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Resource Conservation and Waste Minimization for Property Networks

**Vasiliki Kazantzi, Abdulaziz M. Almutlaq and
Mahmoud M. El-Halwagi**
*Department of Chemical Engineering
Texas A&M University*

Dominic C.Y. Foo and Zainuddin A. Manan
*Chemical Engineering Pilot Plant (CEPP)
Universiti Teknologi Malaysia*



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Outline



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





Objective



Objective

Motivation

Problem

Optimality

Procedure

Case study

Conclusions

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





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.)



Motivation



Objective

*Need a new design paradigm:
based on properties and functionalities*

Motivation

Problem

Property Integration

Optimality

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

Procedure

Case study

Conclusions



Previews Work on Property Integration



Objective

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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



Objective of this Work



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Objective

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

Motivation

Problem

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

Optimality

Objectives:

Procedure

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

Case study

Conclusions



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_j^{in} , that satisfies the following constraint:

$$p_j^{min} < p_j^{in} < p_j^{max}$$

Given is also:

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



Problem Representation



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Objective

Motivation

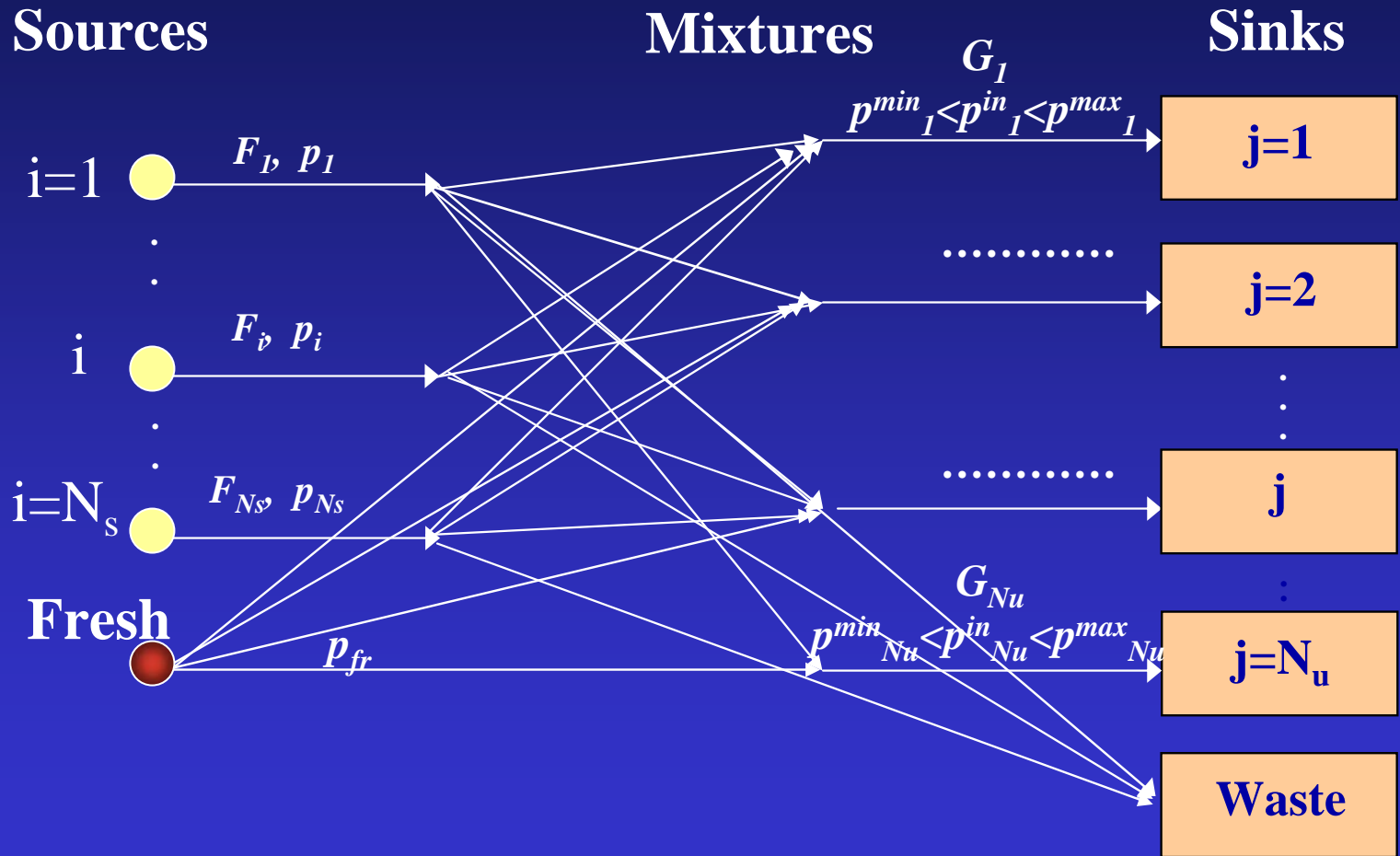
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Property Mixing Rule



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

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

For a stream i and fresh entering sink j :

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

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

where

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



Optimization Formulation



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Objective

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

Motivation

subject to :

Problem

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

Optimality

$$G_j = f_{fr,j} + \sum_{i=1}^{N_s} f_{i,j} \quad \text{for } j = 1, 2, \dots, N_u$$

Procedure

$$G_j \psi_j^{in} = \sum_{i=1}^{N_s} f_{i,j} \psi_i + f_{fr,j} \psi_{fr} \quad \text{for } j = 1, 2, \dots, N_u$$

Case study

$$p_j^{\min} \leq p_j^{in} \leq p_j^{\max} \quad \text{or} \quad \psi_j^{\min} \leq \psi_j^{in} \leq \psi_j^{\max} \quad \text{for } j = 1, 2, \dots, N_u$$

$$f_{i,j} \geq 0 \quad \text{for } i = 1, 2, \dots, N_s \quad j = 1, 2, \dots, N_u$$

