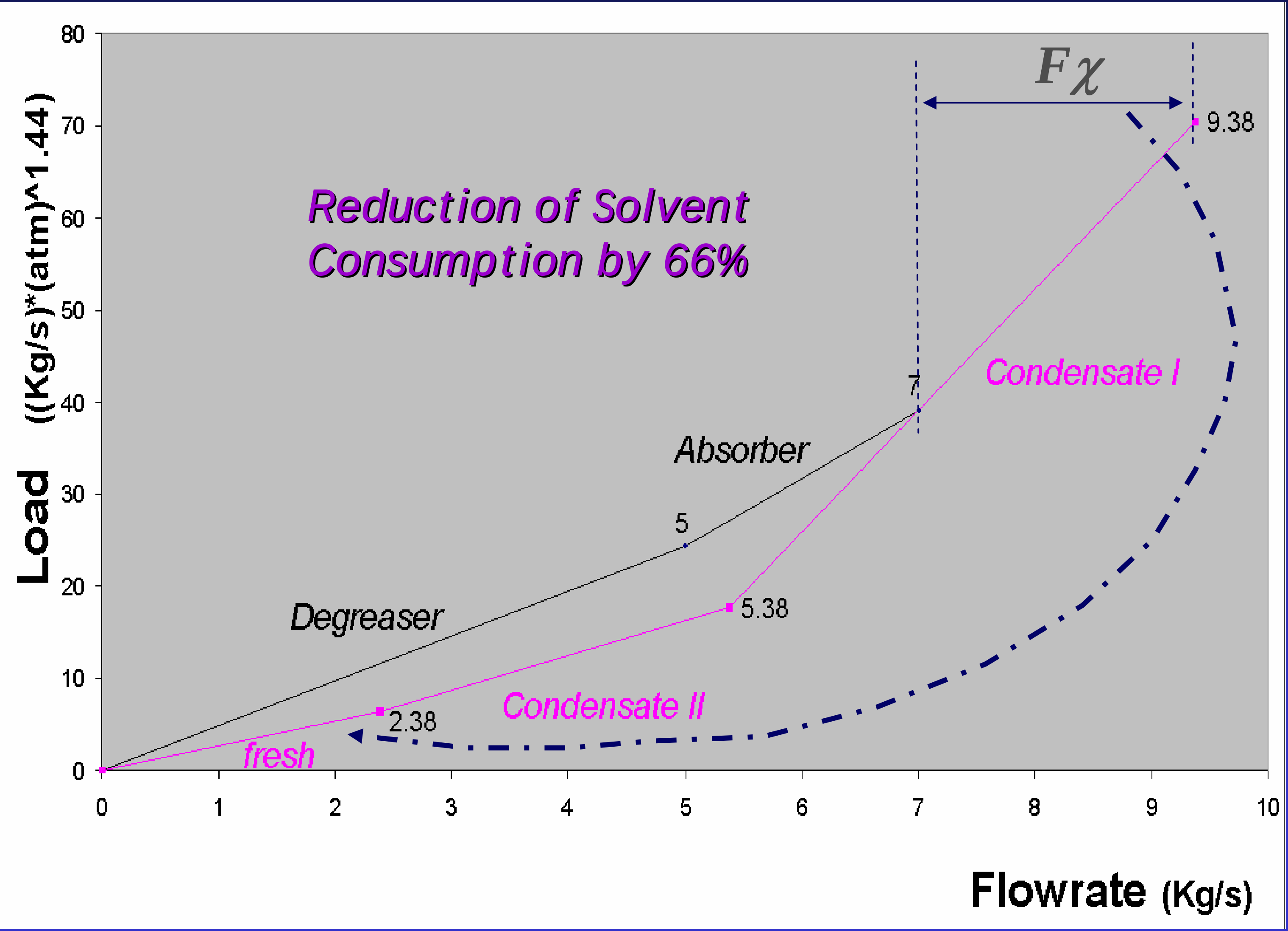

