Sustainable Design of Industrial Processes: Integration of Sustainability into the Curriculum

Presenters:

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2017 ASEE Summer School for Chemical Engineering Faculty

Wednesday, August 2, 2017 9:30 am-noon, Thursday August 3, 2017, 9:30 am-noon

Outline

- Overview of NSF Sustainable Manufacturing Advances in Research and Technology (SMART) Coordination Network (Huang)
- Overview of educational modules on sustainable manufacturing (Eden)
- Concepts, tools, and examples on sustainable design for inclusion in the senior-level design course(s) or an elective (El-Halwagi)

Workshop Learning Outcomes

By the end of the workshop, you should be able to perform the following:

- Introduce principles of sustainability and computer-aided modules into chemical engineering curriculum
- Evaluate overall mass targets (fresh usage, waste discharge, yield, etc.) for a given process
- Evaluate targets for minimum heating and cooling utilities
- Use integrated economic and other sustainability criteria in the assessment and screening of process design alternatives

Part I:

Overview of NSF Sustainable Manufacturing Advances in Research and Technology (SMART) Coordination Network

Yinlun Huang
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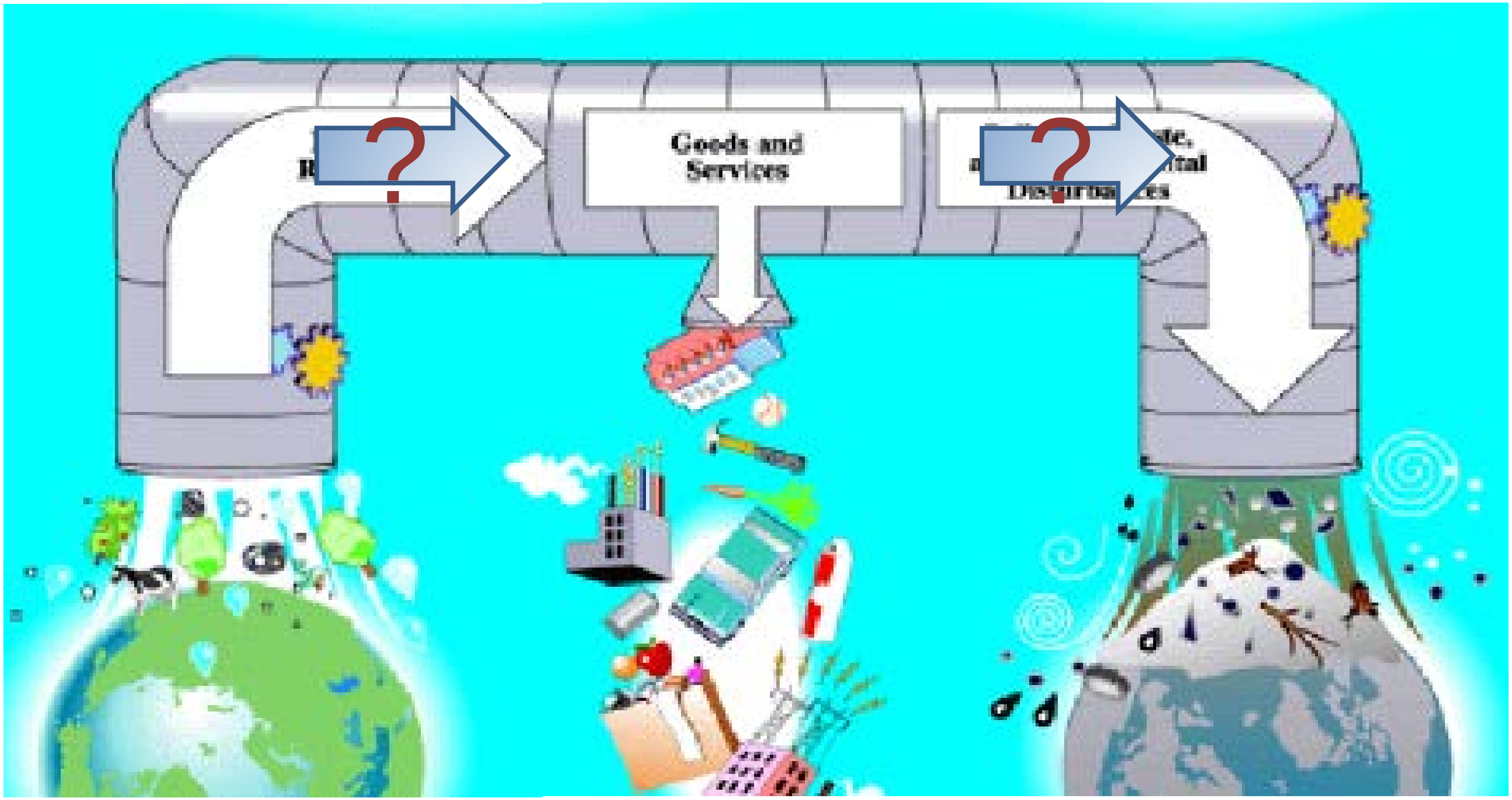
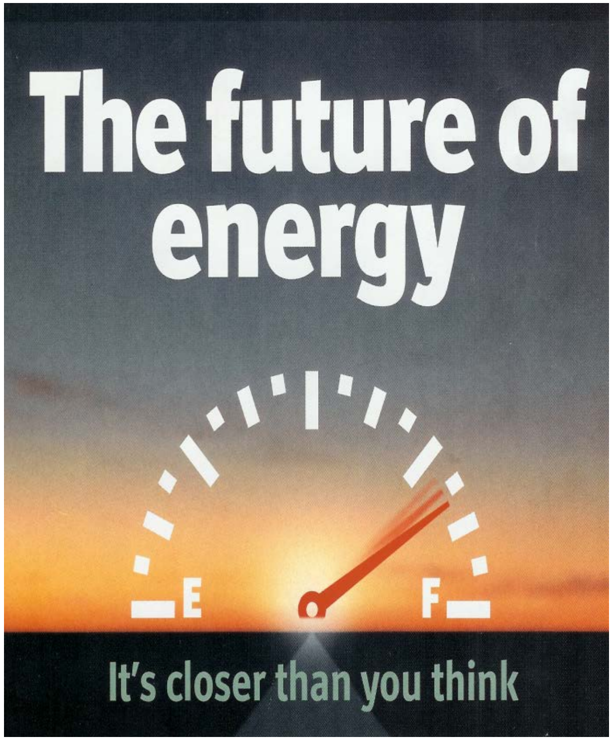
Centuries of Human Activities

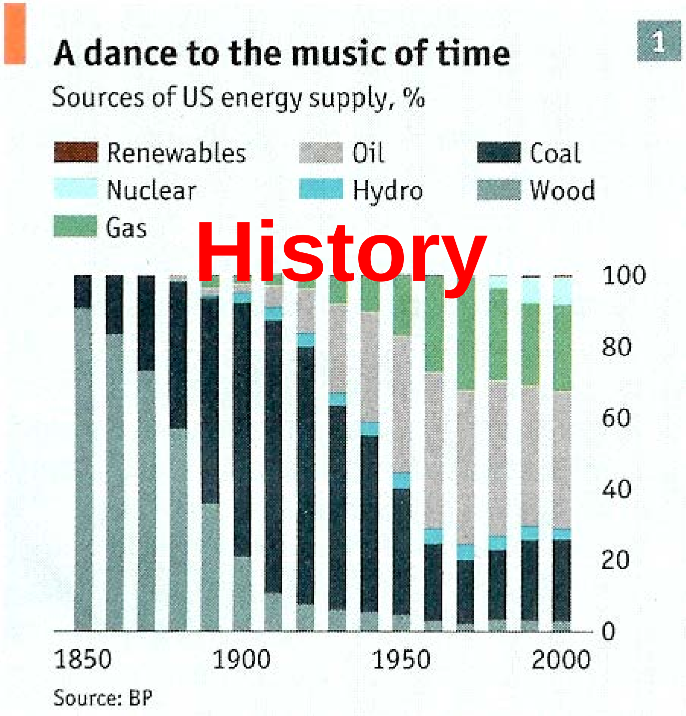
Depleting resources

Increasing wealth

Damaging the Earth

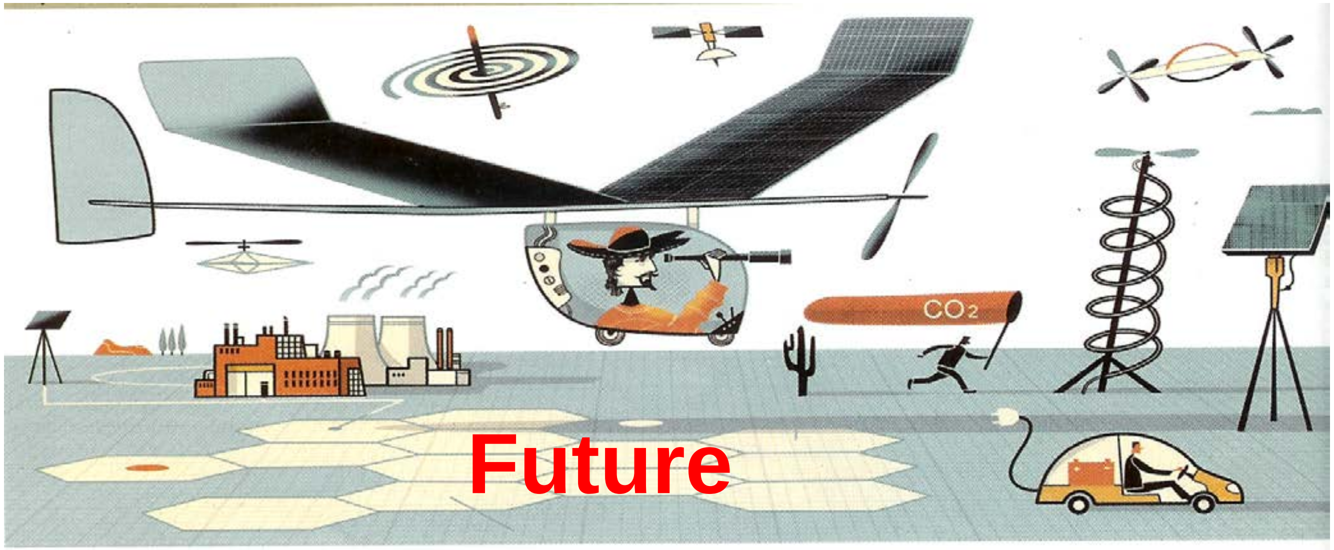






History

Today



Future

Global Challenges

A growing and aging world population

Urbanization

Energy requirements and climate protection

Globalization and new markets

Megatrends

- Energy and Resources
- Housing and Construction
- Health and Nutrition
- Mobility and Communication
- Demographic Change

Sustainability: What Does It Mean to Us

Definition (one of "hundreds"):

- "Development that meets needs of present without compromising ability of future generations to meet their own needs*" – Brudtland, 1987

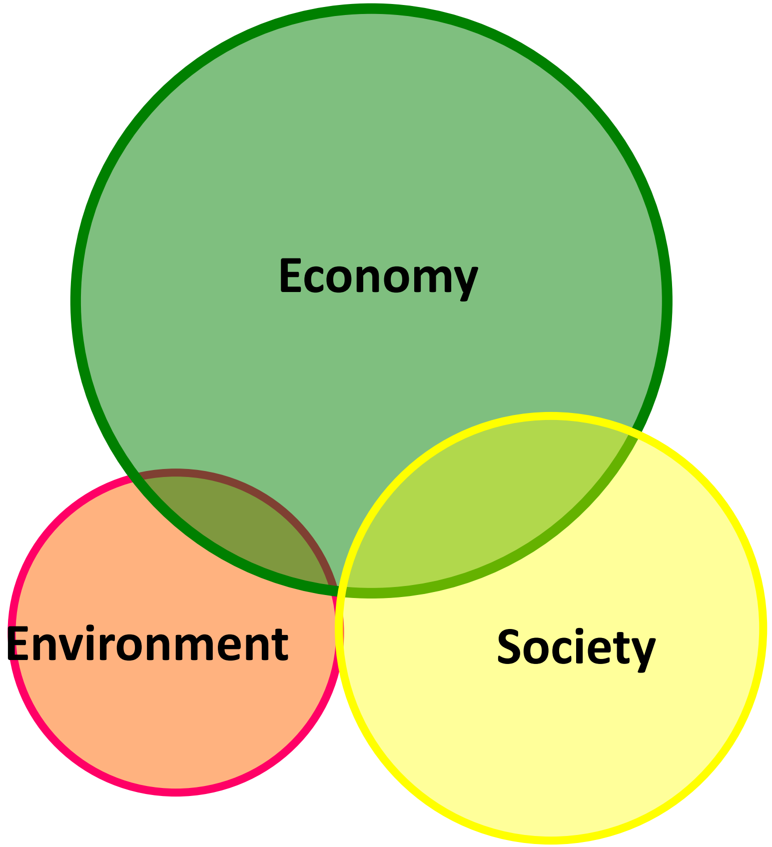
Sustainable Development

- A rich concept for helping shape human society's interaction with the biosphere
- "Triple-bottom-lines" based balance
- Systems of interest: global to local, human to physical, macro to micro, etc.
- Features of systems: multiscale, complex, uncertain, unpredictable, moving target

SD: An Engineer's View

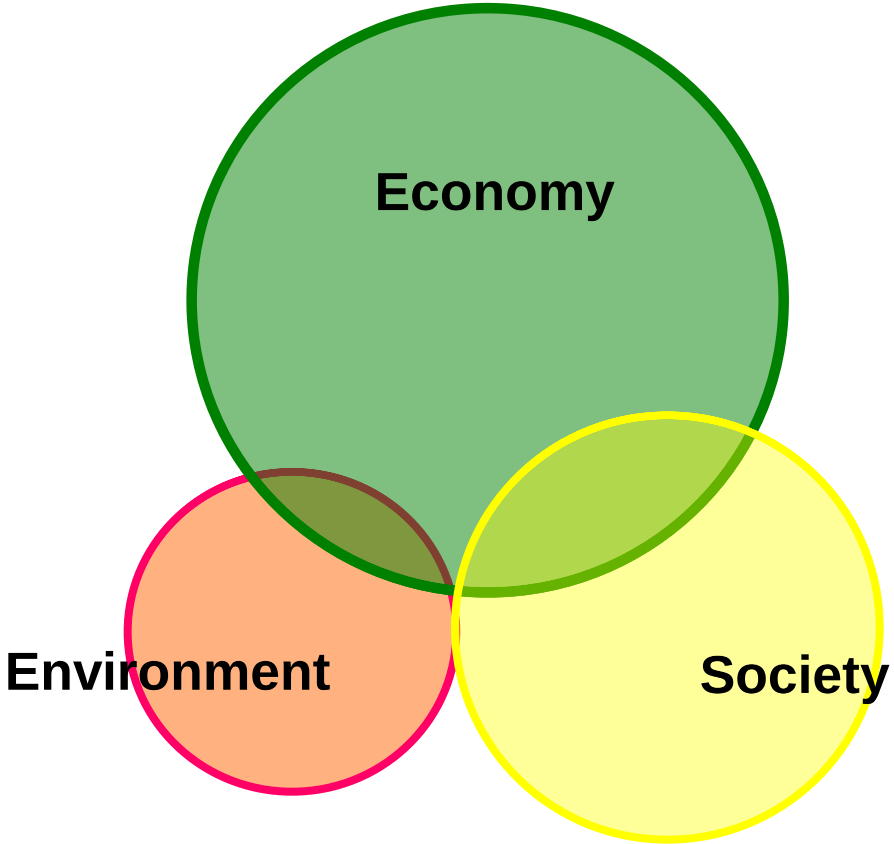
- Modern society: a highly heterogeneous system, experiencing numerous types of "reactions", and having countless "transport phenomena" at all time and length scales
- Ergodicity: the tendency of a system to move towards equilibrium, maximizing entropy, and minimizing free energy
- Human society does not settle down into stable patterns for long; it constantly innovates, grows, and changes, posing a challenge for those trying to adjust human's interactions with the biosphere.
- Human societies are dynamic, open systems far from equilibrium and must evolve and adapt to survive.

Reality and Unacceptable Approach



- **Economic prosperity first**
- **Social responsibility emphasized insufficiently**
- **Environmental quality suffered**

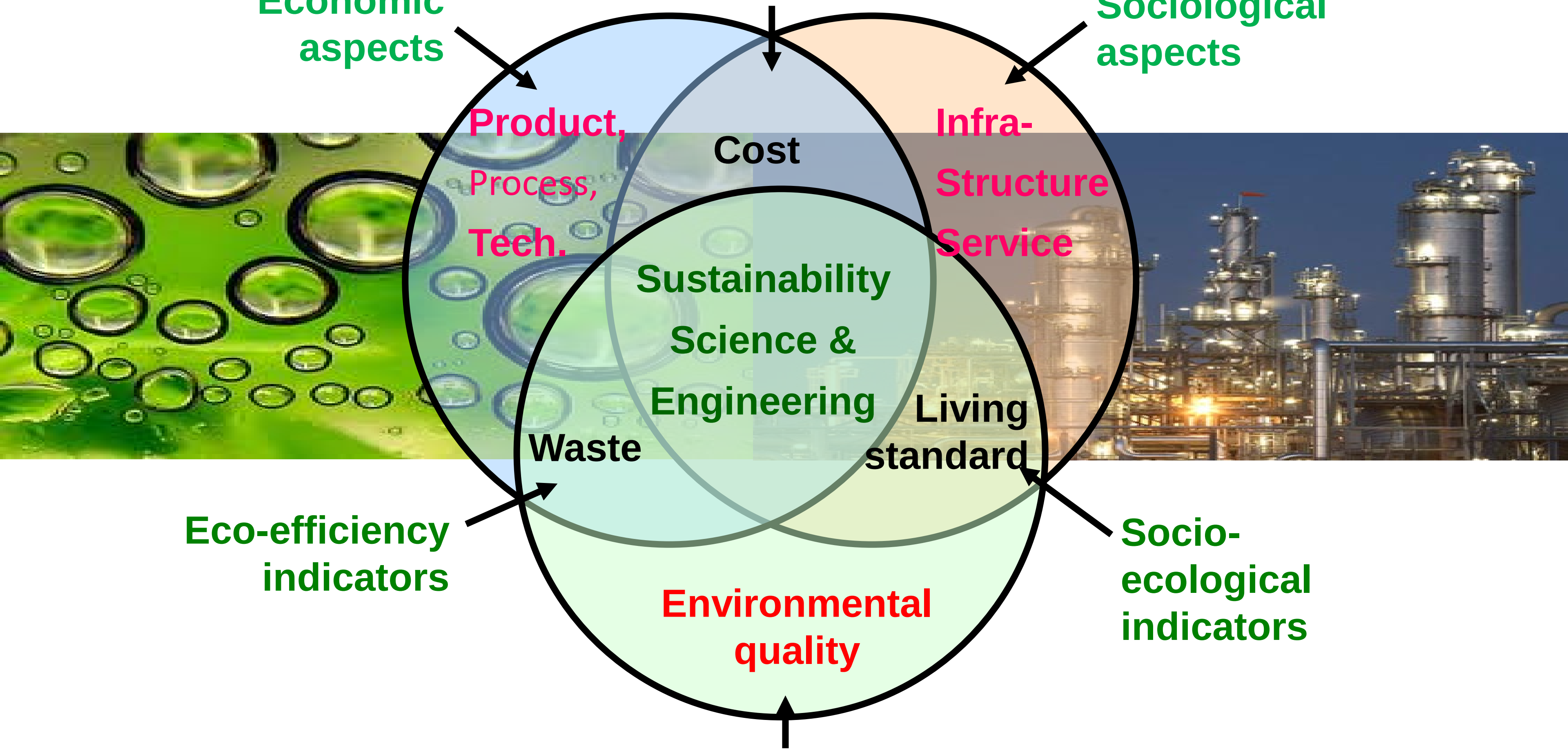
Towards Balanced Development



We want to achieve simultaneously

- economic prosperity
  &
- environmental cleanness
  &
- societal satisfaction

Engineering Sustainability: A Need to Re-engineer Engineering Systems



Socio-economic indicators

Economic aspects

Sociological aspects

Product, Process, Tech.