Conclusions

$$f_{fr,j} \geq 0 \quad \text{for } j = 1, 2, \dots, N_u$$



Derivation of Optimality Conditions



Objective

Motivation

Problem

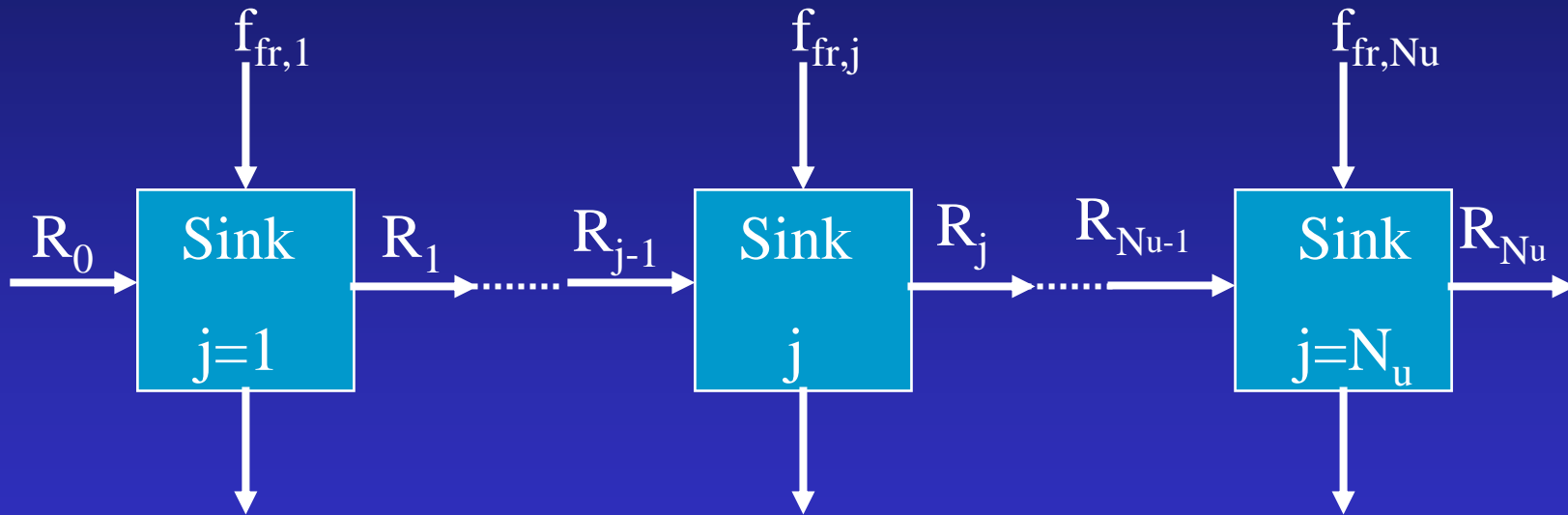
Optimality

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*Parametric optimization through dynamic programming
(Bellman's Principle)*



$$R_j = [R_{1,j}, R_{2,j}, \dots, R_{i,j}, \dots, R_{N_s,j}]$$

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



Optimality Conditions



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Objective

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

Motivation

Sink Optimality Conditions

Problem

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. $\psi_{N_u}^{in} = \psi_{N_u}^{max}$

Optimality

Source Prioritization Optimality Conditions

Procedure

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

Case study

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

Conclusions

Use source and sink optimality conditions in graphical representation



Graphical Targeting Procedure



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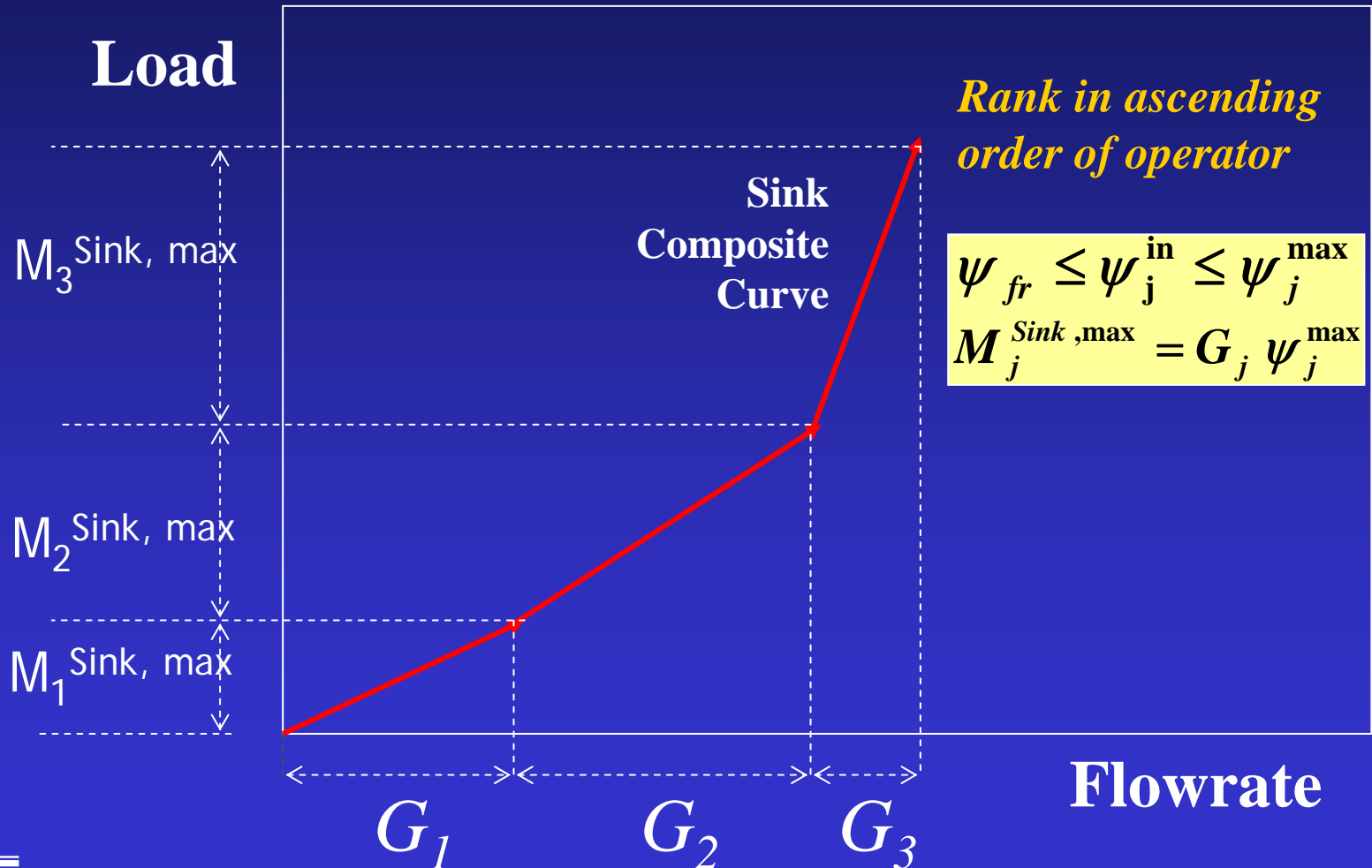
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Sink Composite Diagram