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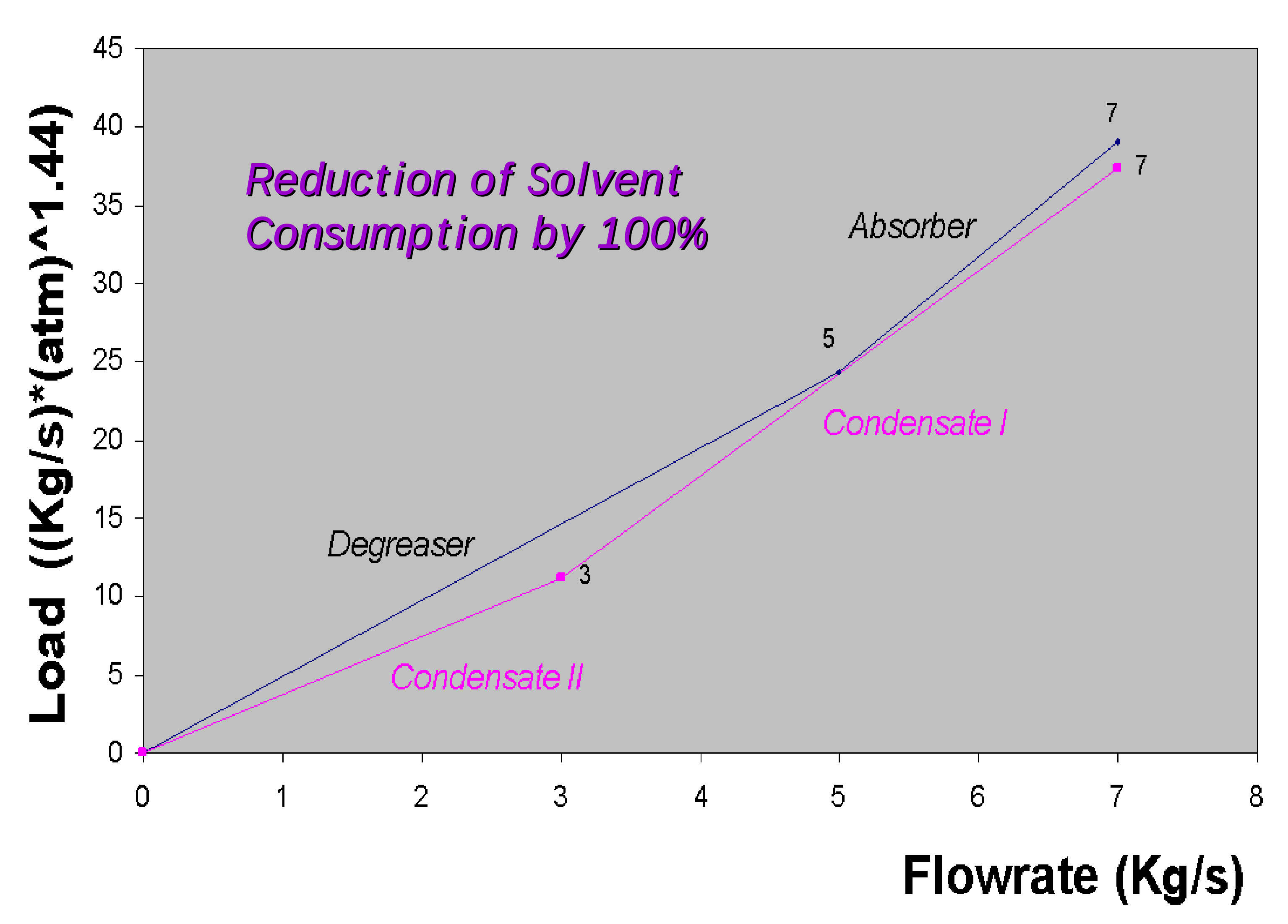