Cost

Infra-Structure Service

Sustainability Science & Engineering

Waste

Living standard

Eco-efficiency indicators

Socio-ecological indicators

Environmental quality

Environmental aspects

Accelerating U.S. Advanced Manufacturing

- PCAST, Oct. 27, 2014

- "The United States has been the leading producer of manufactured goods for more than 100 years."
- "The United States has long thrived as a result of its ability to manufacture goods and sell them to global markets."
- "U.S. strengths in manufacturing innovation and technologies that have sustained American leadership in manufacturing are under threat from new and growing competition abroad."

A renewed national effort has been made to secure U.S. leadership in emerging technologies that will create high-quality jobs and enhance America's global competitiveness.

Sustainable Manufacturing

- **DOC and EPA Definition:**

  Sustainable manufacturing is "the creation of manufactured products through economically-sound processes that minimize negative environmental impacts while conserving energy and natural resources".

  Sustainable manufacturing also "enhances employee, community, and product safety, which are all social issues."

SMART CN – Leadership Team

Principal Investigators/Executive Committee


Y. Huang
Wayne State U


T. Edgar
U Texas


M. El-Halwagi
Texas A&M U


C. Davidson
Syracuse U


M. Eden
Auburn U

Development Director of Educational Modules


D. Sengupta
Gas and Fuels Research Center,
Texas A&M U

Steering Committee


L. Achenie
Virginia Tech.


D. Allen
U Texas


B. Bakshi
Ohio State U


B. English
U Tennessee


D. Fasenfast
Wayne State U


I. Grossmann
Carnegie Mellon U


K. High
Clemson U


I. Jawahir
U Kentucky


C. Maravelias
U Wisconsin


K. Ogden
U Arizona


M. Rezac
Kansas State U


F. Shadman
U Arizona

SMART CN – Collaboration Organizations

Domestic

- **AIChE - Institute for Sustainability (IfS)**
- **CACHE Corporation**
- **Center for Advanced Process Decision-Making, Carnegie Mellon U.**
- **Center for Sustainable Engineering, Syracuse U.**
- **Industrial and Urban Sustainability Group (I&US), Wayne State U.**
- **Institute for Sustainable Manufacturing (ISM), U. of Kentucky**
- **National Alliance for Advanced Biofuels and Bioproducts (NAABB)**
- **National Center for Manufacturing Sciences (NCMS)**
- **National Council for Advanced Manufacturing (NCFAM)**
- **NSF ISRC Engineering Center for Environmentally Benign Semiconductor Manufacturing, U. of Arizona**
- **Smart Manufacturing Leadership Coalition**
- **Texas-Wisconsin-California Control Consortium, Austin, TX**
- **The Industrial & Urban Sustainability (I&US) Group, Wayne State U.**

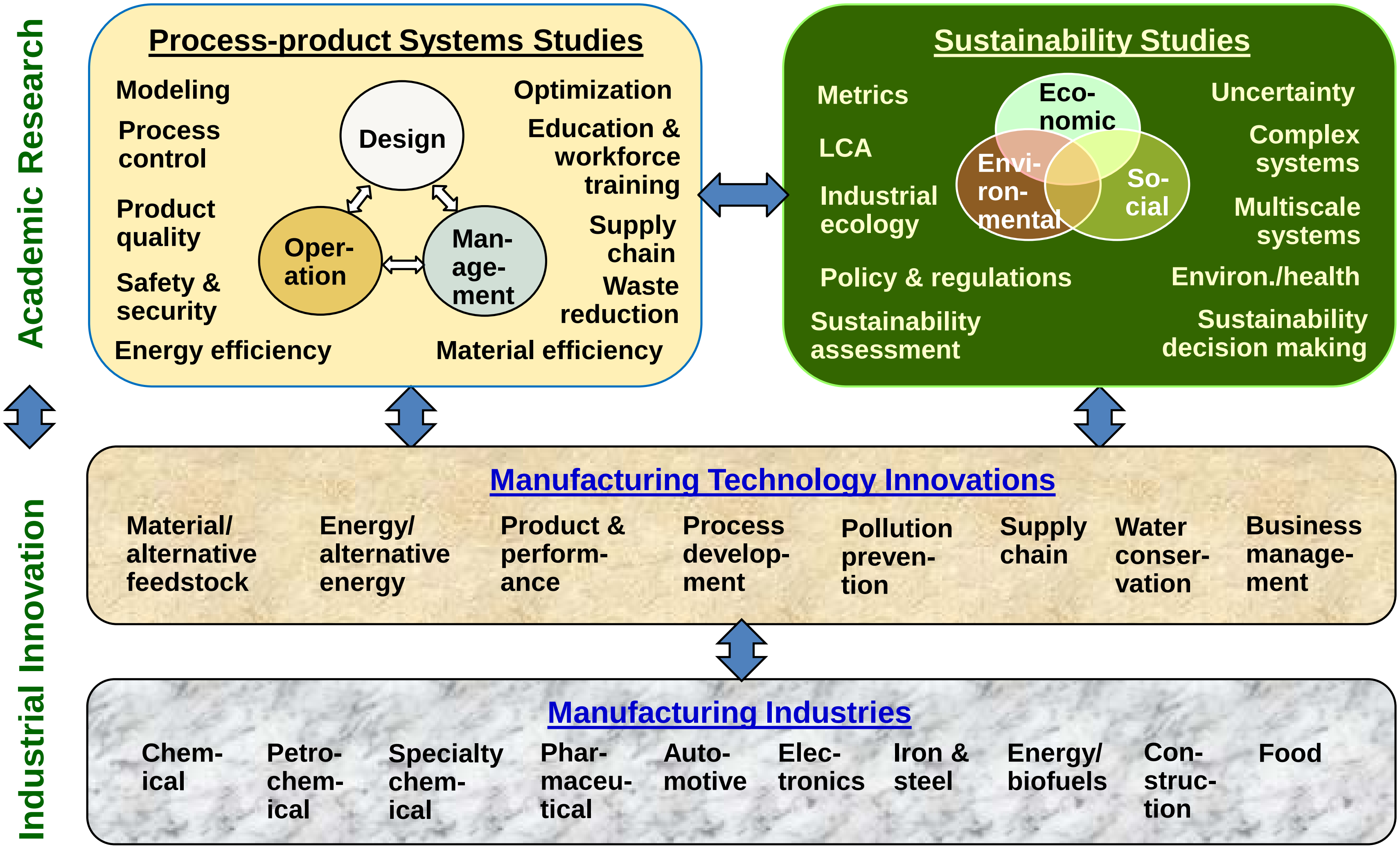
International

- **Denmark, Germany, China, Norway, Singapore, Japan, India**

Project Tasks

1. To conduct comprehensive and in-depth review of the frontier research and technological development for sustainable manufacturing
2. To define roadmaps for manufacturing sustainability and identify bottlenecks in a number of focused research areas via workshops
3. To coordinate research through sharing knowledge, resources, software, and results
4. To establish partnerships with industrial groups to expedite technology innovation
5. To conduct education and outreach to a wide range of stakeholders

Academic and Industrial Collaboration on Sustainable Manufacturing



Academic Research

Industrial Innovation

Process-product Systems Studies

Modeling

Process control

Product quality

Safety & security

Energy efficiency

Design

Operation

Management

Optimization

Education & workforce training

Supply chain

Waste reduction

Material efficiency

Sustainability Studies

Metrics

LCA

Industrial ecology

Policy & regulations

Sustainability assessment

Economic

Environmental

Social

Uncertainty

Complex systems

Multiscale systems

Environ./health

Sustainability decision making

Manufacturing Technology Innovations

Material/ alternative feedstock

Energy/ alternative energy

Product & performance

Process development

Pollution prevention

Supply chain

Water conservation

Business management

Manufacturing Industries

Chemical

Petrochemical

Specialty chemical

Pharmaceutical

Automotive

Electronics

Iron & steel

Energy/ biofuels

Construction

Food

Part II:

Overview of Educational Modules on Sustainable Manufacturing

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Tutorial on the SMART-CN Educational Modules for Incorporation in the Advanced Undergraduate or Graduate Engineering Curriculum

Debalina Sengupta[1]*, Yinlun Huang[2], Thomas F. Edgar[3], Cliff I. Davidson[4], Mario R. Eden[5], Mahmoud M. El-Halwagi[1]

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[2] Chemical Engineering and Materials Science, Wayne State University
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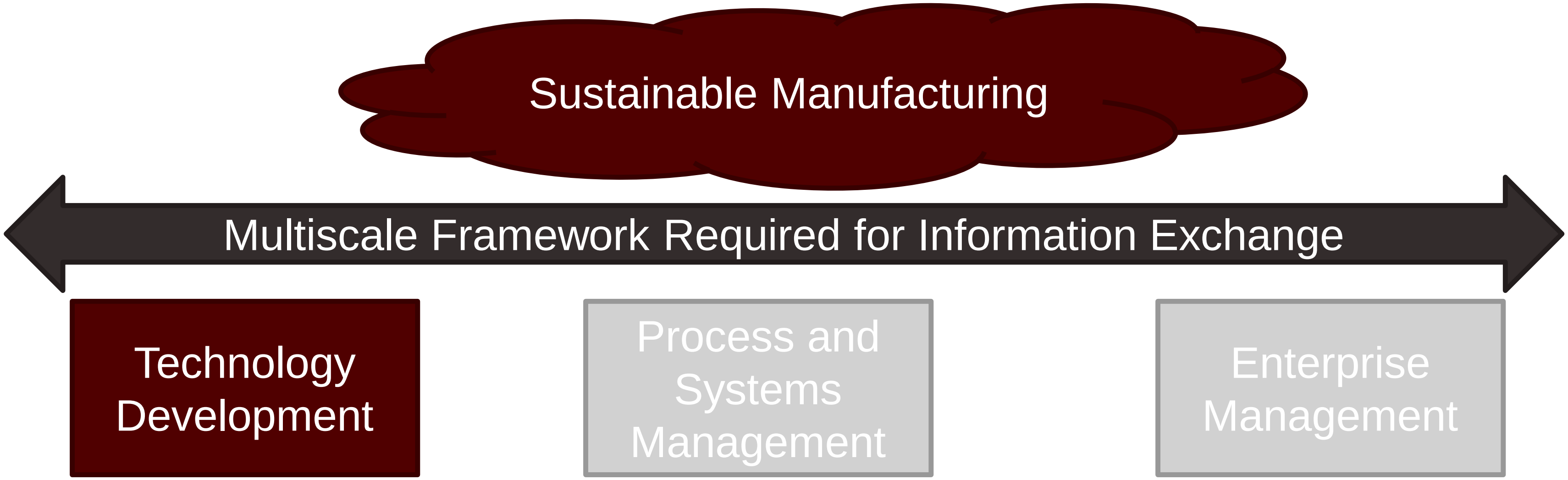
Presented at the AIChE Annual Meeting,
San Francisco, November 14, 2016

Outline

- SMART – CN Education Vision
- Modules Development
- Future Modules

SMART – CN Education Vision



Sustainable Manufacturing

Multiscale Framework Required for Information Exchange

Technology Development

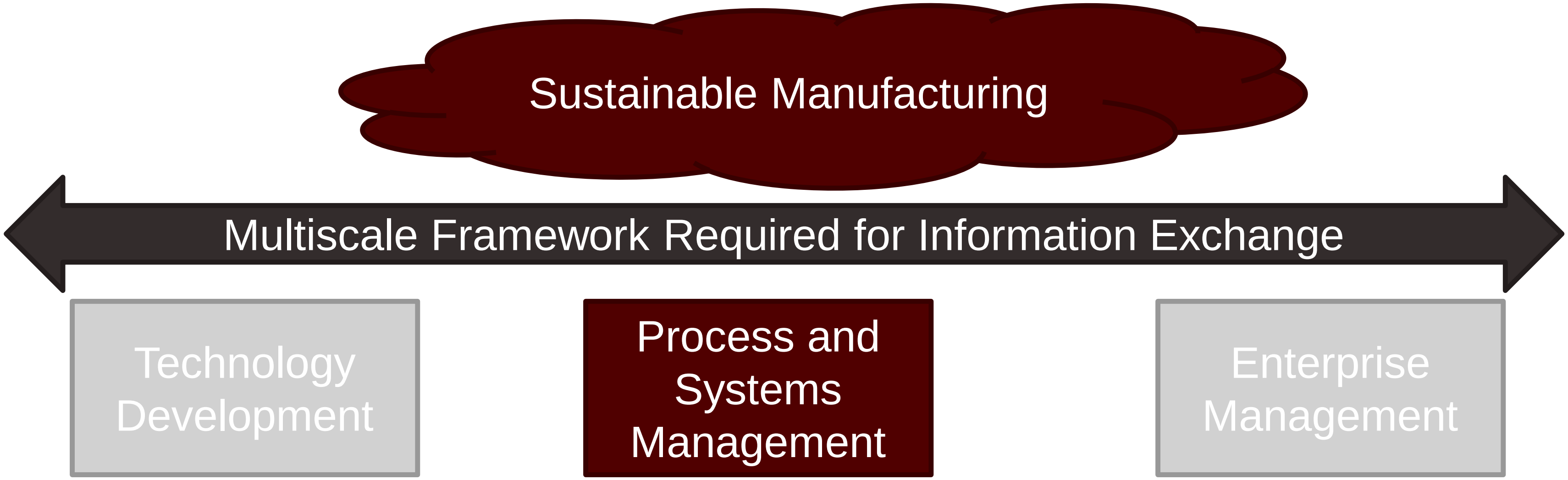
Process and Systems Management

Enterprise Management

- **New Product Development** –Thermodynamics, chemistry, molecular modeling
- **Alternative Feedstock and Materials** – Chemical properties for new feedstock, seamless integration into design software
- **New Pathways and Processes** – catalysis, reaction pathway synthesis, environmental releases

Learning criteria for students/workforce: *Identify (develop if necessary) indicators and metrics for assessment and management of sustainable technologies*

SMART – CN Education Vision



Sustainable Manufacturing

Multiscale Framework Required for Information Exchange

Technology Development

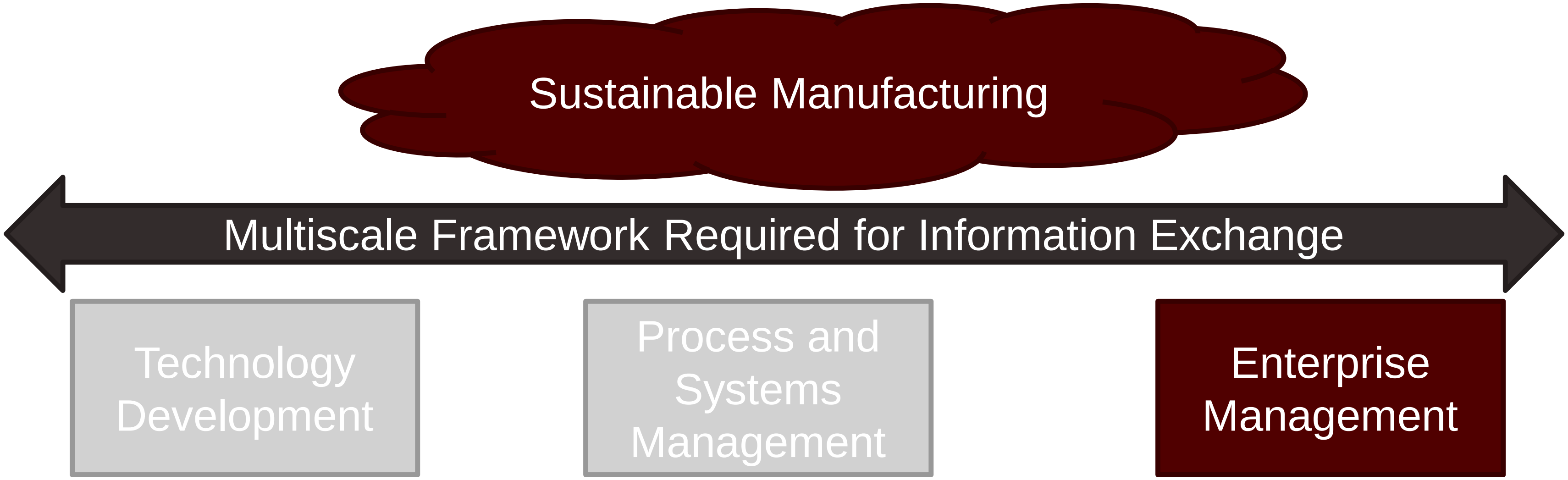
Process and Systems Management

Enterprise Management

- **Process Design** – process integration, process intensification, process optimization
- **Plant Operations** – advanced control systems, process safety, environmental control systems
- **Materials and Energy Management** –can be integrated into process design area through the integration and intensification methods

Learning criteria for students/workforce: *Identify (develop if necessary) technologies, indicators and metrics for assessment and management of process systems. Incorporate this knowledge into various stages of design and operations*

SMART – CN Education Vision



- **Supply Chain Management and Logistics Optimization** – life cycle assessment (for environmental impact assessment), optimization (for logistics, cost), life cycle optimization (for both economic and environmental assessment of supply chain)
- **Information Management** – tools, data, information related to success stories, case studies for enterprise managers
- **Enterprise Framework** – systems analysis for studying impacts of entire supply chain

Learning criteria for students/workforce: *Identify (develop if necessary) methodologies for systematic analysis of sustainability of enterprise. Crucial to include all aspects of sustainability, such as economic, environmental, and social. Can be expanded to include cross-cutting areas such as safety.*

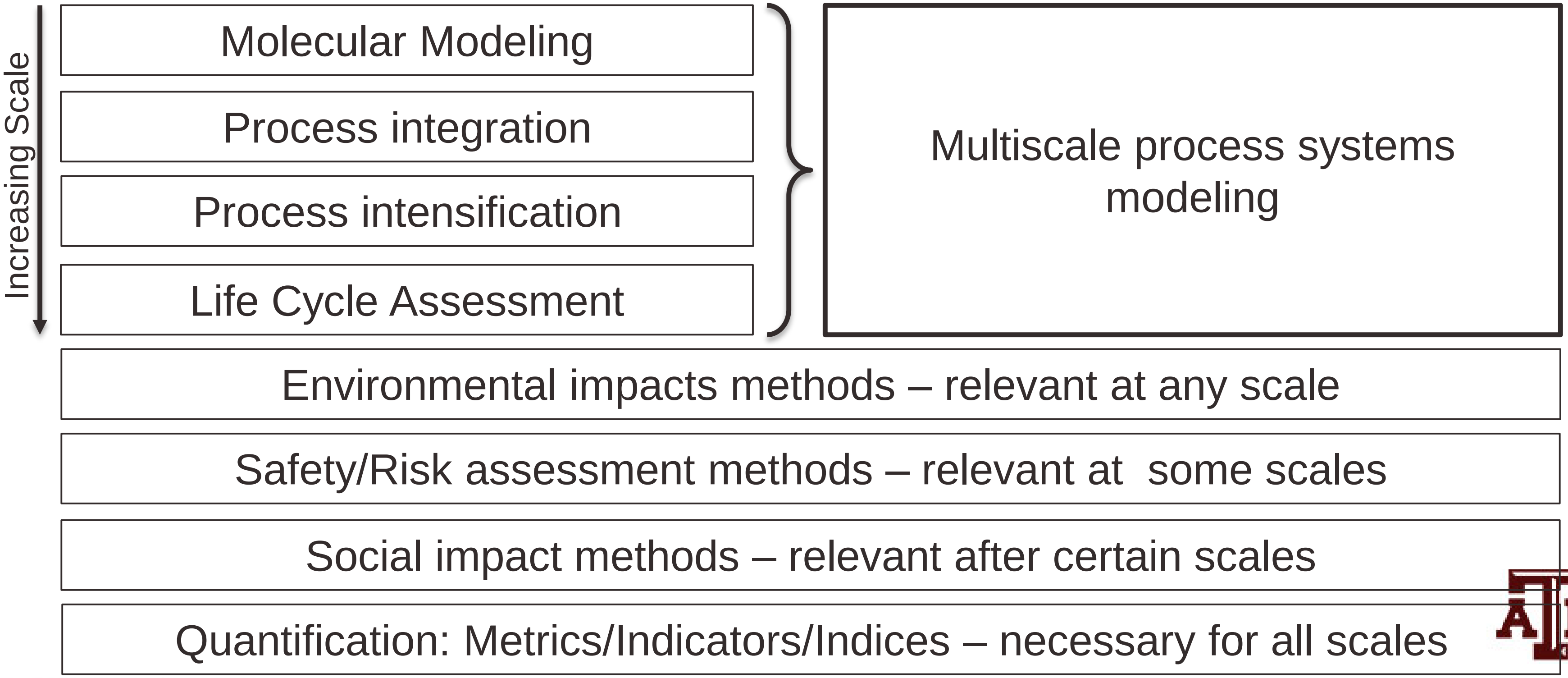
Course Type 1 – Integrating into Existing Coursework

- The approach for this course is to develop modules which **COMPLEMENT** existing engineering discipline course curriculum with sustainability approaches.
- Instructors may choose to incorporate the case studies in these modules into the individual courses.
- Social criteria is not included in this section. It is expected to be incorporated into existing liberal arts coursework that students have to take in their degree.