Graphical Targeting Procedure



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Source Composite Diagram

Objective

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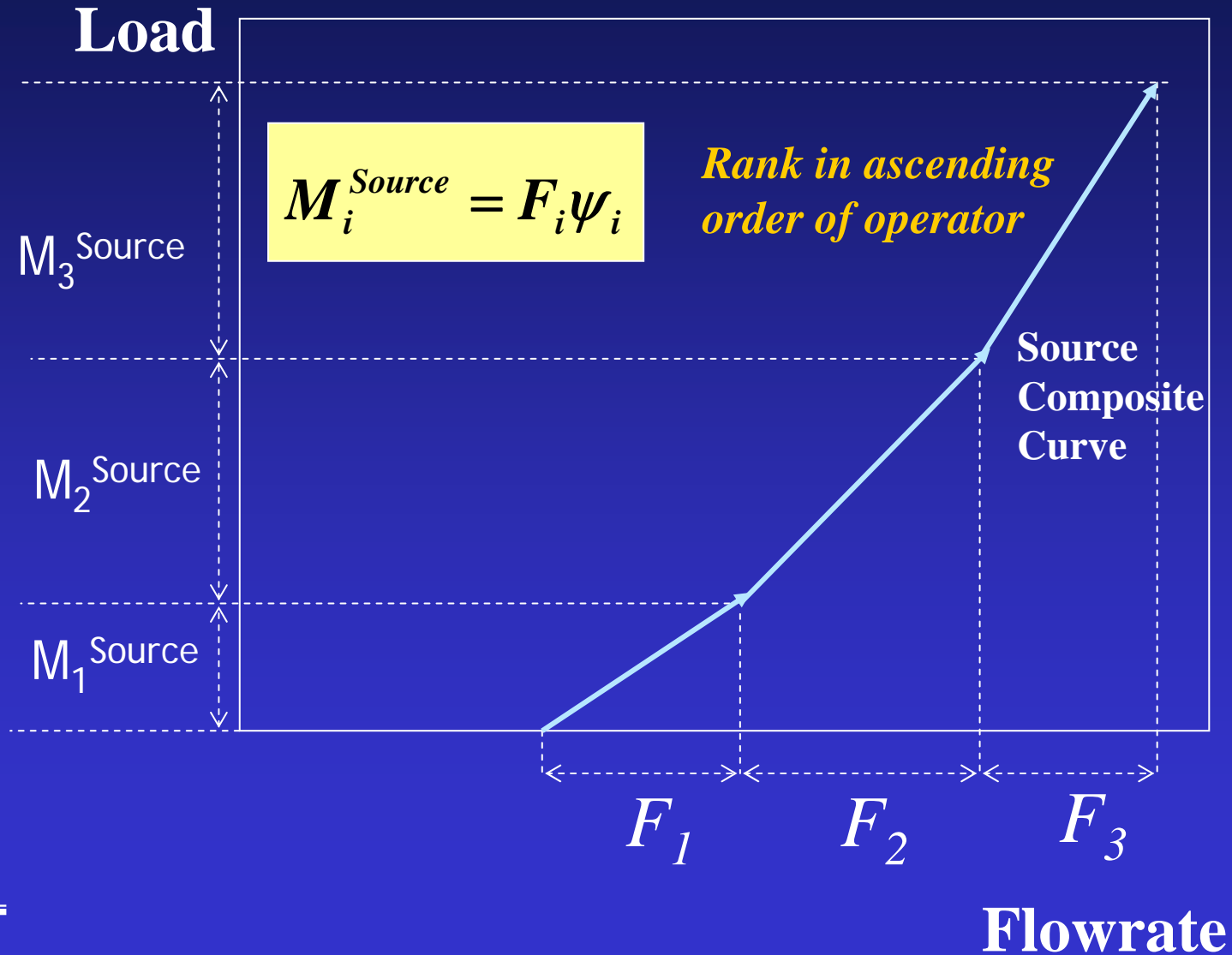
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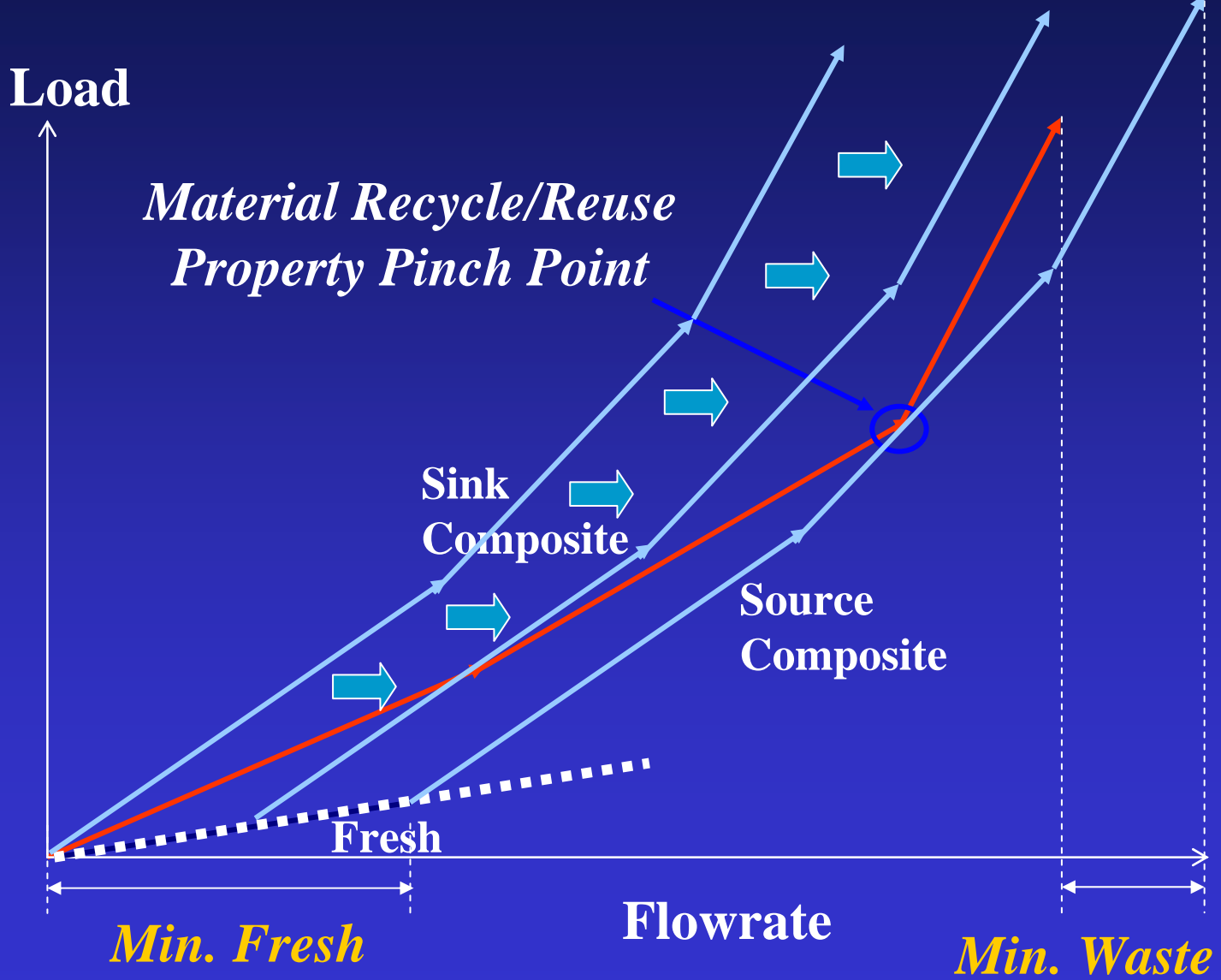
Property-based Material Recycle Pinch Diagram