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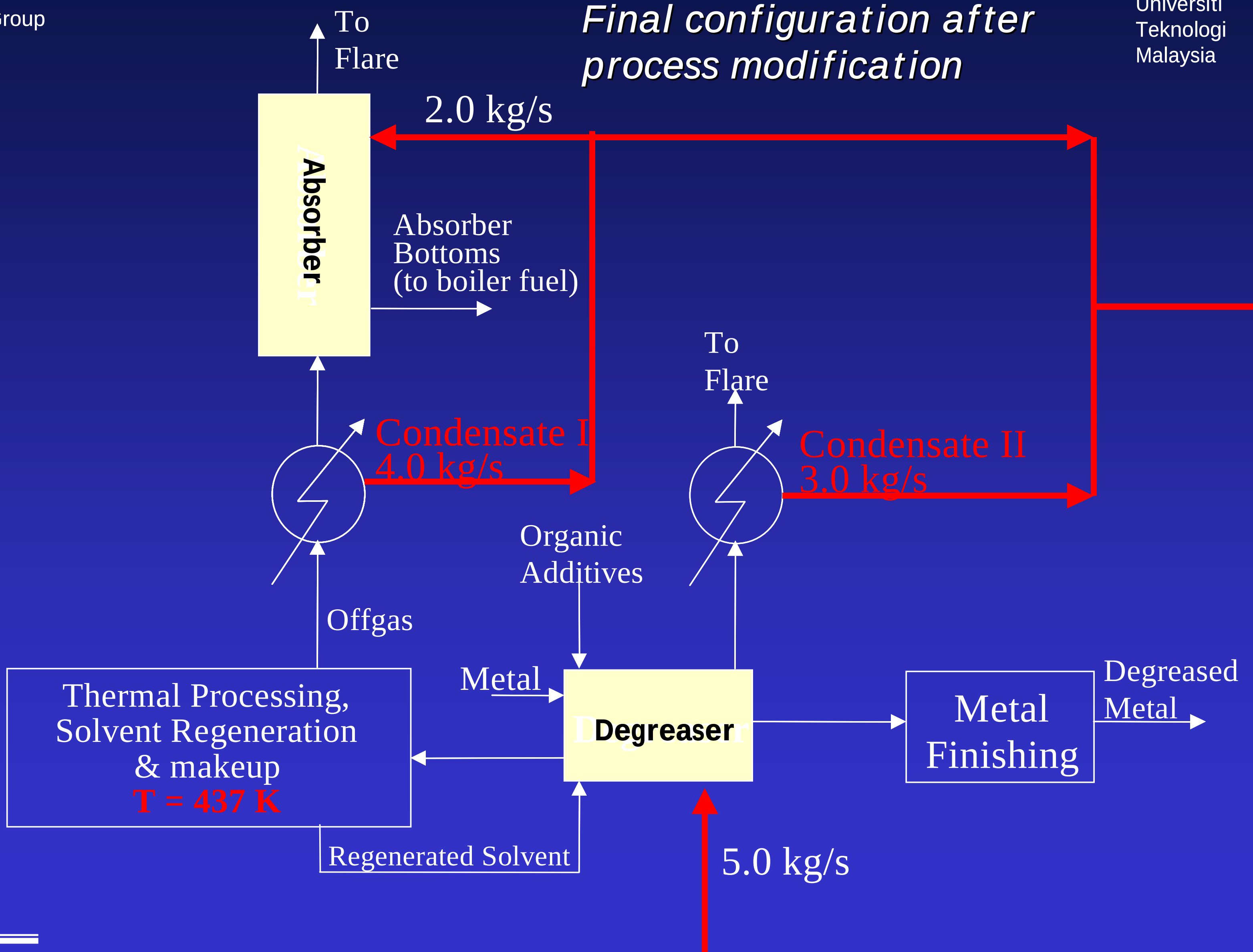
Final configuration after process modification



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Conclusions

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- New property-based pinch analysis and visualization technique for maximum integration of process sources and units
- Optimality conditions derived using dynamic programming principles
- Graphical-based insights for property interception strategies and enhanced reuse
- Novel, non-iterative and systematic algebraic procedure for identifying rigorous targets in a process with property constraints

Future Work

- Investigate New Approach for Multiple Properties
- Optimize Process Performance and Properties
- Integrate Process and Material Synthesis Combining Process Integration and Optimization Principles with Material Design Strategies