Thermodynamics Mass Transfer Heat Transfer Reaction Engineering Transport Phenomena	Molecular modeling Green chemistry Environmental impact potential Resource use Energy use
Engineering Design	Process integration Process intensification Process safety Metrics/Indicators/Indices
Process Control and Optimization	Environmental control variables Optimum points for economic and environmental issues
Supply Chain/Operations Management	Life Cycle Assessment Supply Chain Optimization

Course Type 2 – Introducing New Coursework

- The approach in this course type is to **ADD** a topic to existing engineering discipline courses, at par with engineering design.
- Suggested title: “Sustainability approaches in Engineering”.
- Single instructor, or a group of instructors, specializing in the individual areas.
- Requires coordination among the instructors to time and devise homework/exams.
- Introduction of certain social aspects require interdisciplinary coordination from social sciences instructors.



Increasing Scale

Molecular Modeling

Process integration

Process intensification

Life Cycle Assessment

Multiscale process systems modeling

Environmental impacts methods – relevant at any scale

Safety/Risk assessment methods – relevant at some scales

Social impact methods – relevant after certain scales

Quantification: Metrics/Indicators/Indices – necessary for all scales

Course Type 3 – Short Courses Directed towards Specific Manufacturing Sector

- The approach for this course is to **CATER** to the needs of existing industry professionals to understand, integrate, and measure sustainability approaches in their sector.
- This may be a classroom instruction course, **Massive Open Online Course** (MOOC), or standard slideshow based course
- Developing this will require the following knowledge and dissemination plan:

Knowledge of Industrial Sectors
(can be categorized based on NAICS/SIC codes)

Knowledge of Sustainability Implementation Areas
(for example, petroleum refineries need to be profitable, safer, low emission, and built in areas such that environmental justice is not violated)

Develop Specific Module Based on the Knowledge of The Sustainability Implementation Area

- Course module takes an existing refinery, follows it through the various stages of design to implementation (Front End Engineering Design, Site Selection, HAZOP/HAZID studies, Environmental Permits and Regulations, Construction and Management, Operations)
- Plugs in the sustainability criteria knowledge (through modules) into the stages of design
- Identify a set of key indicators and metrics required to assess sustainability over the life cycle of the sector

Example: Petroleum Refining Manufacturing Industry

Course Type 1- Structure

Outline/Overview (Word® document)

- **Introduction** *(max 500 words, excluding figures)*
  - *Key aspects of module, e.g. "What is LCA?", "Why is LCA needed?", "Overview, framework for LCA"*
- **Rationale: <Life Cycle Assessment> for ensuring Sustainable Engineering** *(max 300 words)*
  - *e.g. Why do we need LCA for sustainable engineering/manufacturing?*
- **Course Content: <LCA theory, methods, tools and databases>** *(max 3000 words to ensure most important information is provided in the text, excludes figures, use of appendices for additional information)*
- **Connections to Existing Core Curriculum** *(max 200 words)*
  - *e.g. Which areas in existing courses can LCA fit into? Who should know about LCA?*
- **Case study** *(max 300 words, short description)*
- **References and Websites for Further Reading**
- **Appendices**

Course Type 1- Structure

Classroom Presentation (Powerpoint® slides)

- ~ 40-50 slides, including case study
- Ready for use by instructor, specific delivery instructions (e.g. when to administer a certain case problem) provided in the notes
- Can also be used by individuals seeking self-study options

Case Study (Word® document)

- No word limits
- Case study can be describing a single problem with multiple example options
- The solutions are provided in most cases, with specific instructions on the solution methods used

Supporting Material

- All supporting material provided (spreadsheets, solution manuals, computer programs, design files)

Module Categories

Methods for Sustainable Manufacturing
Focus on the method of assessment of sustainability

Sustainable Manufacturing Processes
Focus on the process(es) for manufacturing

Dedicated Assessment Tools
Assessment platforms for Sustainable Manufacturing

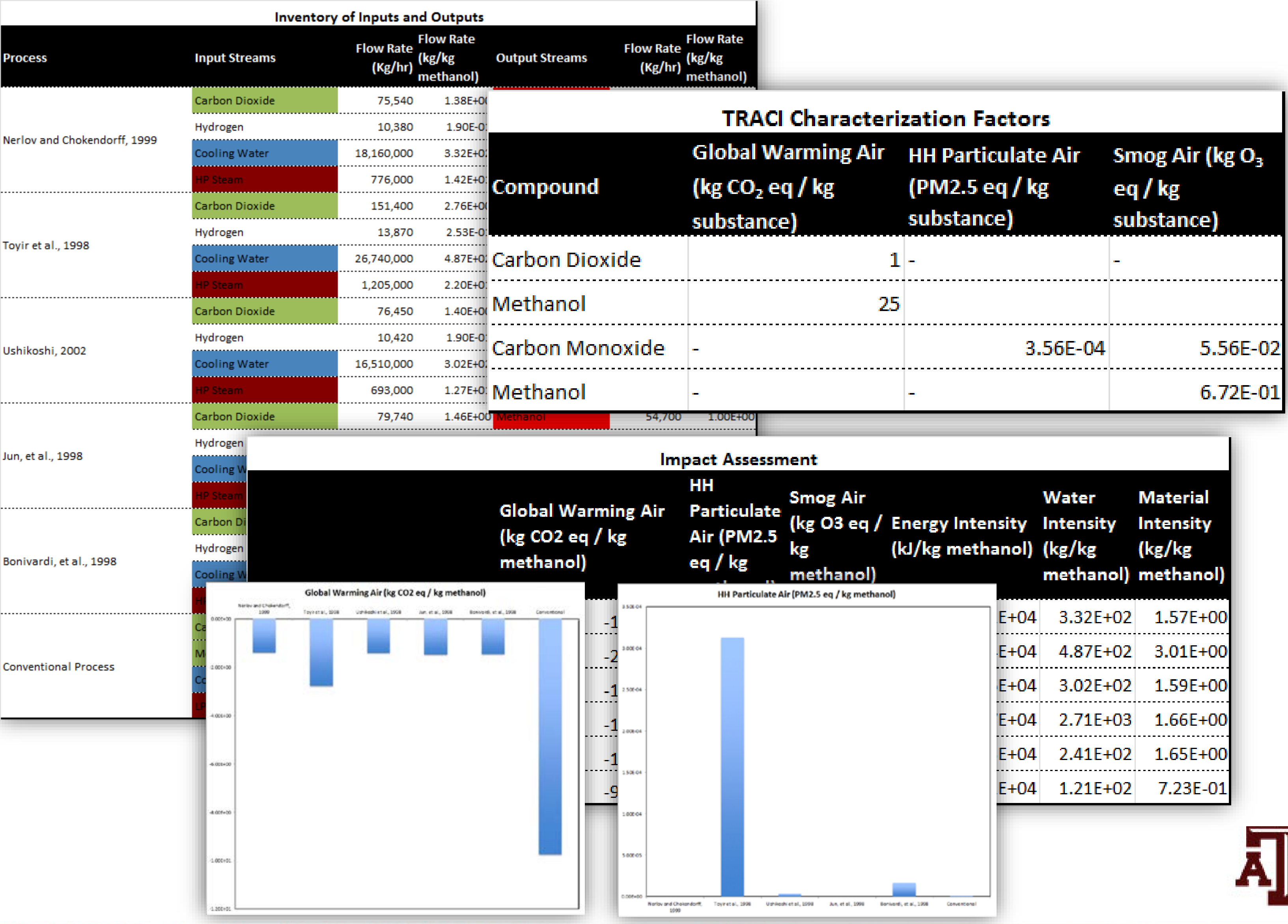
Modules

Module Name	Developer/ University	Module Content
Assessment of the Presidential Green Chemistry Award Winners using Green Chemistry Metrics	Christopher L. Kitchens/Clemson University	***Method Topic*****:** This module evaluates the work that has received the Presidential Green Chemistry Challenge Award using green chemistry metrics, principles, and design strategies. ***Assessment Tools*****:** The first part is to perform a critical review of the awarded technology. The second part of the assignment requires students to contact the award winners by whatever means necessary, and interview them on 1) what the PGCC Award has meant to them and their career and 2) what personal benefit have they gained from working the award winning technology ***Supporting Documents*****:** Sample interview responses, assessment of Ibuprofen production by green technology, awarded Green Chemistry award in 1997 ***Learning Outcomes*****:** Develop an appreciation of the Green Chemistry pathways and challenges through a case study based approach on the awarded winners

Modules

Module Name	Developer/ University	Module Content
Life Cycle Assessment for Sustainable Manufacturing	Debalina Sengupta, Texas A&M University	***Method topic*: Provides overview of life cycle assessment methodology as outlined in the ISO standards, Emphasize the utility for the LCA methods for manufacturing sustainability ***Assessment tools*: Case study for a chemical production process choice for methanol, assignment set ***Supporting documents*: spreadsheet tool demonstrating case study ***Learning Outcomes*: Understand the role of process engineers in providing effective inventory data for LCA, conduct screening level LCA studies for sustainable manufacturing

LCA Module Example



Inventory of Inputs and Outputs

Process	Input Streams	Flow Rate (Kg/hr)	Flow Rate (kg/kg methanol)	Output Streams	Flow Rate (Kg/hr)	Flow Rate (kg/kg methanol)
Nerlov and Chokendorff, 1999	Carbon Dioxide	75,540	1.38E+0			
	Hydrogen	10,380	1.90E-0			
	Cooling Water	18,160,000	3.32E+0			
	HP Steam	776,000	1.42E+0			
Toyir et al., 1998	Carbon Dioxide	151,400	2.76E+0			
	Hydrogen	13,870	2.53E-0			
	Cooling Water	26,740,000	4.87E+0			
	HP Steam	1,205,000	2.20E+0			
Ushikoshi, 2002	Carbon Dioxide	76,450	1.40E+0			
	Hydrogen	10,420	1.90E-0			
	Cooling Water	16,510,000	3.02E+0			
	HP Steam	693,000	1.27E+0			
Jun, et al., 1998	Carbon Dioxide	79,740	1.46E+00	Methanol	54,700	1.00E+00
	Hydrogen					
	Cooling W					
	HP Steam					
Bonivardi, et al., 1998	Carbon Di					
	Hydrogen					
	Cooling W					
	H					
Conventional Process	Ca					
	M					
	Co					
	LP					

TRACI Characterization Factors

Compound	Global Warming Air (kg CO_2 eq / kg substance)	HH Particulate Air (PM2.5 eq / kg substance)	Smog Air (kg O_3 eq / kg substance)
Carbon Dioxide	1	-	-
Methanol	25		
Carbon Monoxide	-	3.56E-04	5.56E-02
Methanol	-	-	6.72E-01

Impact Assessment

	Global Warming Air (kg CO2 eq / kg methanol)	HH Particulate Air (PM2.5 eq / kg	Smog Air (kg O3 eq / kg methanol)	Energy Intensity (kJ/kg methanol)	Water Intensity (kg/kg methanol)	Material Intensity (kg/kg methanol)
	-1			E+04	3.32E+02	1.57E+00
	-2			E+04	4.87E+02	3.01E+00
	-1			E+04	3.02E+02	1.59E+00
	-1			E+04	2.71E+03	1.66E+00
	-1			E+04	2.41E+02	1.65E+00
	-9			E+04	1.21E+02	7.23E-01

Global Warming Air (kg CO2 eq / kg methanol)

HH Particulate Air (PM2.5 eq / kg methanol)

Modules

Module Name	Developer/ University	Module Content
Sustainability Metrics and Sustainability Footprint Method	Debalina Sengupta, Texas A&M University	***Method topic*: ** Provides overview of methods to compute sustainability metrics. It also gives a method compute overall sustainability by aggregating metrics. ***Assessment tools*: ** Two case studies are presented on automotive shredder residue treatment method and on automobile fender formulation. ***Supporting documents*: ** spreadsheet tool demonstrating case study ***Learning Outcomes*: ** Understand the metrics used for measuring sustainability, compute these metrics, and then use the sustainability footprint method to decide which is the best option among these.

Modules

Module Name	Developer/ University	Module Content
Green Chemistry to Manufacture Specialty Chemicals from Renewable Resources	Jeffrey R. Seay, Assistant Professor, University of Kentucky	***Method Topic*: Introduces the concept of green chemistry for green design of processes, gives three methods for assessing “greener” processes: The WAR Algorithm for computing the potential environmental impact (PEI) of a process, Life Cycle Assessment for assessing environmental and other impacts, and inherently safe process design. ***Assessment Tools*: Case study for assessing sustainability of acrolein production, assignment set for pre-test on sustainability and five guided enquiry activities. ***Supporting Documents*: Aspen Plus design files for acrolein production ***Learning Outcomes*: Learn the theory for green chemistry, green engineering, and sustainability assessment methods

Modules

Module Name	Developer/ University	Module Content
Sustainability Root Cause Analysis (SRCA)	Helen H. Lou, Professor, Lamar University	***Method Topic*: Demonstrates Sustainability Root Cause Analysis (SRCA) as a tool to determine the bottlenecks for a system's progress towards sustainability. The framework is built on the combination of Pareto chart and the Fishbone diagram, in conjunction with a set of sustainability metrics (economics, environmental and safety). ***Assessment Tools*: Three case studies with assignment set on steam reforming of methane, polygeneration, and LNG process ***Supporting Documents*: ASPEN Plus design files for the case studies ***Learning Outcomes*: Learn how to combine quality assessment method of Root Cause Analysis (RCA) and sustainability metrics to determine a sustainable manufacturing process

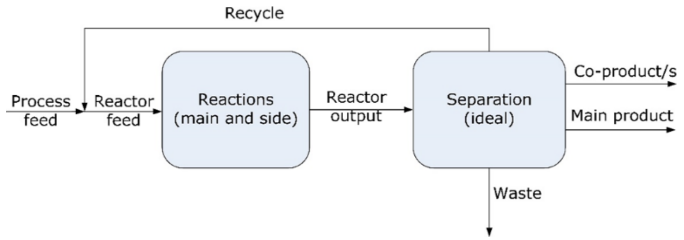
Modules

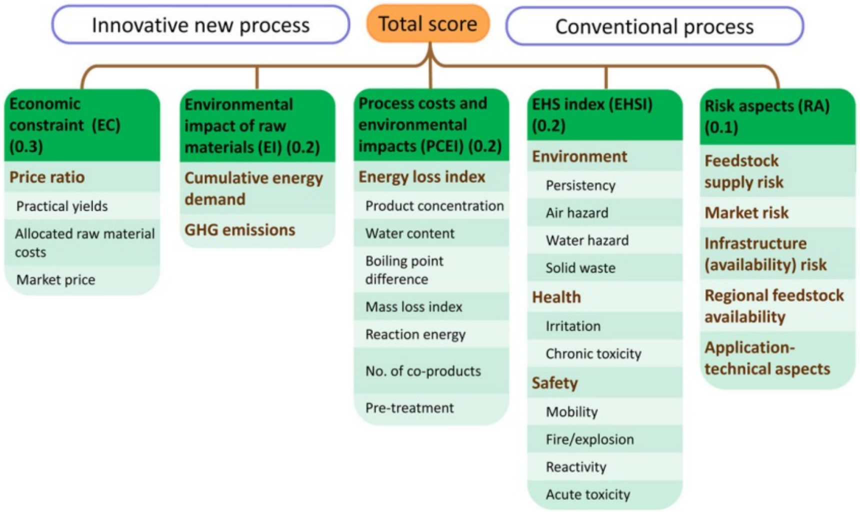
Module Name	Developer/ University	Module Content
Optimization and Uncertainty for Green Design and Industrial Symbiosis	Dr. Urmila Diwekar, Vishwamitra Research Institute and Dr. Yogendra Shastri, IIT Bombay	***Method Topic*****:** Demonstrates the use of optimization methods for sustainable manufacturing. Incorporates systems theory as a valuable tool to enable the integration of multi-scale, multi-disciplinary components using an informational and computational platform. ***Assessment Tools*****:** A case study on mercury waste management from coal power plants, divided into several sub-modules to demonstrate model formulation and solving. ***Supporting Documents*****:** GAMS codes, solution files ***Learning Outcomes*****:** Learn how to use optimization methods as a tool to formulate and solve issues related to sustainable manufacturing

Modules

Module Name	**Developer/ University**	**Module Content**
Early Stage Sustainability Analysis Tool - EarlySim	Akshay Patel/SustAnalyze /Utrecht University	***Tool*: This module provides an early stage chemical process assessment tool. The tool can be used for sustainability assessment in the areas of economic constraints, environmental impact of raw materials, process costs and environmental impact, EHS index, and Risk aspects. ***Assessment Tools*: The module provides a link to a tool available online, instructions on how to use the tool and learning modules. ***Supporting Documents*: Dedicated tool online access, Learning modules, walkthrough for case studies ***Learning Outcomes*: Learn to analyze sustainability issues through a tool based learning environment

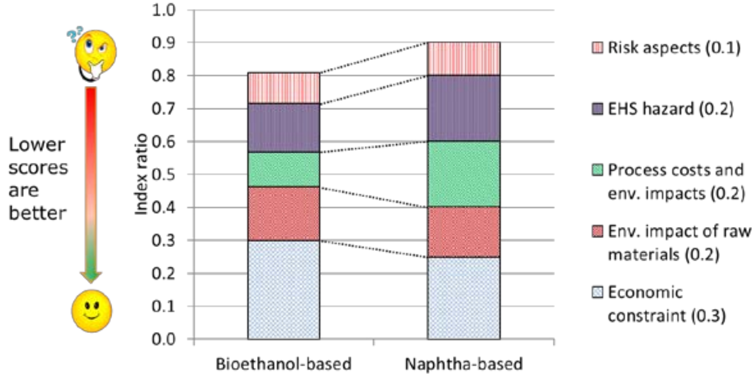
EarlySim Tool





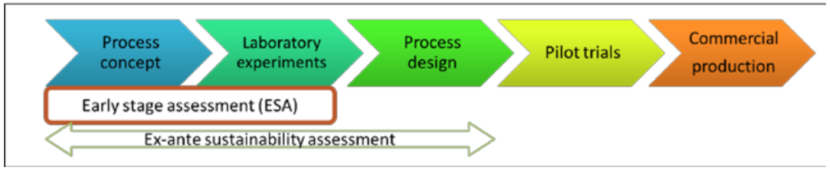
Innovative new process | Total score | Conventional process

- **Economic constraint (EC) (0.3)**
  - **Price ratio**
    - Practical yields
    - Allocated raw material costs
    - Market price
- **Environmental impact of raw materials (EI) (0.2)**
  - **Cumulative energy demand**
  - **GHG emissions**
- **Process costs and environmental impacts (PCEI) (0.2)**
  - **Energy loss index**
    - Product concentration
    - Water content
    - Boiling point difference
    - Mass loss index
    - Reaction energy
    - No. of co-products
    - Pre-treatment
- **EHS index (EHSI) (0.2)**
  - **Environment**
    - Persistency
    - Air hazard
    - Water hazard
    - Solid waste
  - **Health**
    - Irritation
    - Chronic toxicity
  - **Safety**
    - Mobility
    - Fire/explosion
    - Reactivity
    - Acute toxicity
- **Risk aspects (RA) (0.1)**
  - **Feedstock supply risk**
  - **Market risk**
  - **Infrastructure (availability) risk**
  - **Regional feedstock availability**
  - **Application-technical aspects**



Index Ratio = 0.90

Bioethanol Score / Naphtha score



Modules

Module Name	Developer/University	Module Content
Atomic Layer Deposition Nano-Manufacturing Technology	Chris Yuan/University of Wisconsin, Milwaukee	***Process Topic*: This module on atomic layer deposition (ALD) focuses on the study of energy usage and exergy efficiency, simulate reactions inside ALD system and analyze ALD deposition and emissions. ***Assessment Tools*: A design of experiments based assessment of ALD process with sustainability considerations, Minitab example to run DOE ***Supporting Documents*: Detailed process description, experimental requirements, and design of experiments description for sustainability assessment of ALD process ***Learning Outcomes*: Learn details of ALD concept, manufacturing steps, model formulation for DOE, and benefits of sustainable manufacturing principles applied to ALD