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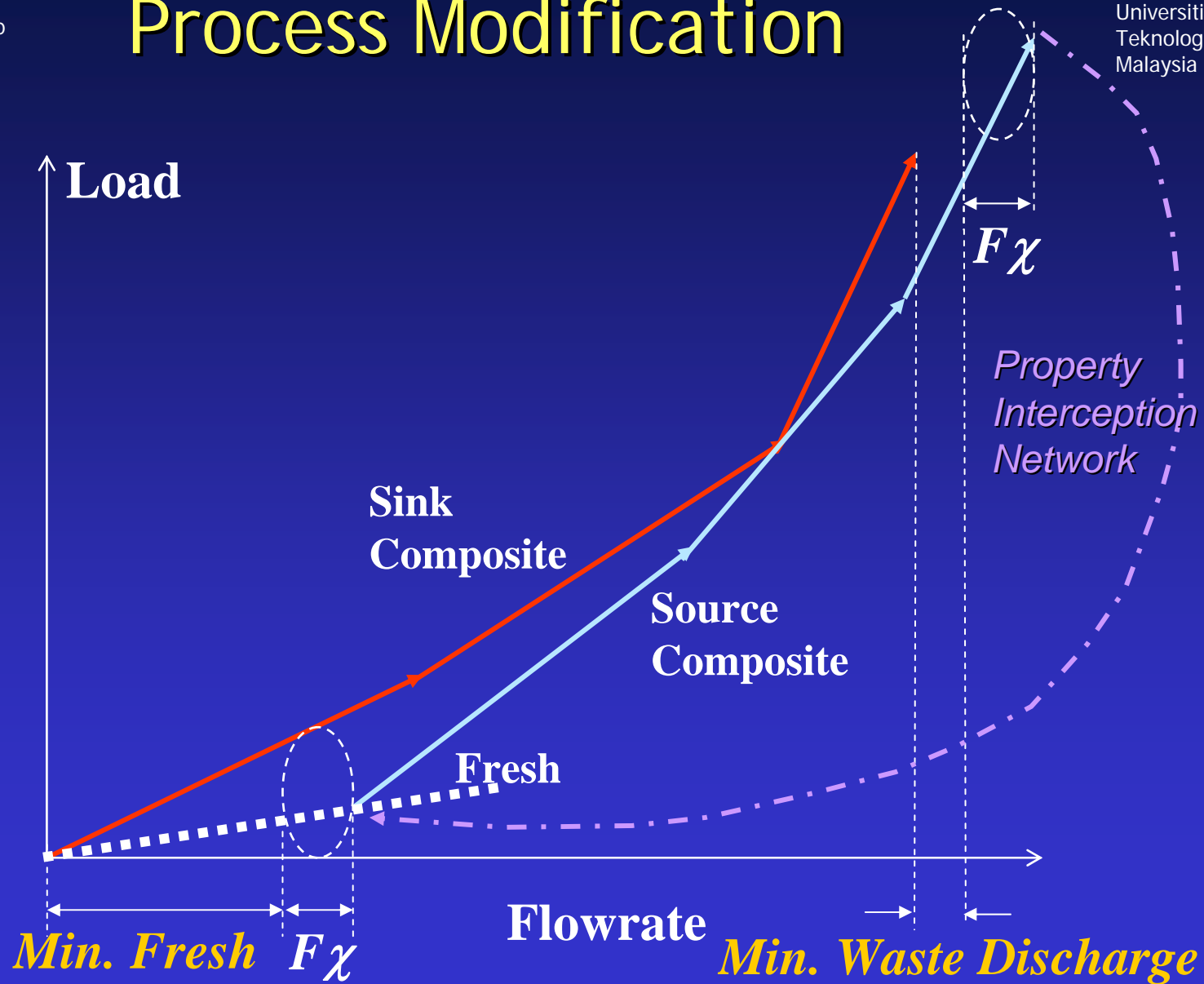
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Implementing Process Modification

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Extension to Other Cases



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Fresh has property operator greater than process streams