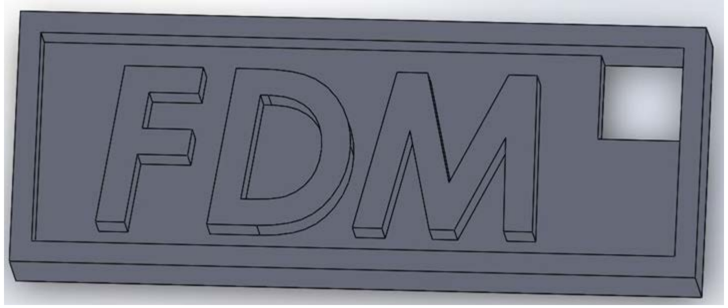
Modules

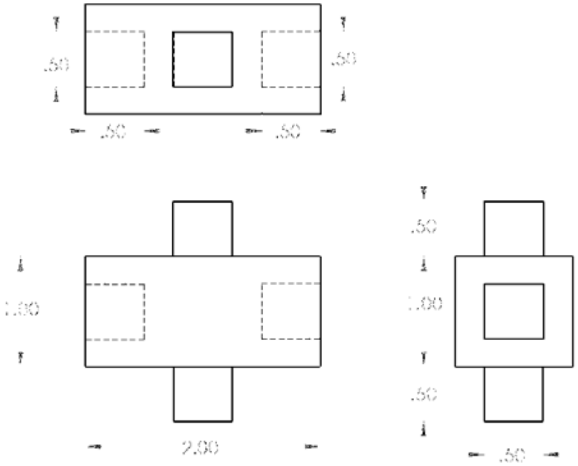
Module Name	**Developer/ University**	**Module Content**
Optimal Design and Operation of Reverse Osmosis Desalination	Mingheng Li/California State Polytechnic	***Process Topic*: Specific energy consumption (SEC) in reverse osmosis (RO) desalination is considered for sustainability of the water treatment process. The module focuses on case studies that help in the optimal design for RO with the sustainability concerns in energy cosumption addressed. ***Assessment Tools*: GAMS program files ***Supporting Documents*: Supporting documentation on RO, homework problems ***Learning Outcomes*: Learn about RO water treatment as a means to provide desalinated water, understand the key sustainability issues with RO desalination, and

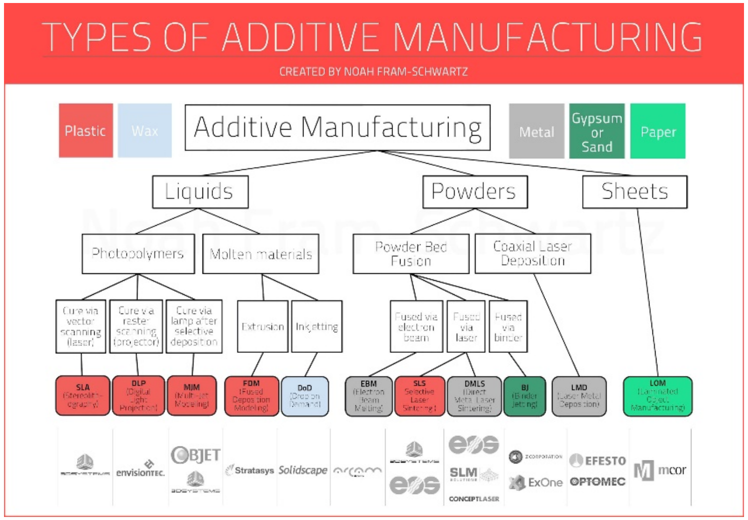
Modules

Module Name	Developer/ University	Module Content
Sustainable Additive Manufacturing	Karl Haapala/Oregon State University	***Process topic*****:** Provides a module that covers additive manufacturing as a means for sustainable manufacturing. This module explains the basics of additive manufacturing, and explores energy analysis as a metric to establish the benefits of AM. ***Assessment tools*****:** Case study in the form of a hands-on laboratory that will educate students about the use of CAD and CAM tools in AM for developing a keychain. ***Supporting documents*****:** CAD exercise file, Powerpoint presentations for different topics covered ***Learning Outcomes*****:** Understand the basics of the new trend in additive manufacturing, have sustainability considerations in design, create effective low cost and low energy consuming manufactured goods.

Additive Manufacturing Module Example







Think-Pair-Share

- What can be done to improve the efficiency of AM processes?
  - Process:
  - Problem:
  - Research:
  - Action:

Modules

Module Name	**Developer/ University**	**Module Content**
Sustainable Mitigation of Carbon Dioxide to Chemicals	Debalina Sengupta and Sherif Khalifa/Texas A&M University and Drexel University	***Process Topic*****:** this module explores CO2 mitigation strategies through the utilization of CO2 into high value chemicals. A superstructure optimization model is formulated and solved for different scenarios. ***Assessment Tools*****:** GAMS program files for several scenarios, homeworks ***Supporting Documents*****:** Case study explanation files, background information documents ***Learning Outcomes*****:** The module is intended to expand the knowledge on CO2 mitigation methods as a means to tackle climate change.

Future Modules

- Currently following modules are under development:
  - Tool:
    - Chemical Complex Analysis tool for Sustainability Analysis
    - Process Modeling and Life Cycle Analysis of 1,3-Propanediol from Fossils and Biomass: Instructor Materials
  - Process:
    - Sustainability of Battery Manufacturing
    - Characterizing and Managing Hydraulic Fracturing Water and Gas Production
    - Sustainable Shale Gas Monetization
    - Electrodialysis Membrane Distillation
  - Method:
    - Process Integration
    - Sustainability Cost Assessment for Manufacturing
    - Water-Energy Nexus
    - Biomass Feedstock Properties
- Help is sought in the academic community for knowledge dissemination and utilization of the modules

Web Resources and Additional Readings

Modules are made available through the following website: Computer Aids in Chemical Engineering “CACHE”:

http://cache.org/super-store

Additional Reading: Sengupta, D., Y. Huang, C. I. Davidson, T. F. Edgar, M. Eden, and M. M. El-Halwagi, “Using Module-Based Learning Methods to Introduce Sustainable Manufacturing in Engineering Curriculum”, Int. J. Sustainability in Higher Education 18(3), 307-328 (2017)

Acknowledgement

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For more information, please contact Dr. Debalina Sengupta
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TEXAS A&M
UNIVERSITY.

Part III:
Concepts, Tools, and Examples on Sustainable Design for Inclusion in the Senior-level Design Course(s) or an Elective

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Professor and Holder of the McFerrin Professorship
The Artie McFerrin Department of Chemical Engineering
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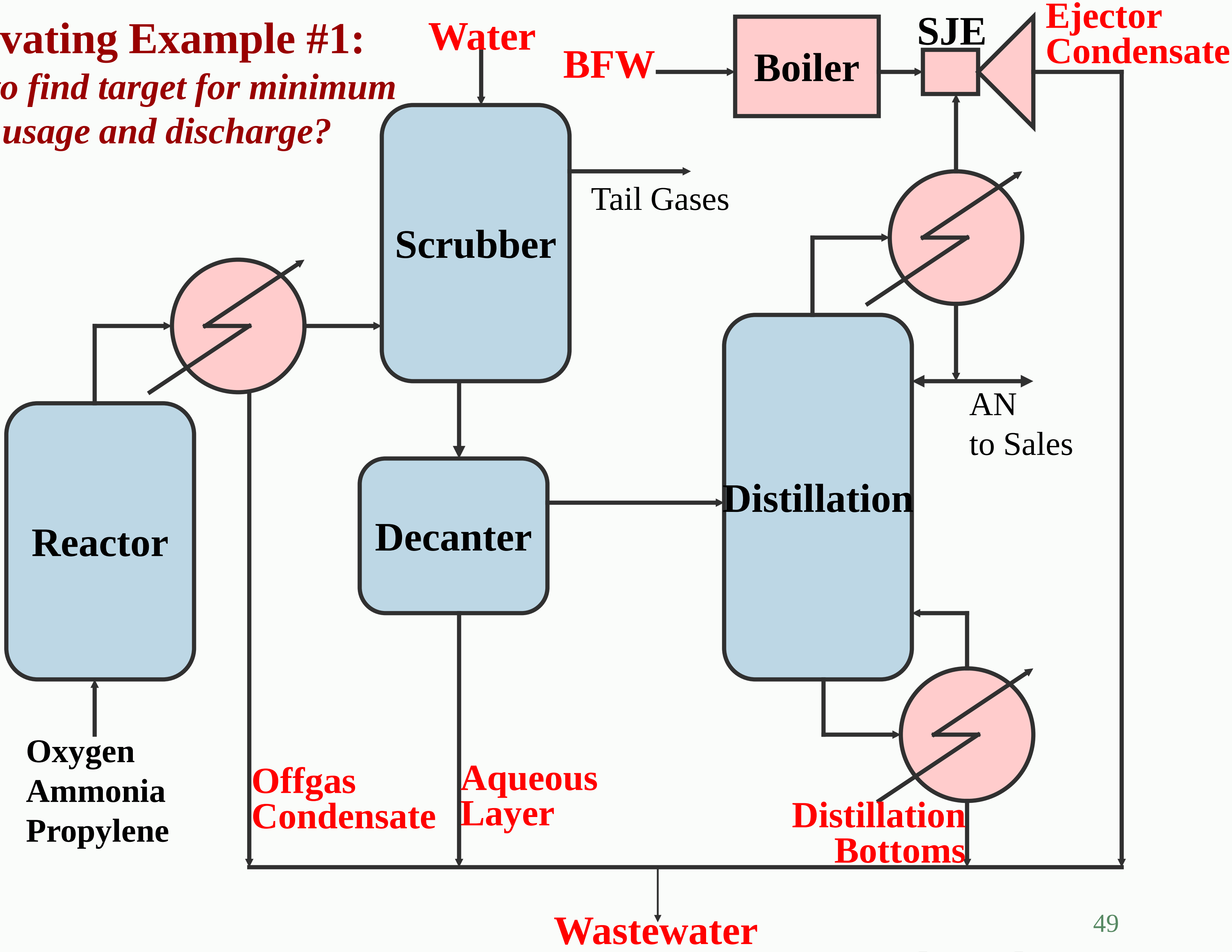
Motivating Example #1:

How to find target for minimum water usage and discharge?



Water

BFW

Boiler

SJE

Ejector Condensate

Scrubber

Tail Gases

Reactor

Decanter

Distillation

AN to Sales

Oxygen
Ammonia
Propylene

Offgas Condensate

Aqueous Layer

Distillation Bottoms

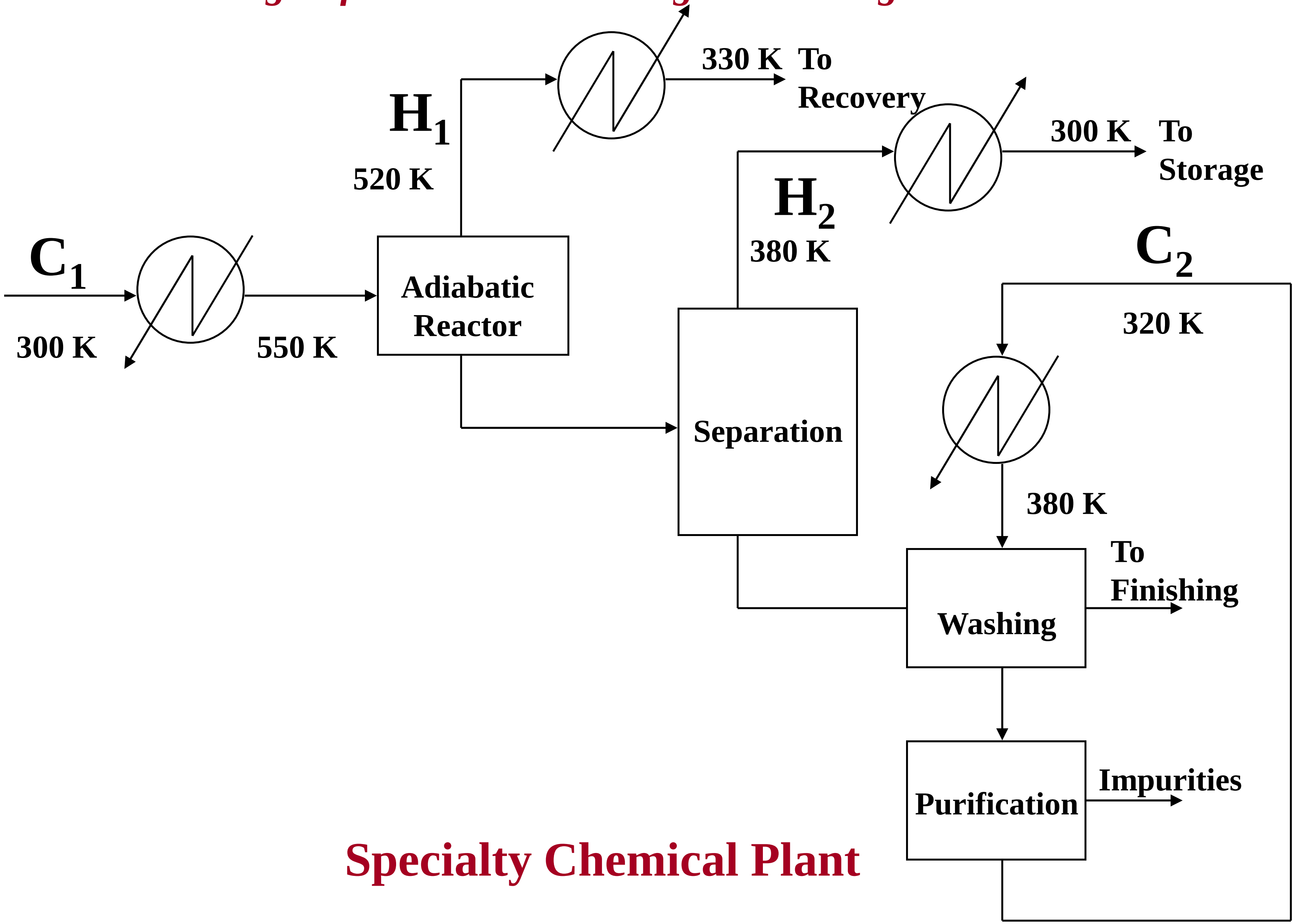
Wastewater (to Biotreatment)

Bottleneck

Motivating Example #2:

What is wrong with this flowsheet from an energy perspective?

What are the targets for minimum heating and cooling utilities?



Specialty Chemical Plant

OBSERVATIONS

- **Numerous alternatives**
- **Intuitively non-obvious solutions**
- **Focus on root causes not symptoms, must go to heart of process**
- **Need a systematic methodology to extract optimum solution**
- **Process must be treated as an integrated system**

Conventional Engineering Approaches

- Brainstorming among experienced engineers

- Evolutionary techniques: copy (or adapt) the last design we or someone else did

- Heuristics based on experience-based rules

Limitations of Conventional Approaches

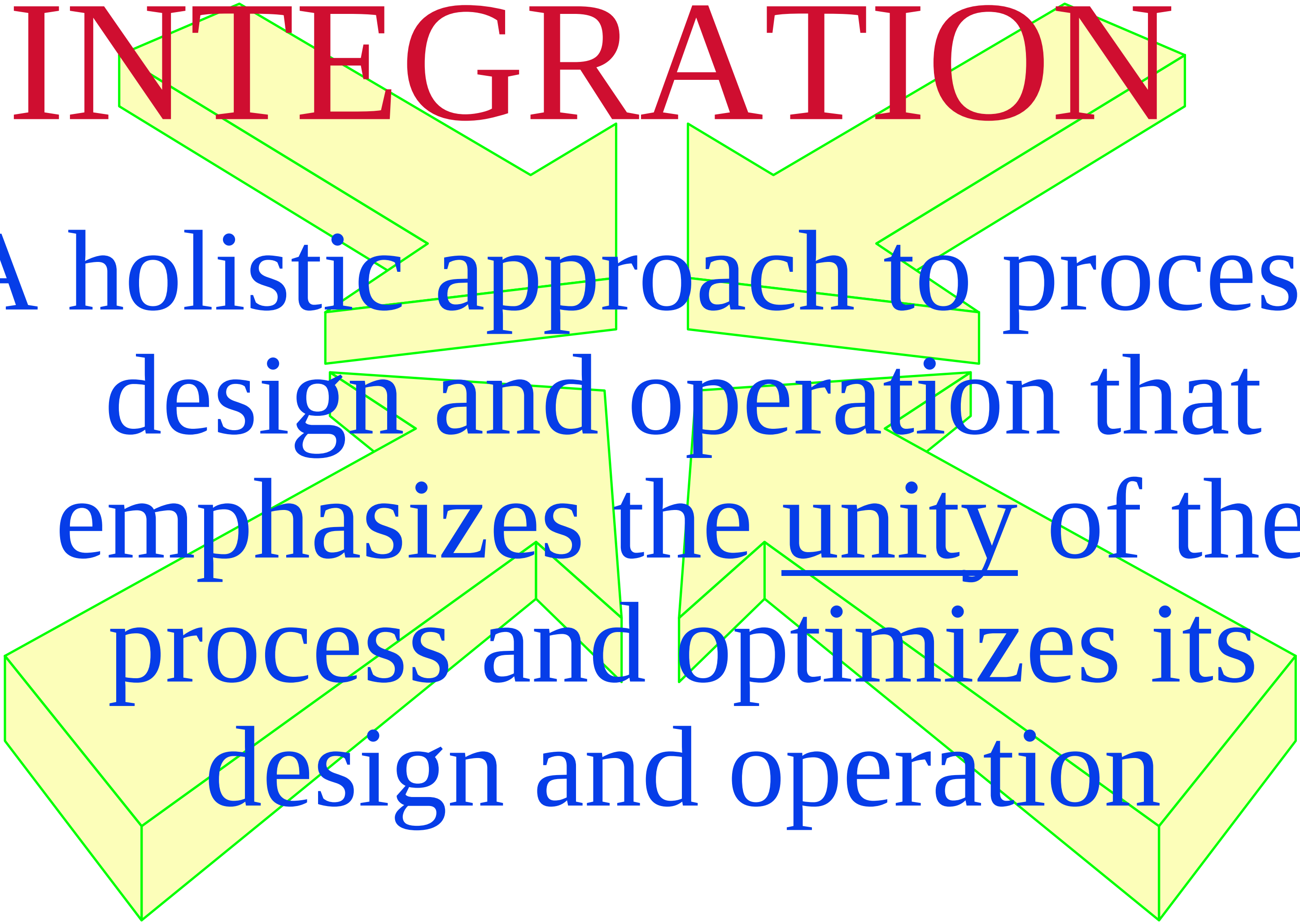
- Time and money intensive
- Cannot enumerate the infinite alternatives
- Is not guaranteed to come close to optimum solutions (except for very simple cases or extreme luck)
- Does not shed light on global insights and key characteristics of the process
- Severely limits groundbreaking and novel ideas.

State of the art:

Systematic, fundamental, and generally applicable techniques can be learned and applied to synthesize optimal designs for improving process performance.

This is possible via *Process Synthesis and Integration*

PROCESS INTEGRATION

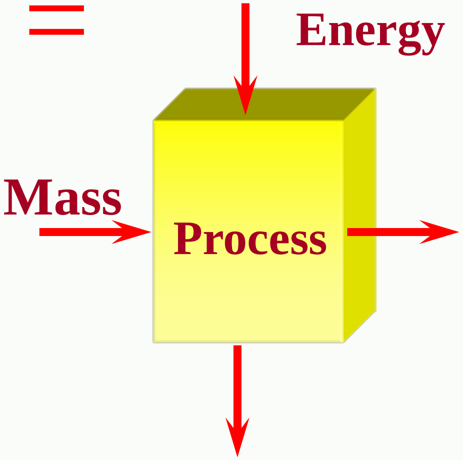


A holistic approach to process design and operation that emphasizes the unity of the process and optimizes its design and operation

PROCESS INTEGRATION =

MASS INTEGRATION +

ENERGY INTEGRATION



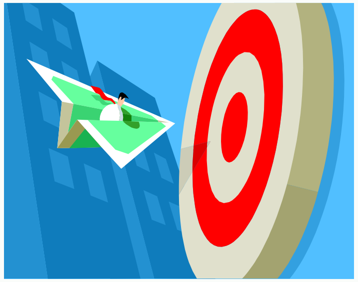
Overall Philosophy

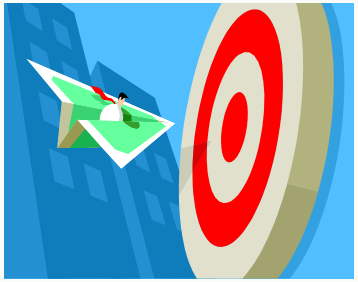
BIG PICTURE FIRST,
DETAILS LATER

FIRST, understand the global picture of the process and develop system insights

LATER, think equipment, detailed simulation, and process details.

TARGETING APPROACH OF PROCESS INTEGRATION





Identification of performance targets for the whole process AHEAD of detailed design!!!

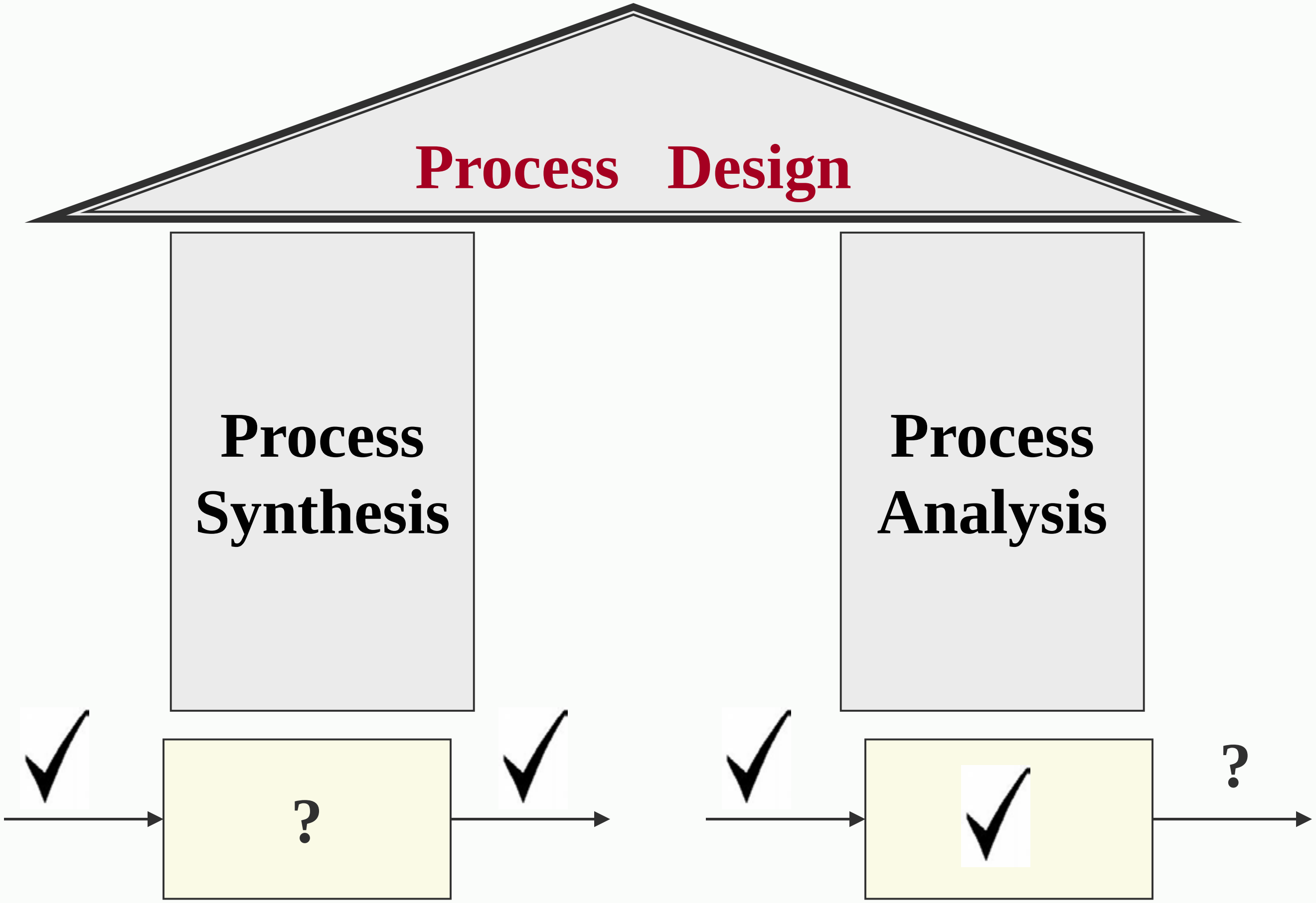
Specific Performance Objectives

- **Profitability improvement (maximization)**
- **Yield enhancement (maximization)**
- **Resource (mass and energy) conservation (minimization)**
- **Pollution prevention/waste minimization (minimization)**

All leading to sustainability

PILLARS OF PROCESS DESIGN

Process Design = Process Synthesis + Process Analysis

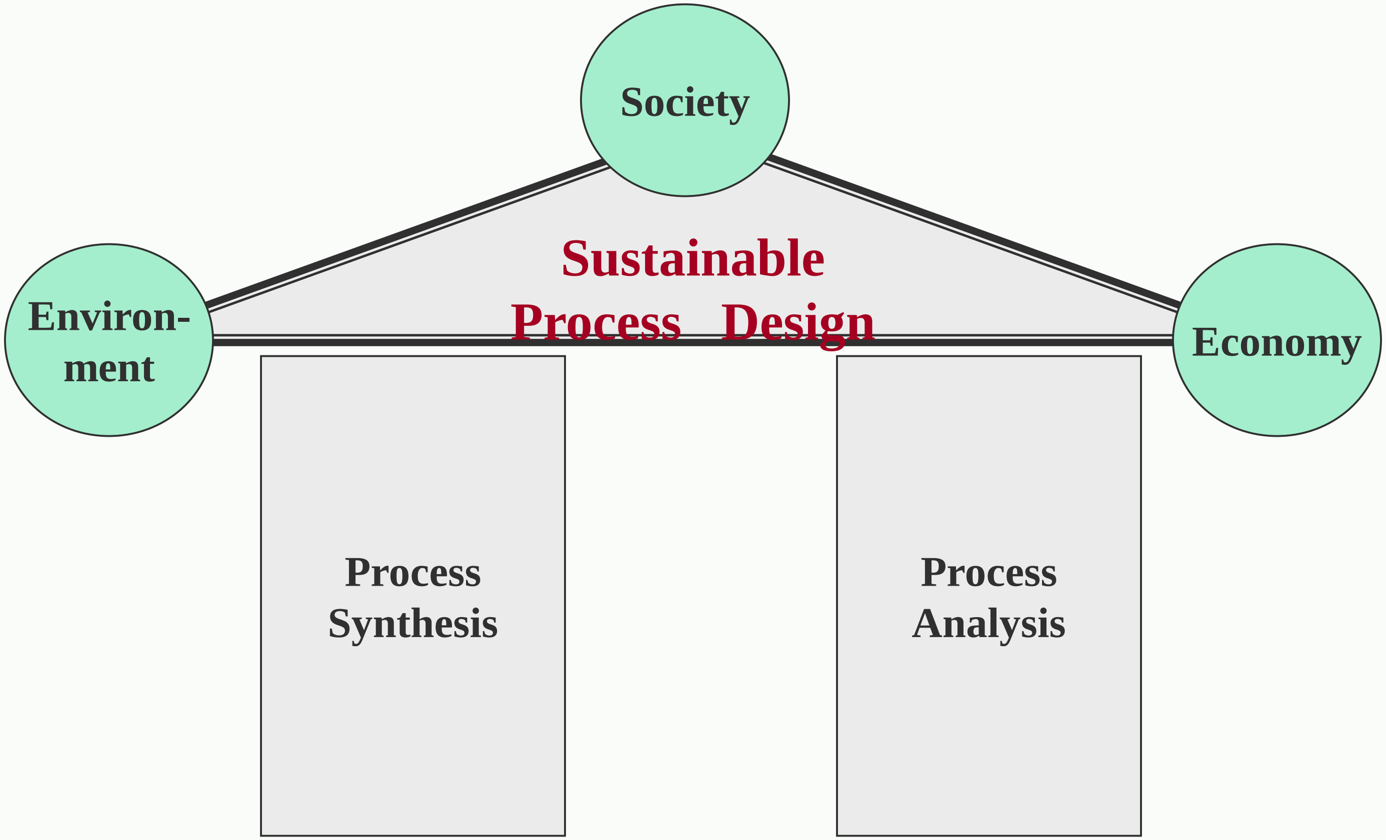


Process Design

Process Synthesis

Process Analysis

WHAT IS SUSTAINABLE PROCESS DESIGN?



Process design activities that lead to economic growth, environmental protection, and social progress for the current generation without compromising the potential of future generations to have an ecosystem which meets their needs.

BENCHMARKING PROCESS PERFORMANCE THROUGH OVERALL MASS TARGETING

- **Benchmarking** : The determination of a standard of excellence against which the process performance can be compared.
- Benchmarking can be systematically performed using targeting.

- **Targeting:** The identification of performance benchmarks that can be **determined ahead of carrying out a detailed design (for new processes) or without conducting an in-depth analysis (for existing processes).**

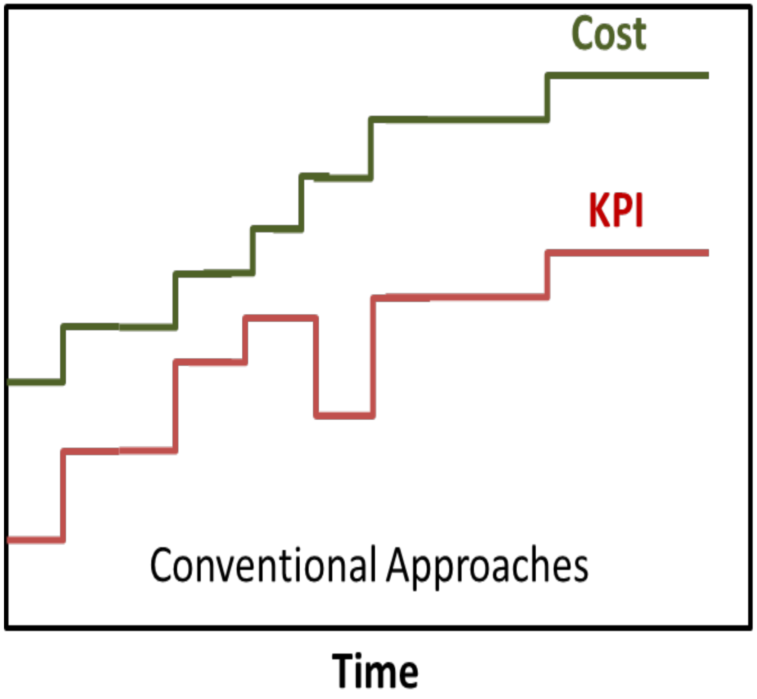
- The overarching philosophy in targeting is "*big picture first, details later*"

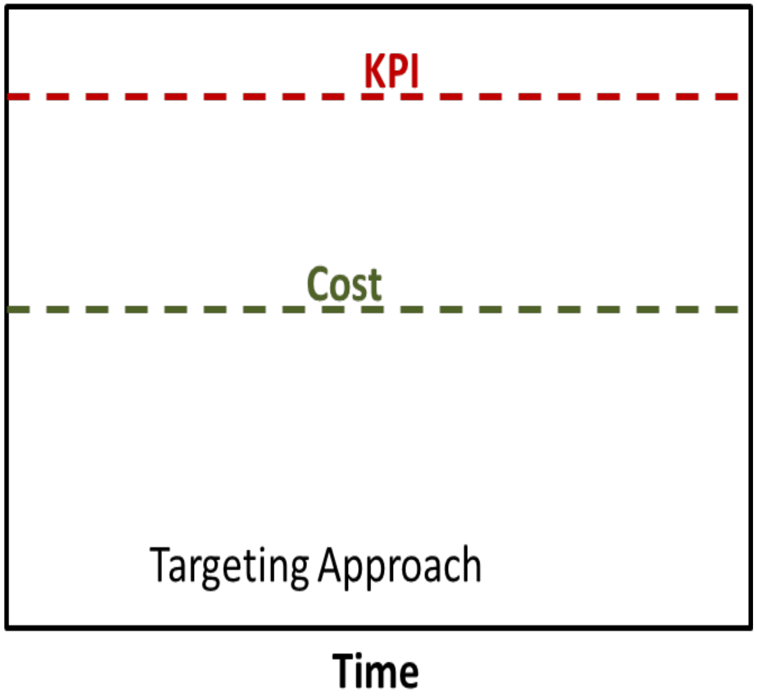
- The emphasis is on using minimum data and calculations to identify performance limits.

Examples of overall mass targets include:

  - Maximum yield of desired products or byproducts
  - Minimum usage of raw materials
  - Minimum usage of material utilities (e.g., solvents, water)
  - Minimum discharge of pollutants and waste streams

Targeting vs. Conventional “Learning Curve” Approaches





OVERALL MASS TARGETING APPROACHES

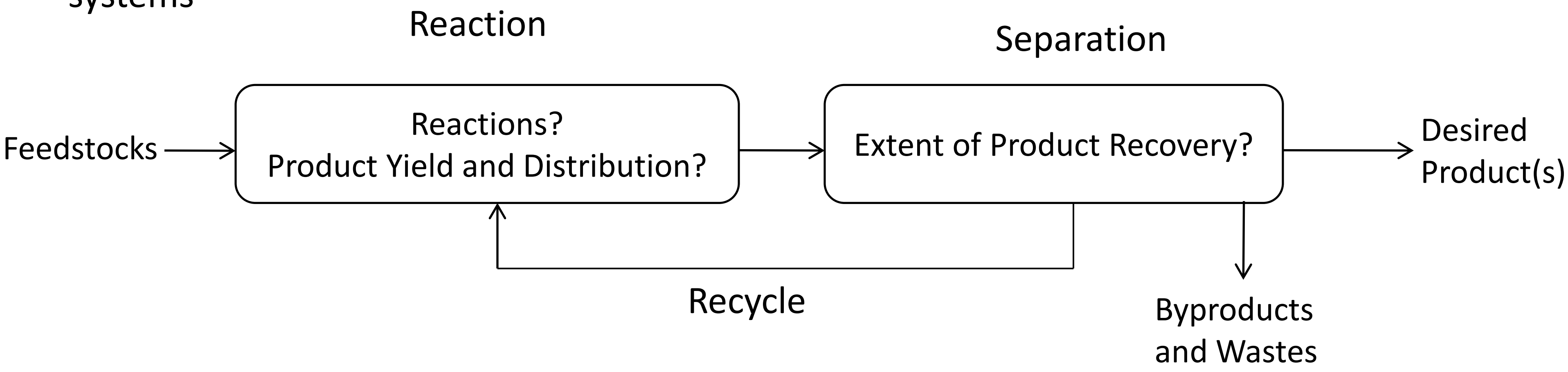
- **Stoichiometric calculations**: when there are very limited data and information for the process (e.g., initial consideration of a new process)

- **Mass integration**: for existing processes or process designs with sufficient details

- **Atomic targeting and industrial symbiosis**: based on tracking specific atoms to establish multi-scale benchmarks for chemical species and for individual or multiple processes

OVERALL MASS TARGETING APPROACHES

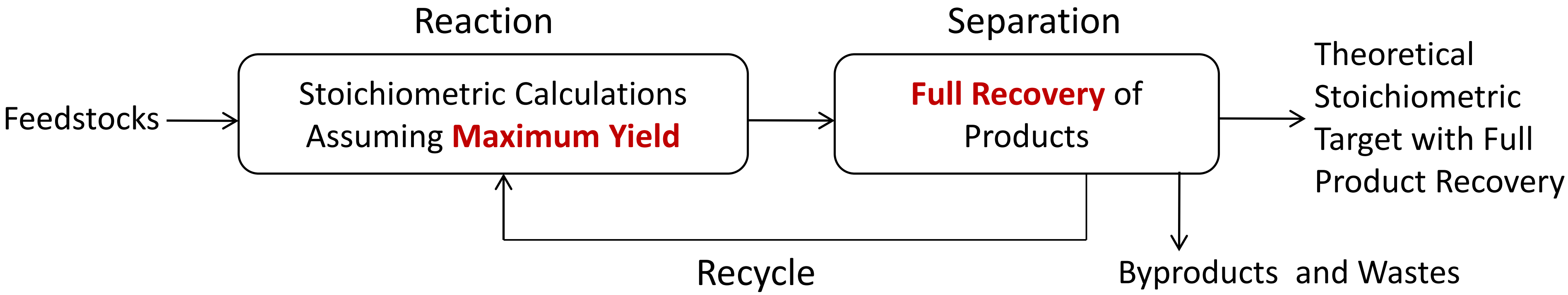
- Given a chemical pathway to convert certain feedstocks into products.
- Interest in designing a process based on this chemical pathway
- Very limited data are available
- Before detailed design, it is desired to perform targeting to estimate the flows of the key feedstocks and products.
- For targeting purposes, consider a generic process with reaction and separation systems



LEVELS OF STOICHIOMETRIC TARGETING

Depending on the type of available data, three levels of stoichiometric targets:

Level I: Theoretical stoichiometric targets with full product recovery: When only the process chemistry is available in the form of an overall reaction, the stoichiometric calculations are carried out assuming **maximum reaction yield** and **full recovery** of the product.



Reaction

Separation

Feedstocks

Stoichiometric Calculations Assuming **Maximum Yield**

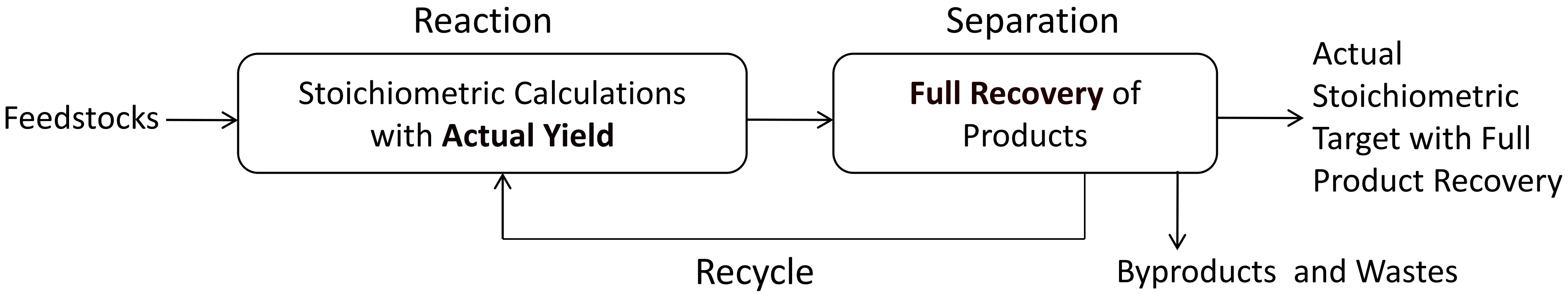
Full Recovery of Products

Theoretical Stoichiometric Target with Full Product Recovery

Recycle

Byproducts and Wastes

Level II: Actual stoichiometric targets without product losses: When the process chemistry is available in the form of an overall reaction along with the actual yield data for the product (from experiments, thermodynamic-equilibrium models, or reaction models), the stoichiometric calculations are carried out using the **actual reaction yield** and **full recovery** of the product


Reaction

Separation

Feedstocks

Stoichiometric Calculations with **Actual Yield**

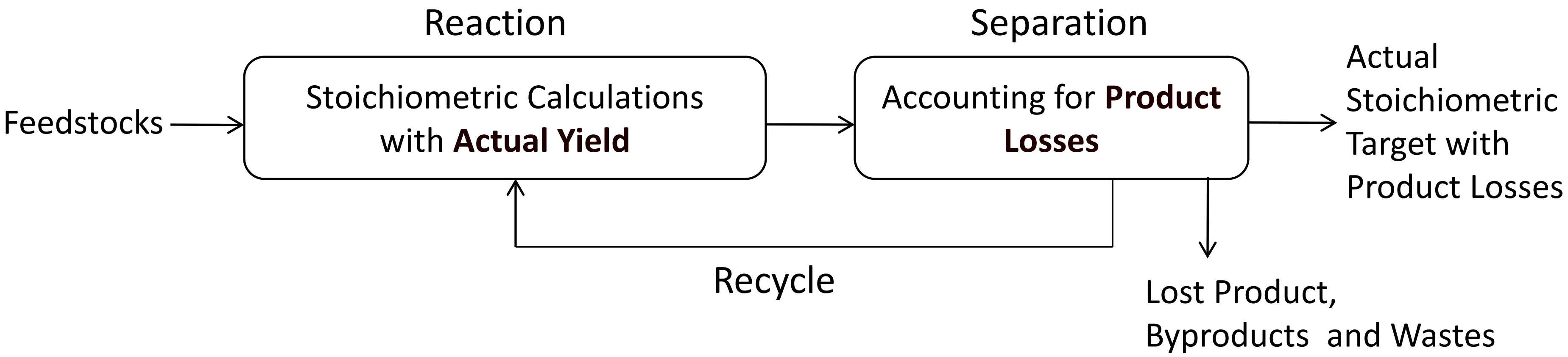
Full Recovery of Products

Actual Stoichiometric Target with Full Product Recovery

Recycle

Byproducts and Wastes

Level III: Actual stoichiometric targets with product losses: When the process chemistry is available in the form of an overall reaction along with data on the actual yield of the product and its expected fractional recovery in the separation systems, the stoichiometric calculations are carried out using the **actual reaction yield** while accounting for the **expected losses** of the product.