Objective

Motivation

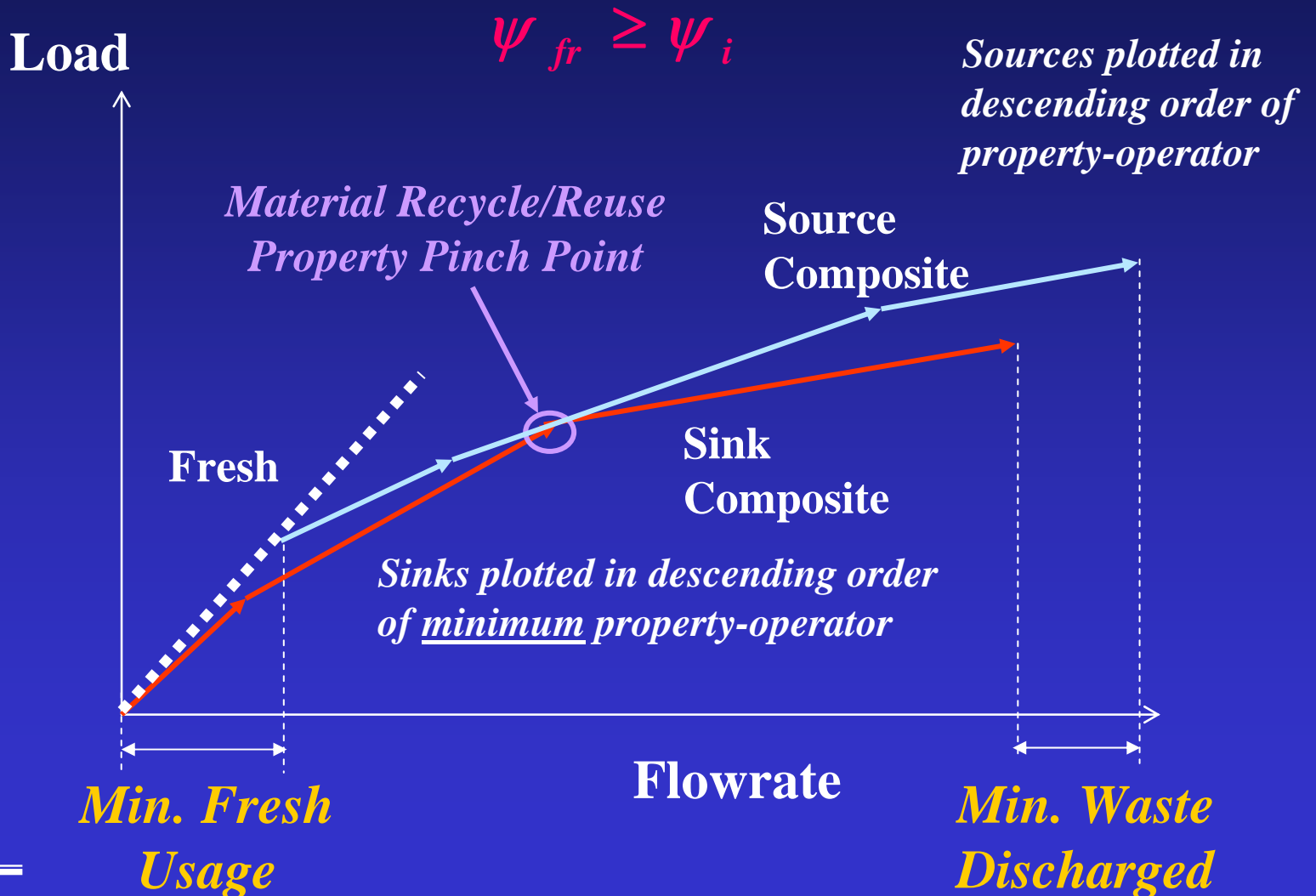
Problem

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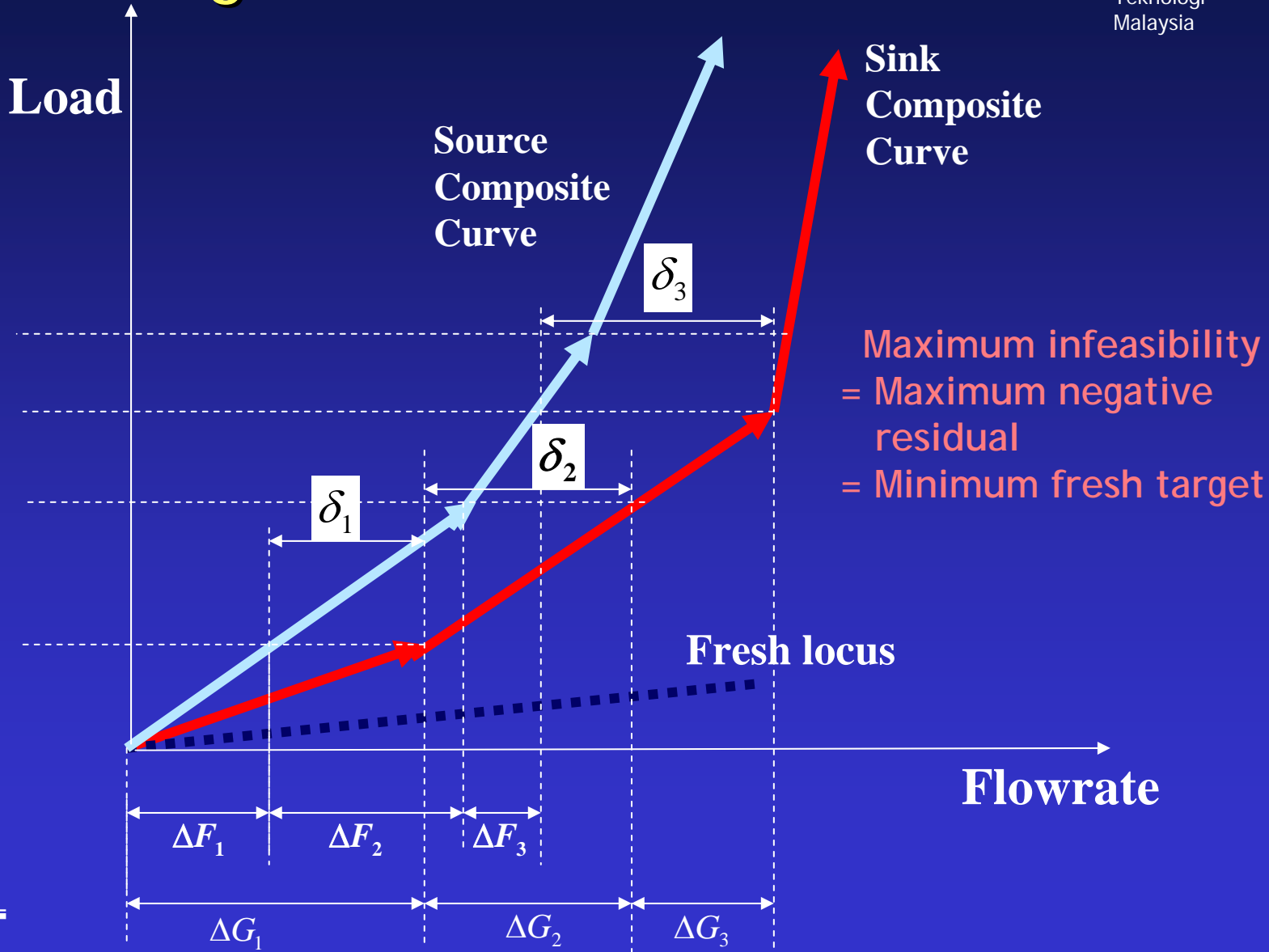
Conclusions





Transformation to Algebraic Procedure

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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		$\frac{\Delta M_2}{\psi_{s,1} - \psi_{fr}}$		$\frac{\Delta M_2}{\psi_{u,2}^{\max} - \psi_{fr}}$
			Source 2	$\frac{\Delta M_3}{\psi_{s,2} - \psi_{fr}}$	Sink 2 $\psi_{u,2}^{\max}$	$\frac{\Delta M_3}{\psi_{u,2}^{\max} - \psi_{fr}}$
	M_{k-1}					
k	M_k	ΔM_k	Source 3	$\frac{\Delta M_k}{\psi_{s \text{ in interval } k} - \psi_{fr}}$	Sink 3	$\frac{\Delta M_k}{\psi_{u \text{ in interval } k}^{\max} - \psi_{fr}}$
	M_{n-1}		Source N_s			
n	M_n	ΔM_n		$\frac{\Delta M_n}{\psi_{s \text{ in interval } n} - \psi_{fr}}$	Sink N_u	$\frac{\Delta M_n}{\psi_{u \text{ in interval } n}^{\max} - \psi_{fr}}$