Reaction

Separation

Feedstocks

Stoichiometric Calculations with **Actual Yield**

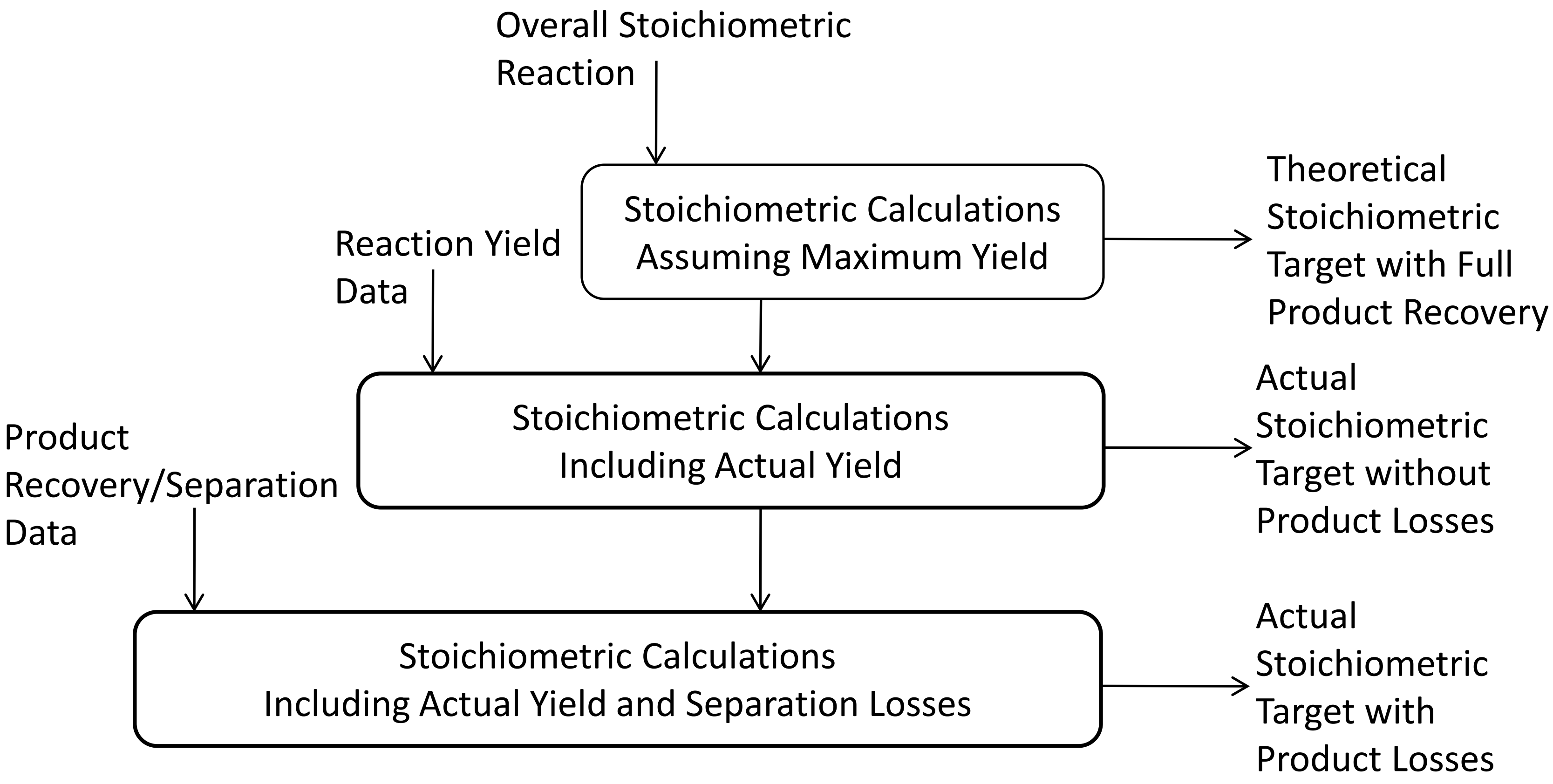
Accounting for **Product Losses**

Actual Stoichiometric Target with Product Losses

Recycle

Lost Product, Byproducts and Wastes

SUMMARY OF THE THREE LEVELS OF STOICHIOMETRIC TARGETING



Overall Stoichiometric Reaction

Stoichiometric Calculations Assuming Maximum Yield

Theoretical Stoichiometric Target with Full Product Recovery

Reaction Yield Data

Stoichiometric Calculations Including Actual Yield

Actual Stoichiometric Target without Product Losses

Product Recovery/Separation Data

Stoichiometric Calculations Including Actual Yield and Separation Losses

Actual Stoichiometric Target with Product Losses

STOICHIOMETRIC-ECONOMIC “STOICHIO-NOMIC” TARGETING

For quick and preliminary targeting using stoichiometric targeting results and simple economic data

Economic Gross Potential “EGP” =

$$\sum_{p=1}^{N_{\text{Products}}} \text{Annual production rate of product p} * \text{Selling price of product p} \quad - \sum_{r=1}^{N_{\text{Reactants}}} \text{Annual feed rate of reactant r} * \text{Purchased price of reactant r}$$

$EGP > 0$ Process may be considered for further analysis

$EGP \leq 0$ Process is not economically viable

Metric for Inspecting Sales and Reactants "MISR"

$$\textbf{MISR} = \frac{\sum_{p=1}^{N_{\text{Products}}} \text{Annual production rate of product p} * \text{Selling price of product p}}{\sum_{r=1}^{N_{\text{Reactants}}} \text{Annual feed rate of reactant r} * \text{Purchased price of reactant r}}$$

MISR $>$ 1 Process may be considered for further analysis

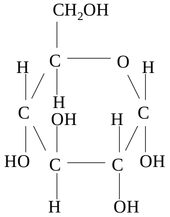
MISR $\leq$ 1 Process is not economically viable

High values of MISR are desirable

Rule of thumb: start the detailed analysis for process candidates with the highest values of MISR

Example 1. Stoichiometric Targeting of Ethanol Production from Glucose

A new process is to be designed for the conversion of 150 MM kg/yr of sugar to ethanol. The sugar is taken to be in the form of glucose



($C_6H_{12}O_6$) and is converted to ethanol (C_2H_5OH) through the following overall fermentation reaction:

$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$$

a. Calculate the maximum theoretical stoichiometric target for ethanol

b. Available experimental data (Krishnan et al., 1999) show that the actual reaction yield that can be obtained is 0.46 kg ethanol/kg glucose. Determine the actual stoichiometric target for ethanol.

c. In separating ethanol from the reaction mixture, it is expected to lose 5% of ethanol with the wastewater stream. What is the actual stoichiometric target for ethanol when the separation losses are accounted for?

Solution:

a. To evaluate the theoretical target for ethanol, let us assume full conversion of glucose according to the overall stoichiometric reaction:

$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$$

Molecular weights: 180 2*46 + 2*44

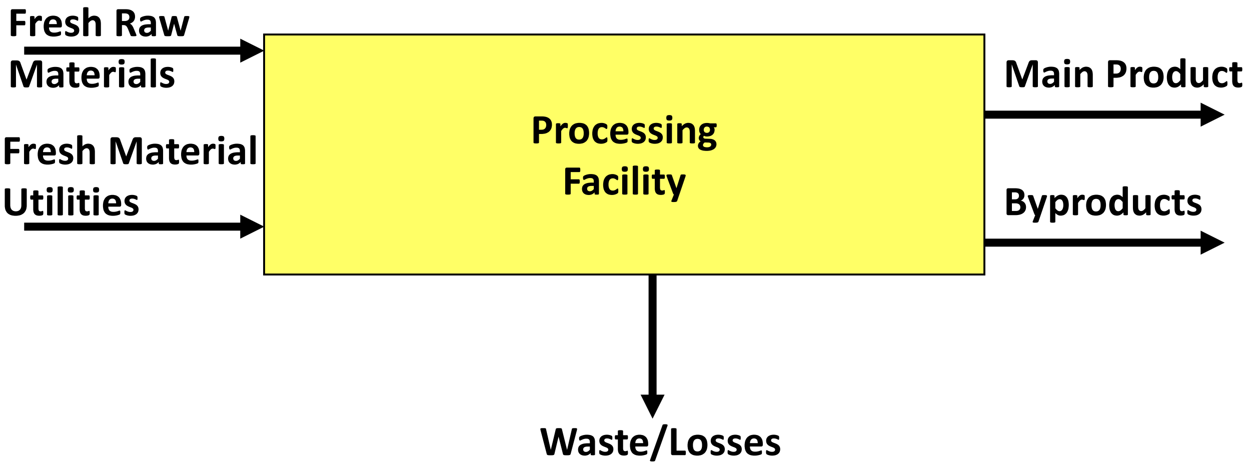
➔ Theoretical yield of ethanol from glucose = $\frac{2*46}{180}$ = 0.51 kg ethanol/kg glucose

For a feed rate of 150 MM kg/yr of glucose,
The theoretical stoichiometric target of ethanol =
0.51 kg ethanol/kg glucose*150 MM kg glucose/yr = 76.5 MM kg ethanol/yr

b. For the reported experimental yield,
The actual stoichiometric target of ethanol =
0.46 kg ethanol/kg glucose*150 MM kg glucose/yr = 69.0 MM kg ethanol/yr
(10% less than the theoretical stoichiometric target)

c. By accounting for 5% loss of ethanol in separation,
The actual stoichiometric target of ethanol with product losses
= 0.95*69.0 = 65.6 MM kg ethanol/yr

OVERALL MASS TARGETING THROUGH MASS INTEGRATION



How to benchmark performance for mass objectives of an existing process or a process design with sufficient details (e.g., flowsheet, mass balance, Process model), the whole process ahead of detailed design?

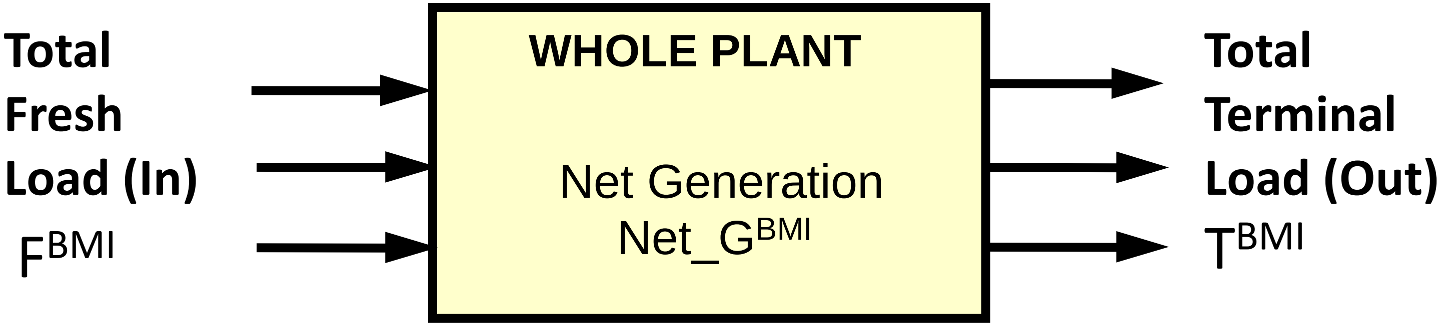
Mass integration is a systematic "big-picture" methodology that provides a fundamental understanding of the global flow of mass within the process and employs this understanding in identifying performance targets and optimizing the generation and routing of species throughout the process

Applications:

- **Minimization of waste discharge/losses**
- **Minimization of purchase of fresh resources (raw materials, material utilities)**
- **Maximization of yield of desired products/byproducts**

Example 1: Reduction of Terminal Losses or Discharge of Waste

- **Terminal Load (out) = Fresh Load (in) + Net Generation**



Total Fresh Load (In)

F^{BMI}

WHOLE PLANT

Net Generation

Net_G^{BMI}

Total Terminal Load (Out)

T^{BMI}

Overall Mass Balance Before Mass Integration (BMI)

$$T^{BMI} = F^{BMI} + Net\_G^{BMI}$$

For fixed generation:

Minimum terminal (out) corresponds to minimum fresh (in)

To minimize fresh:

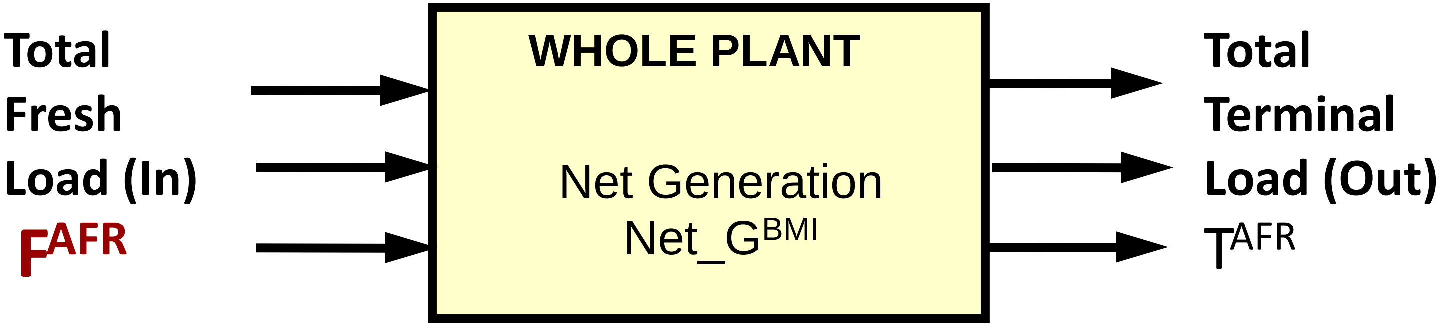
1. Adjust design and operating variables
2. Maximize recycle to replace fresh usage

1. Adjust Design and Operating Variables to Reduce Fresh

- **What are the design and operating variables in the process that influence fresh consumption?**
- **Which ones are allowed to be changed (manipulated variables)?**
- **How is fresh usage related to these design and operating variables?**

Fresh Usage = f (manipulated design variables, manipulated operating variables)

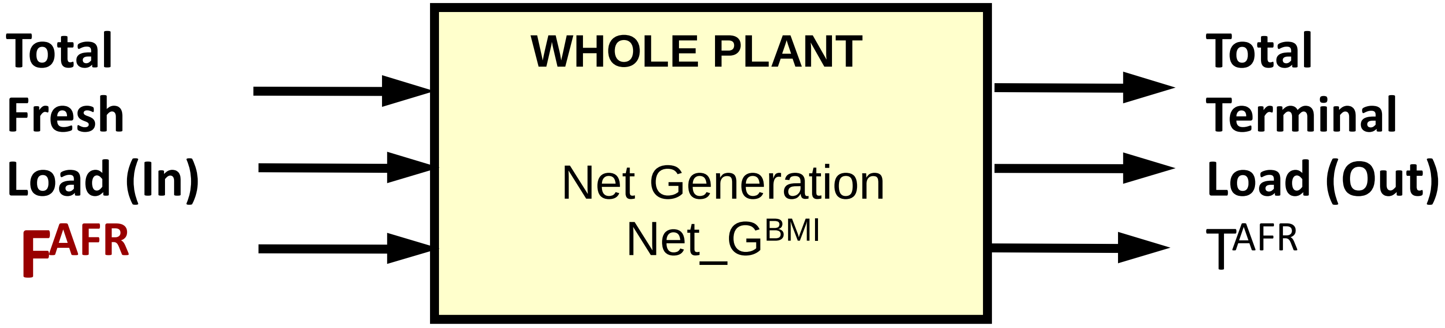
F^{AFR}= minimize f (manipulated design variables, manipulated operating variables)



Overall Mass Balance after Fresh Reduction

$$T^{AFR} = F^{AFR} + Net\_G^{BMI}$$

2. Maximize Recycle to Reduce Fresh Usage



Total Fresh Load (In) F^{AFR}

WHOLE PLANT

Net Generation Net_G^{BMI}

Total Terminal Load (Out) T^{AFR}

Overall Mass Balance after Fresh Reduction

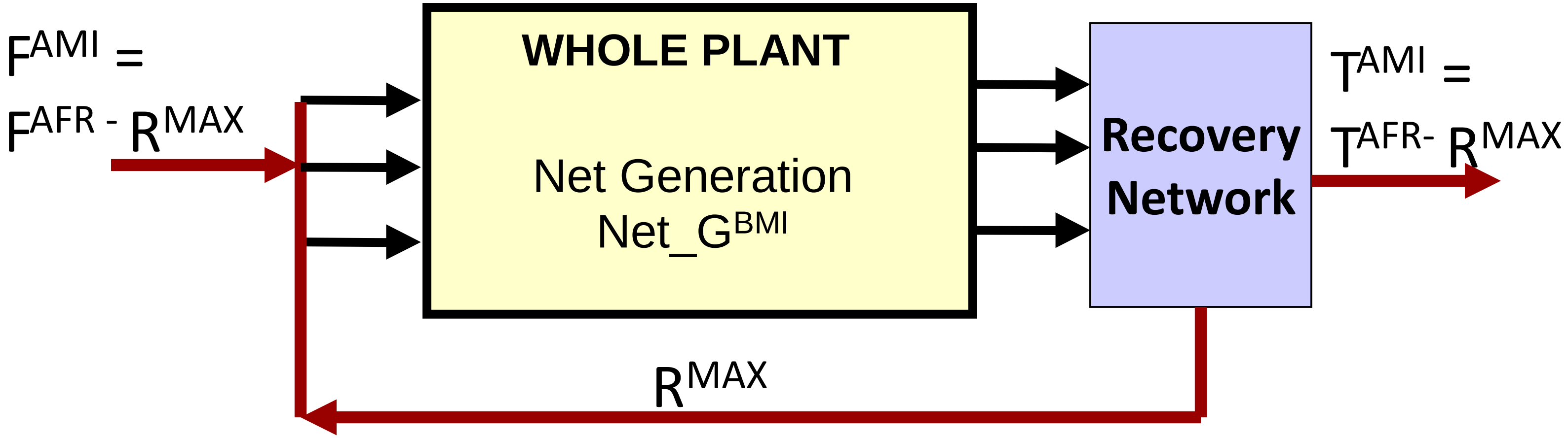
$$T^{AFR} = F^{AFR} + Net\_G^{BMI}$$

Need to replace maximum load of fresh load with recycled terminal load

What is maximum recyclable load?

Recycle Rules to Reduce Terminal Load (continued):

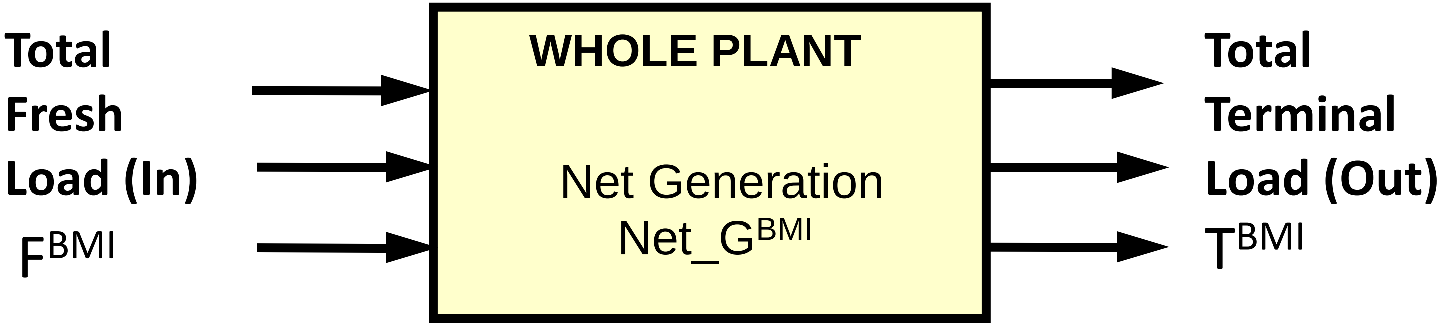
- Recovery devices can recover (almost) all terminal load and render acceptable quality to replace fresh feed. During targeting, cost and details of recovery are not relevant (yet)
- Maximize recycle from outlet path to fresh inlets (can recycle the smaller of the two loads: total recovered terminal vs. total needed fresh). R^{max} = argmin $\{F^{AFR}, T^{AFR}\}$



Target After Mass Integration (AMI)

Example 2: Reduction of Terminal Losses or Discharge of Waste for Variable Generation

- **Terminal Load (out) = Fresh Load (in) + Net Generation**



Overall Mass Balance Before Mass Integration (BMI)

$$T^{BMI} = F^{BMI} + Net\_G^{BMI}$$

Minimize generation of waste
(or targeted species)

Minimize fresh:

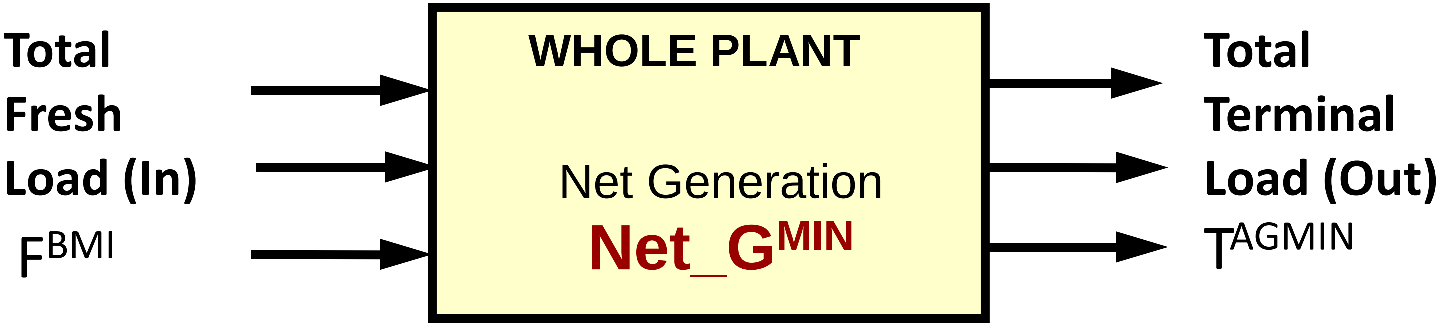
1. Adjust design and operating variables
2. Maximize recycle to replace fresh usage

When generation and fresh cannot be decoupled, see : Noureldin, M. B. and M. M. El-Halwagi, 2000, “Pollution-Prevention Targets through Integrated Design and Operation", Comp. Chem. Eng., 24, 1445-1453.

Minimizing Generation of Waste

Minimize generation (or maximize depletion) of targeted species (e.g., Describe generation quantitatively then identify values of design and operating conditions of reactors to minimize generation)

Terminal Load (out) = Fresh Load (in) + Generation (- Depletion)

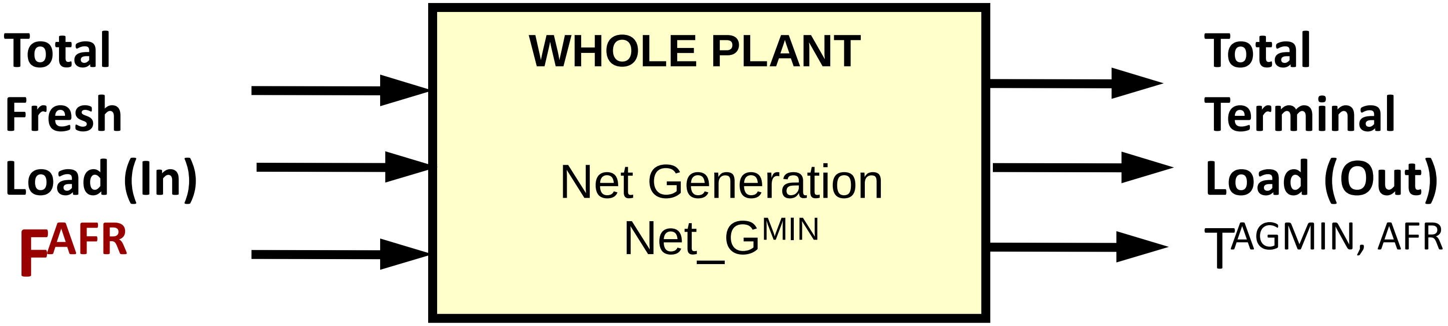


Overall Mass Balance after Minimization of Generation

$$T^{AGMIN} = F^{BMI} + Net\_G^{MIN}$$

Adjust Design and Operating Variables to Reduce Fresh

Terminal Load (out) = Fresh Load (in) + Generation (- Depletion)

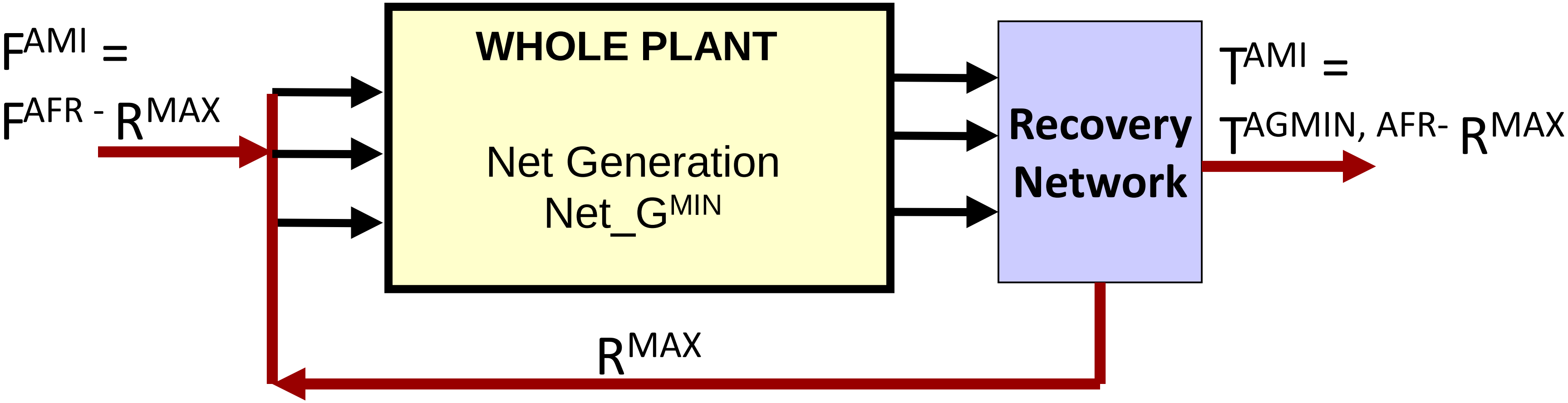


Overall Mass Balance after Fresh Reduction and Minimization of Generation

$$T^{AGMIN, AFR} = F^{AFR} + Net\_G^{MIN}$$

Recycle Rules to Reduce Terminal Load (continued):

- **Recovery devices can recover (almost) all terminal load and render acceptable quality to replace fresh feed. During targeting, cost and details of recovery are not relevant (yet)**
- **Maximize recycle from outlet path to fresh inlets (can recycle the smaller of the two loads: total recovered terminal vs. total needed fresh). $R^{max} = \text{argmin}\,\{F^{AFR}, T^{AGMIN, AFR}\}$**



$F^{AMI} =$

$F^{AFR} - R^{MAX}$

WHOLE PLANT

Net Generation

Net_G^{MIN}

Recovery Network

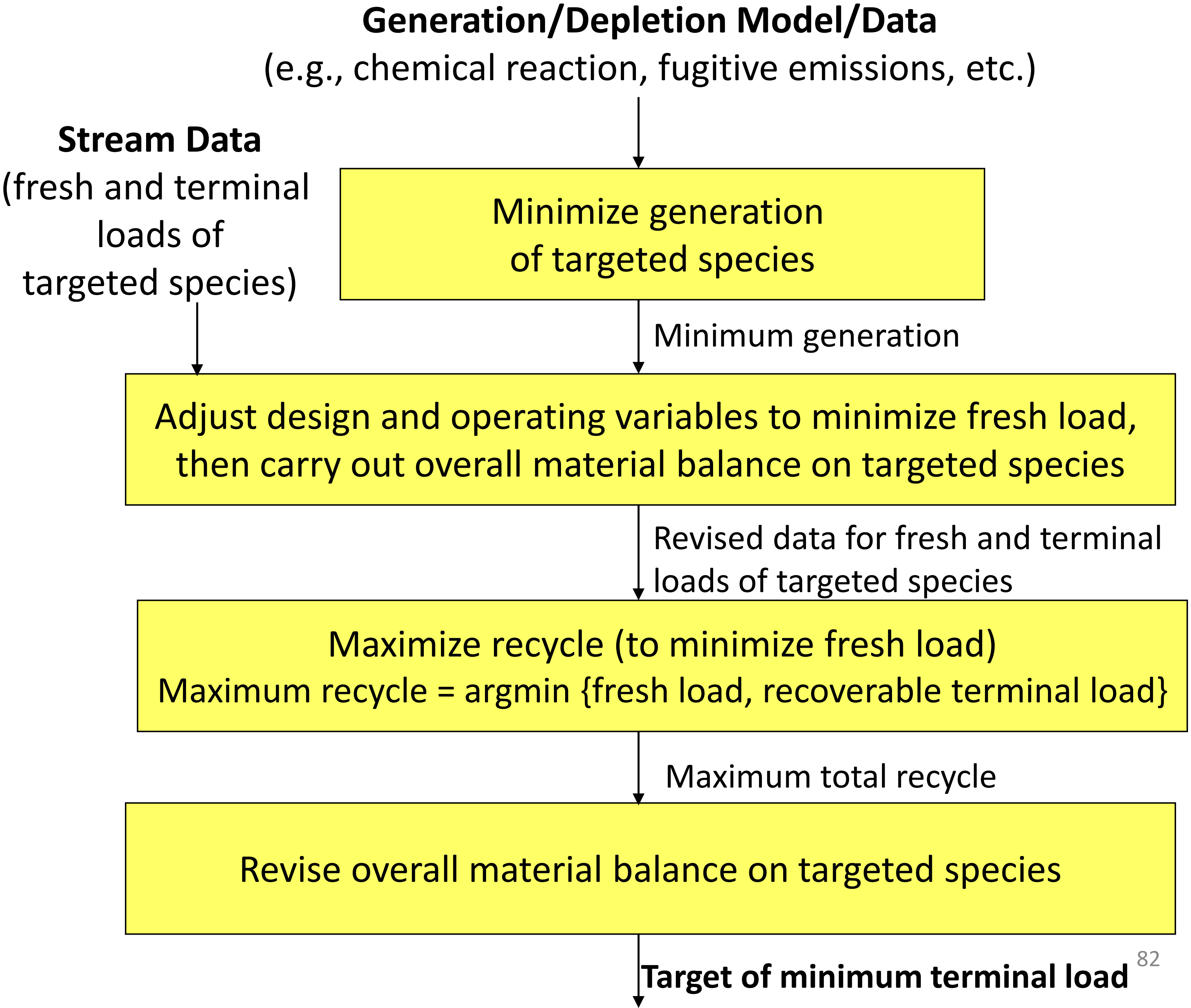
$T^{AMI} =$

$T^{AGMIN, AFR} - R^{MAX}$

R^{MAX}

Target After Mass Integration (AMI)

TARGETING PROCEDURE TO MINIMIZE TERMINAL LOSS OR WASTE DISCHARGE



Generation/Depletion Model/Data
(e.g., chemical reaction, fugitive emissions, etc.)

Stream Data
(fresh and terminal
loads of
targeted species)

Minimize generation
of targeted species

Minimum generation

Adjust design and operating variables to minimize fresh load,
then carry out overall material balance on targeted species

Revised data for fresh and terminal
loads of targeted species

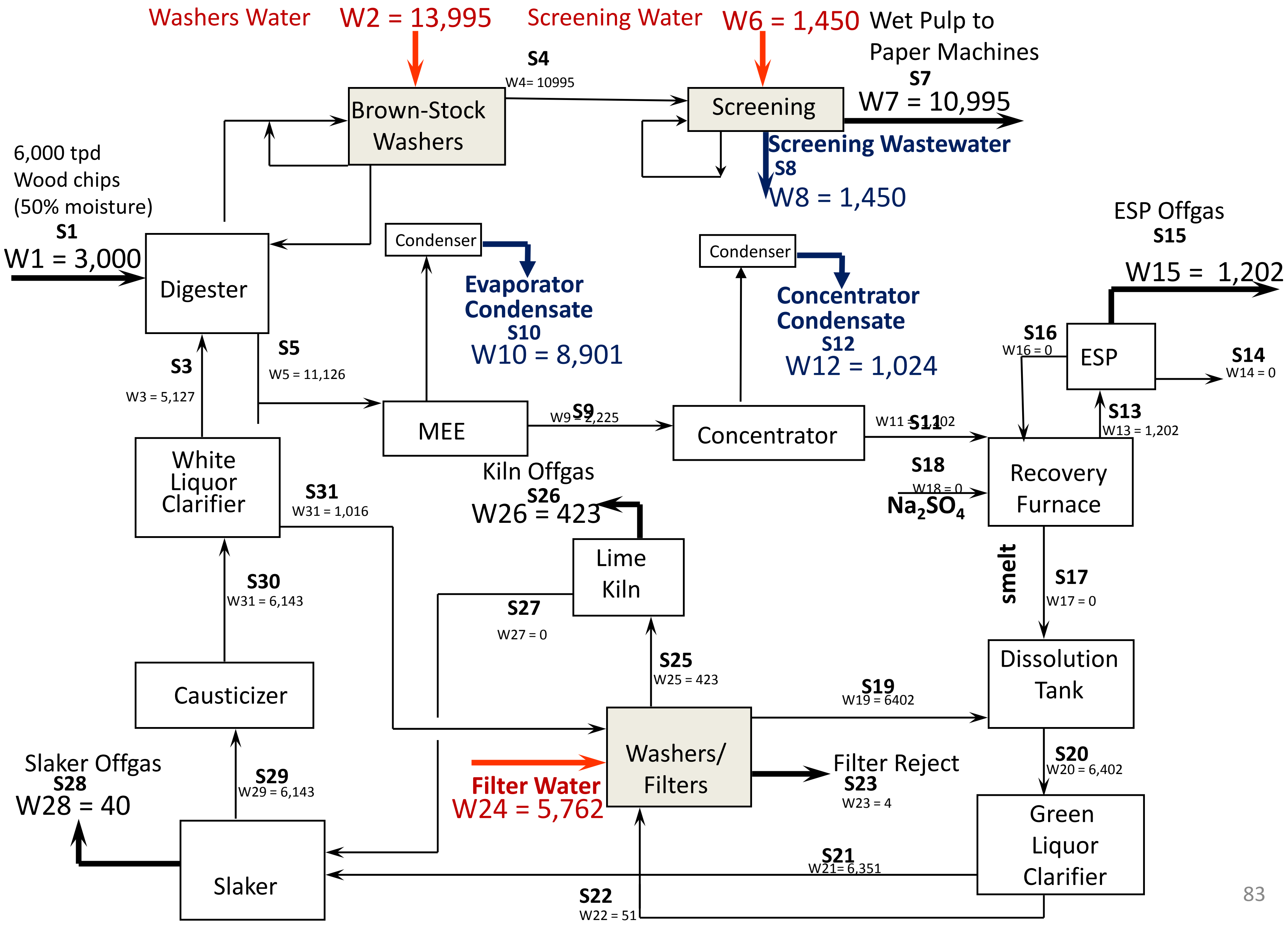
Maximize recycle (to minimize fresh load)
Maximum recycle = argmin {fresh load, recoverable terminal load}

Maximum total recycle

Revise overall material balance on targeted species

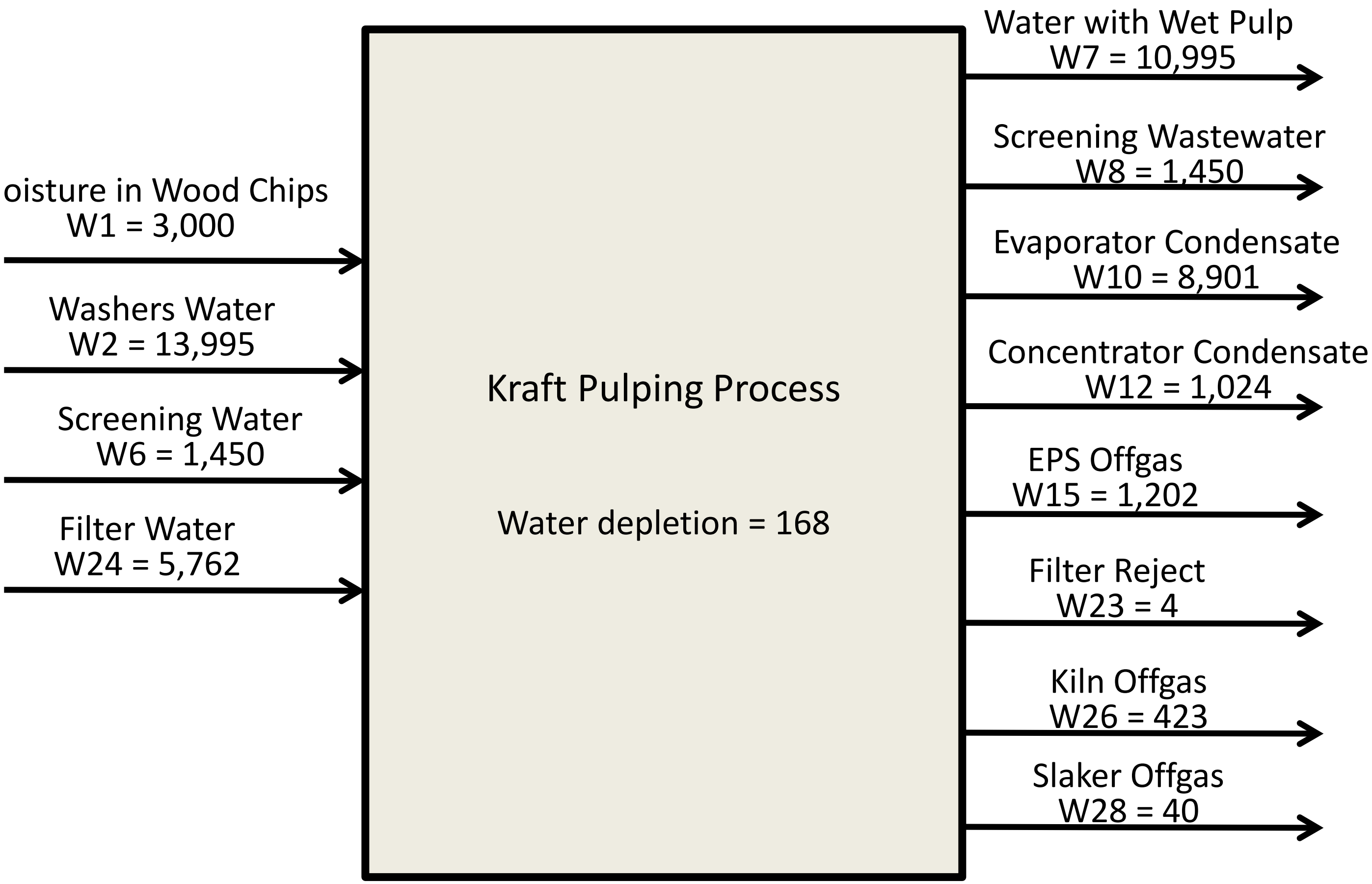
Target of minimum terminal load

Example 3.6. Minimizing Fresh Water Usage in a Pulping Mill



Source: Lovelady, E. M., M. M. El-Halwagi, and G. Krishnagopalan, "An Integrated Approach to the Optimization of Water Usage and Discharge in Pulp and Paper Plants", Int. J. of Environ. and Pollution (IJEP) 29(1-3), 274-307 (2007)