Cascade Diagram



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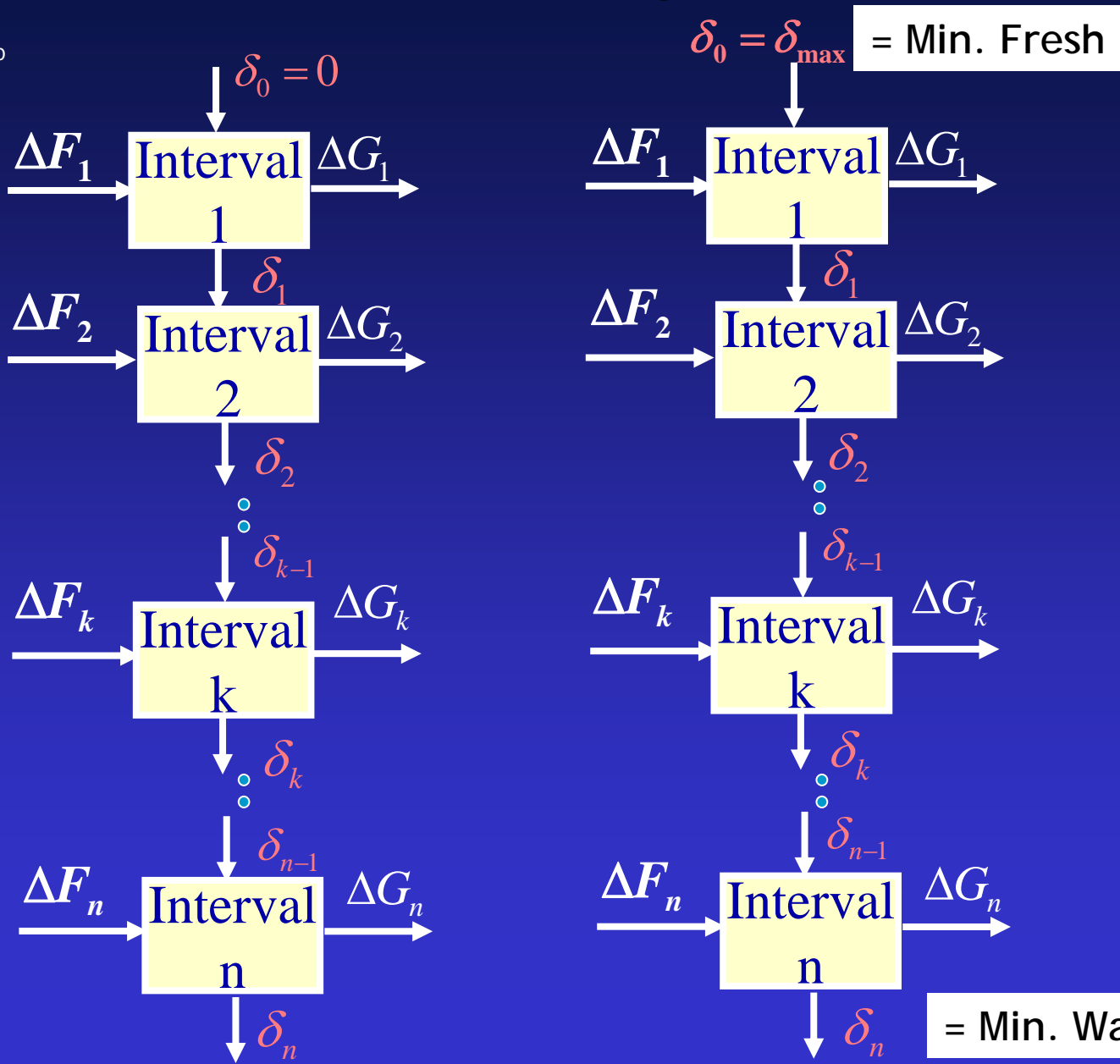
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Case Study



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Property Mixing Rule

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

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Objective

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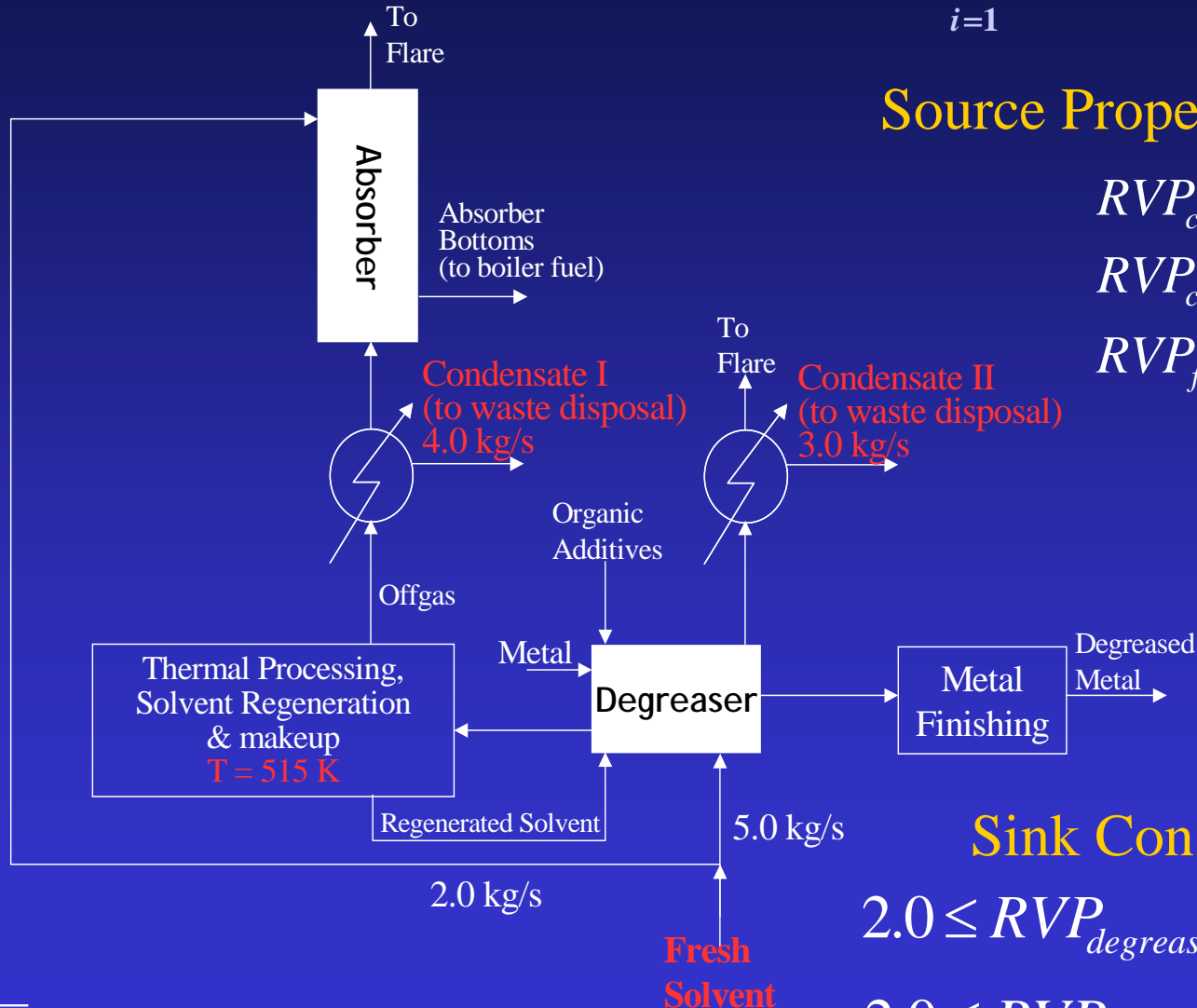
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Source Property Values

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

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

$$RVP_{fresh} = 2.0\text{ atm}$$

Sink Constraints

$$2.0 \leq RVP_{degreaser}(\text{atm}) \leq 3.0$$

$$2.0 \leq RVP_{absorber}(\text{atm}) \leq 4.0$$



Case Study



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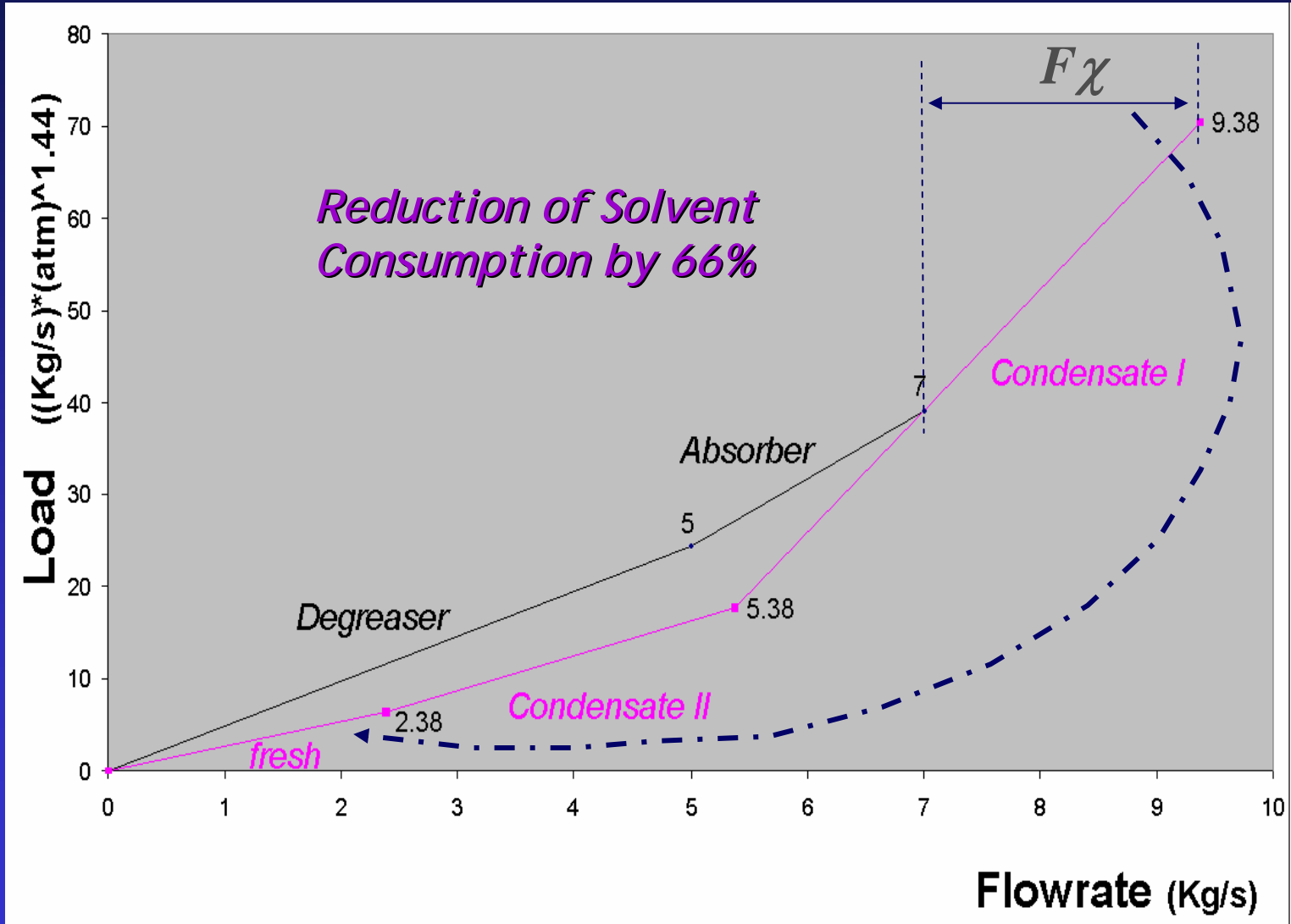
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Case Study



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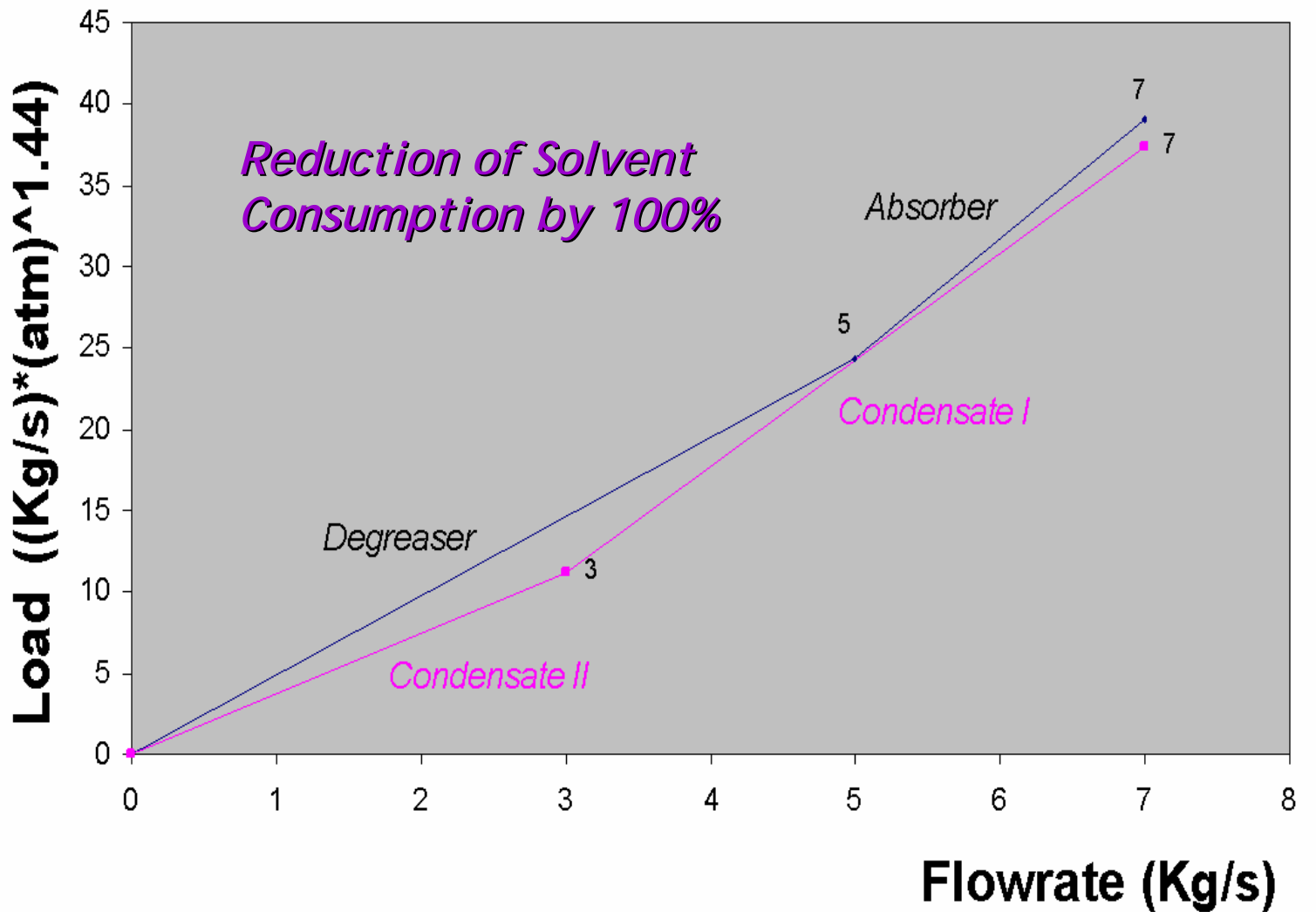
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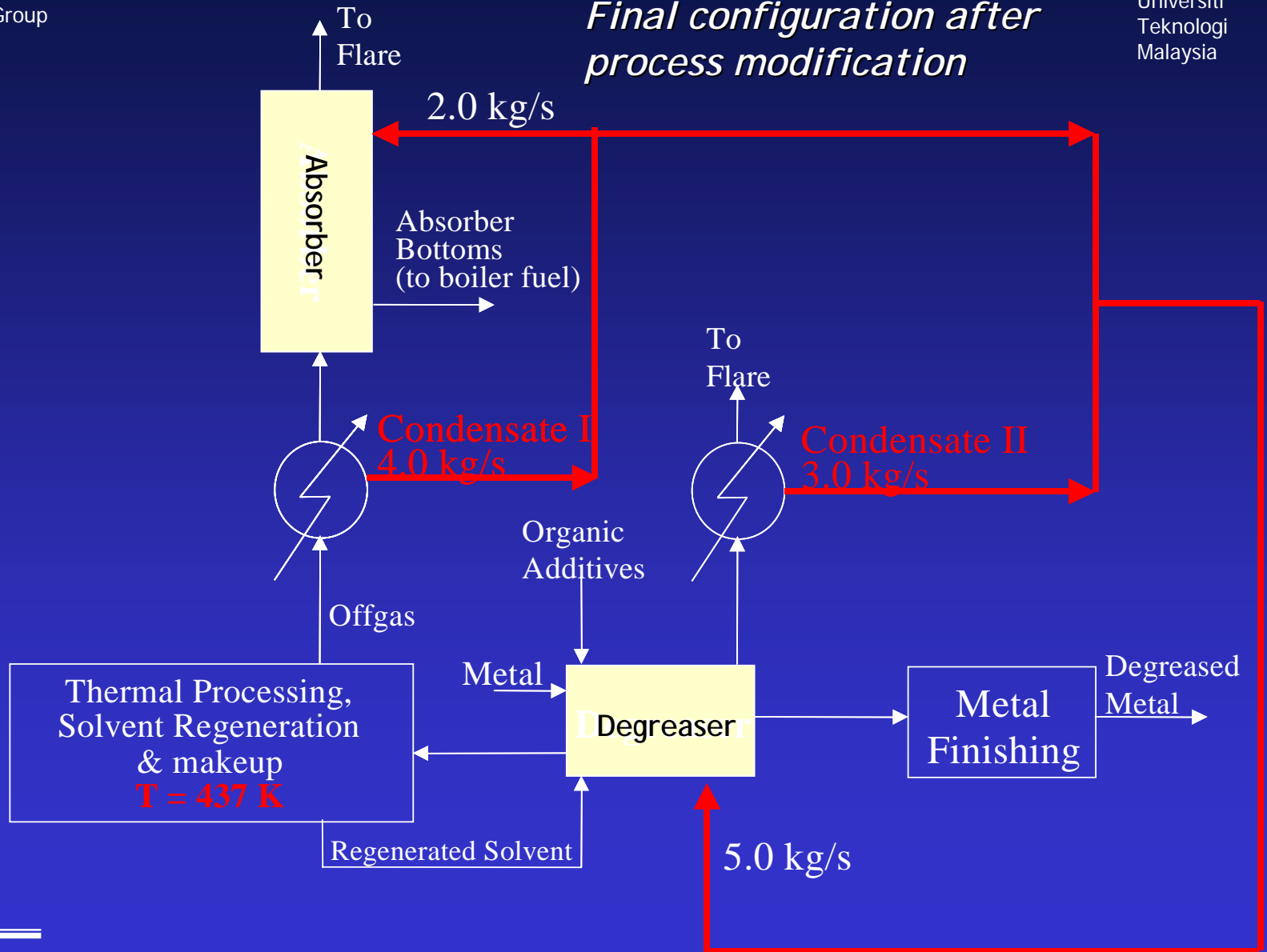
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Final configuration after process modification





Conclusions



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Conclusions

- 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



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Conclusions

- 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