Overall (Big-Picture) Water Balance



Moisture in Wood Chips
W1 = 3,000

Washers Water
W2 = 13,995

Screening Water
W6 = 1,450

Filter Water
W24 = 5,762

Kraft Pulping Process

Water depletion = 168

Water with Wet Pulp
W7 = 10,995

Screening Wastewater
W8 = 1,450

Evaporator Condensate
W10 = 8,901

Concentrator Condensate
W12 = 1,024

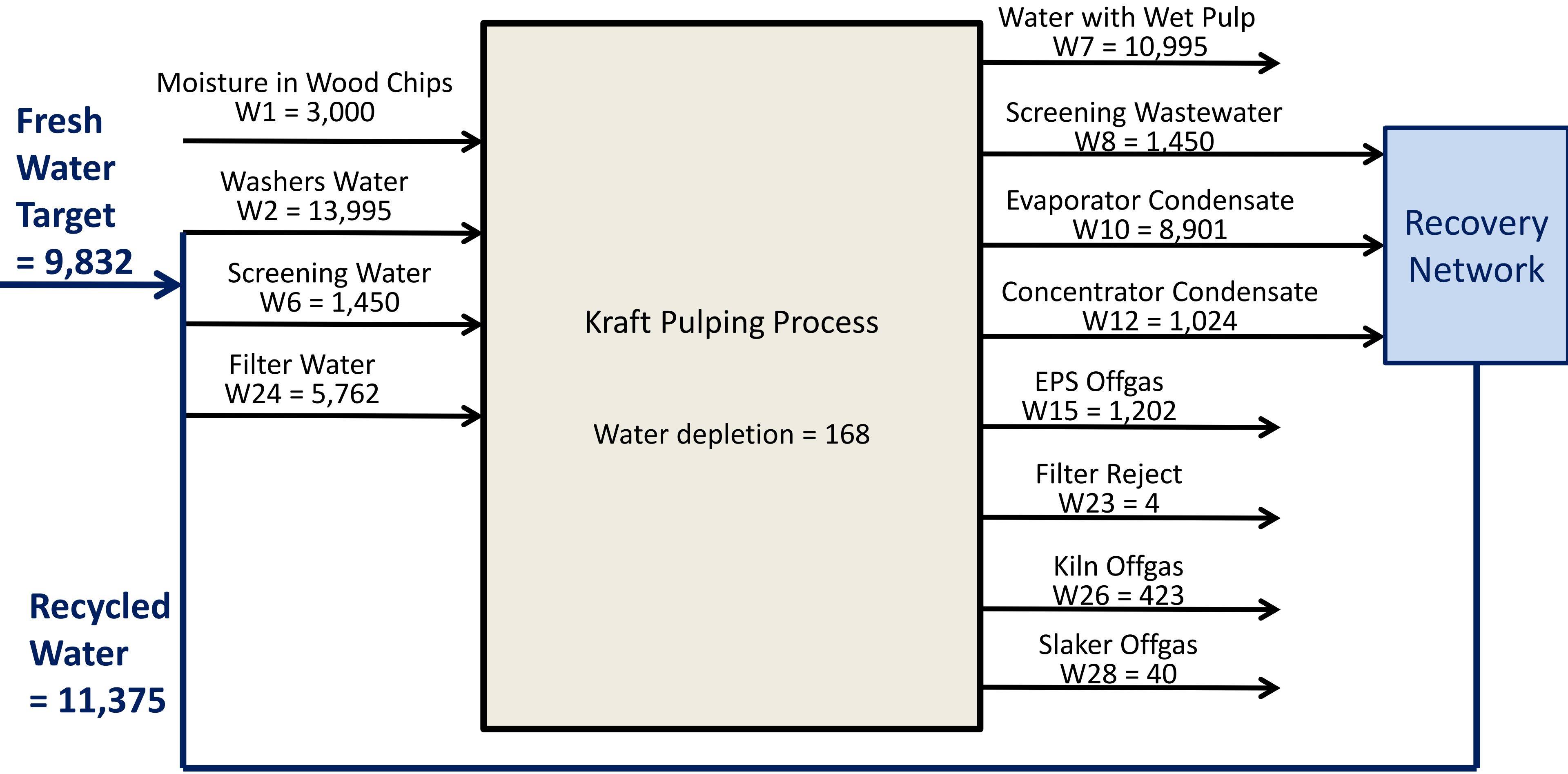
EPS Offgas
W15 = 1,202

Filter Reject
W23 = 4

Kiln Offgas
W26 = 423

Slaker Offgas
W28 = 40

Overall Water Targeting



Fresh Water Target = 9,832

Moisture in Wood Chips
W1 = 3,000

Washers Water
W2 = 13,995

Screening Water
W6 = 1,450

Filter Water
W24 = 5,762

Recycled Water = 11,375

Kraft Pulping Process

Water depletion = 168

Water with Wet Pulp
W7 = 10,995

Screening Wastewater
W8 = 1,450

Evaporator Condensate
W10 = 8,901

Concentrator Condensate
W12 = 1,024

EPS Offgas
W15 = 1,202

Filter Reject
W23 = 4

Kiln Offgas
W26 = 423

Slaker Offgas
W28 = 40

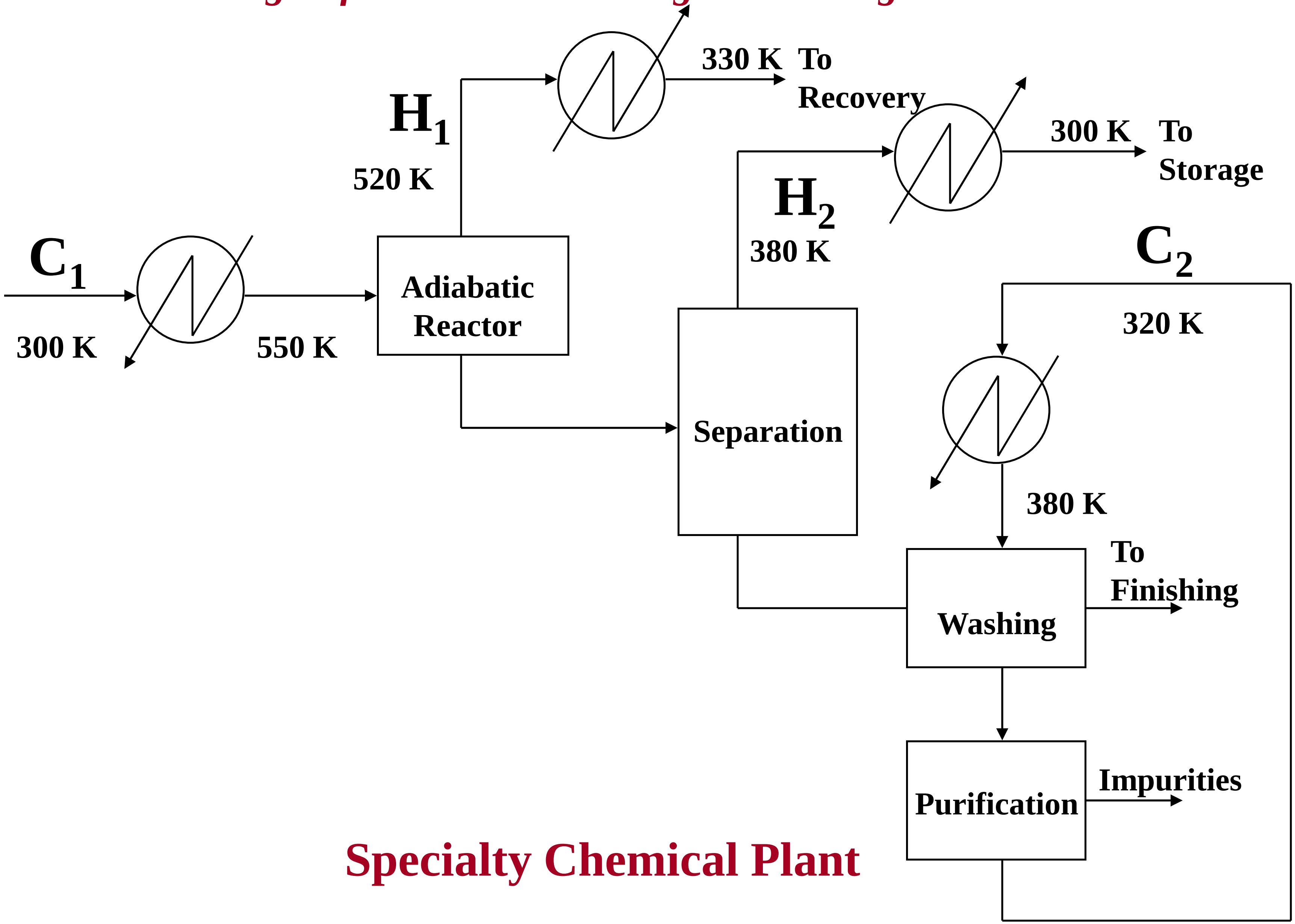
Recovery Network

HEAT INTEGRATION

Motivating Example #2:

What is wrong with this flowsheet from an energy perspective?

What are the targets for minimum heating and cooling utilities?



Specialty Chemical Plant

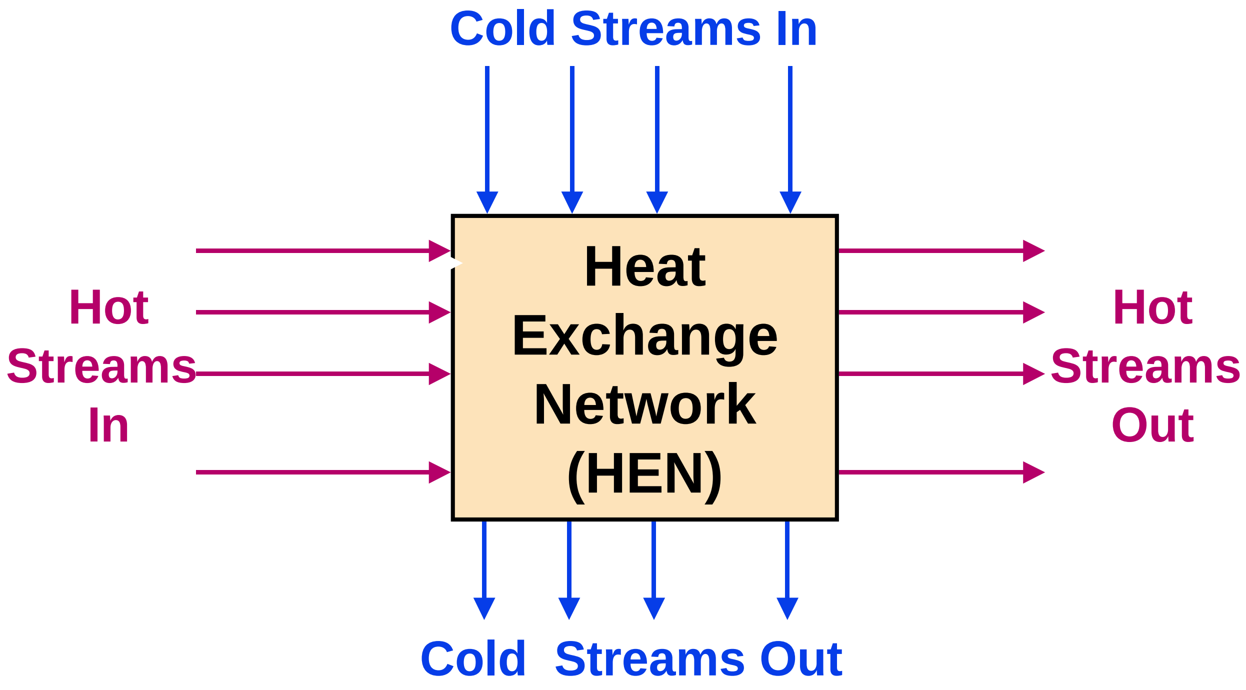
HEAT EXCHANGE NETWORKS (HENs)

Problem Statement:

Given a number N_H of process hot streams (to be cooled)
and a number N_C of process cold streams (to be heated),
it is desired to synthesize a cost-effective network of heat exchangers
that can transfer heat from the hot streams to the cold streams.

Given also are the heat capacity (flowrate x specific heat)
of each process hot stream, $FC_{P,u}$; its supply (inlet) temperature, T_{us};
and its target (outlet) temperature, T_{ut}, where $u = 1,2,\ldots,N\mathrm{H}$.

In addition, the heat capacity, $fc_{P,v}$, supply and target temperatures,
tvs and tvt, are given for each process cold stream, where $v = 1,2,.,N\mathrm{C}$.
Available for service are N_{HU} heating utilities and N_{CU} cooling utilities
whose supply and target temperatures (but not flowrates) are known.



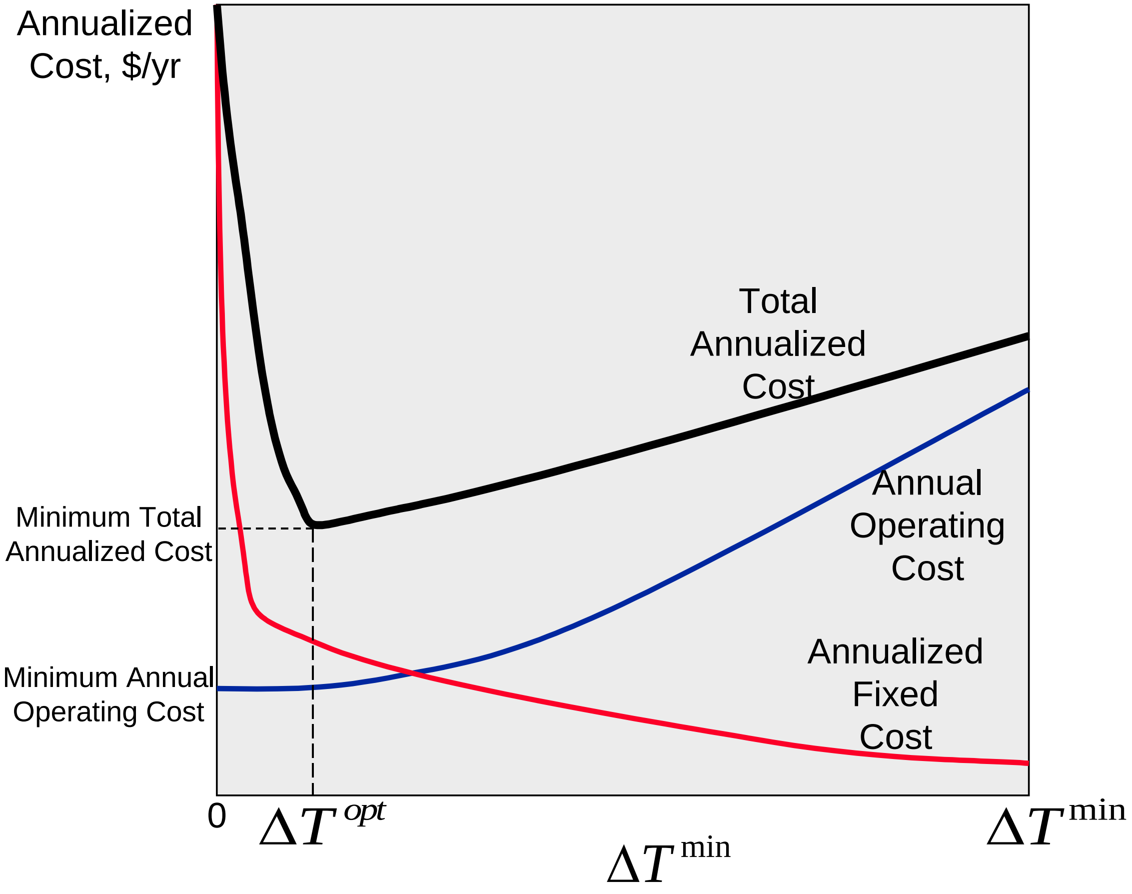
Which heating/cooling utilities should be employed ?

- What is the optimal heat load to be removed/added by each utility?
- How should the hot and cold streams be matched (i.e., stream pairings)?
- What is the optimal system configuration (e.g., how should the heat exchangers be arranged? Is there any stream splitting and mixing ?)

Practical Feasibility of Heat Transfer

Thermal equilibrium: T = t

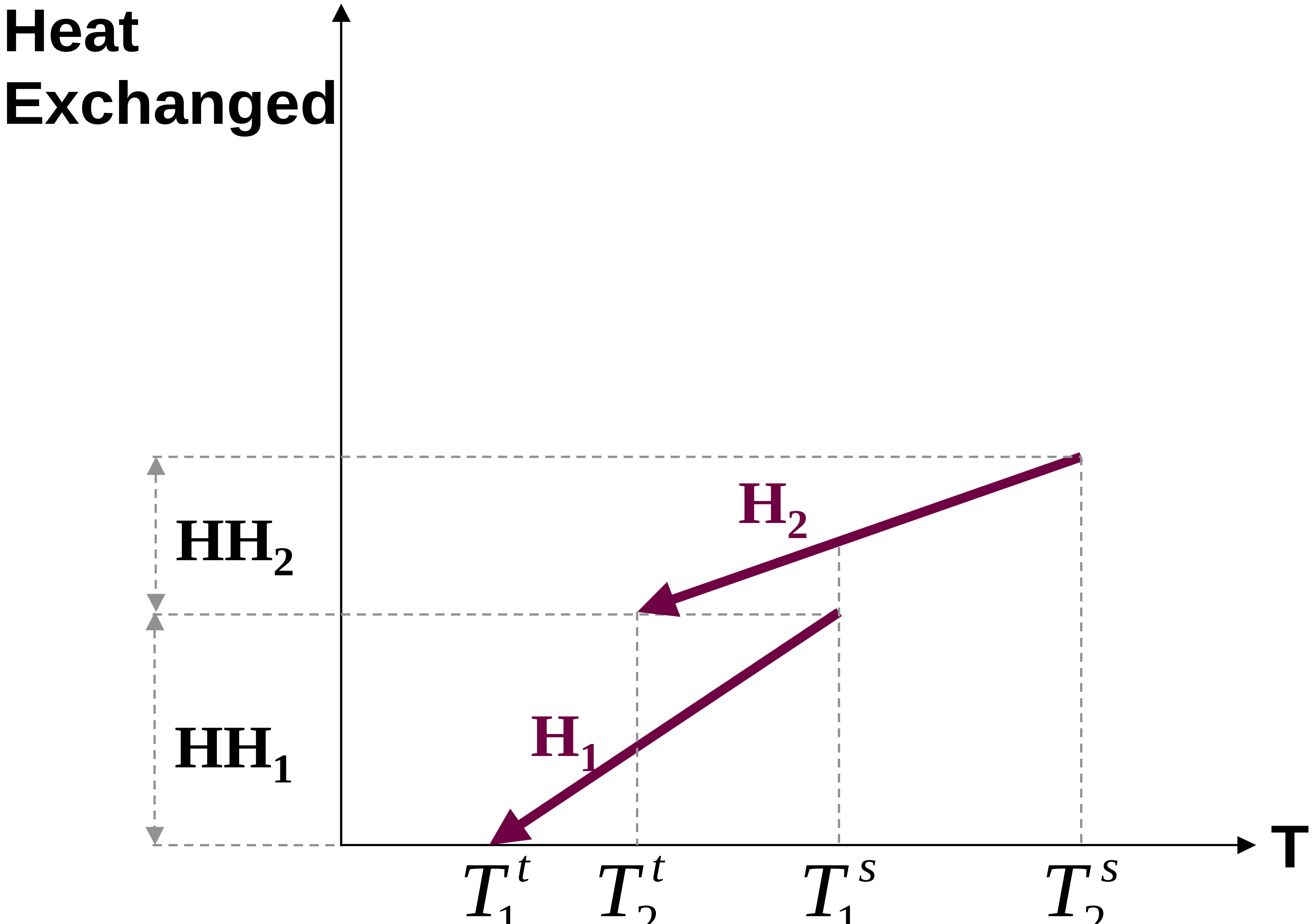
Practically-feasible heat transfer: $T = t + \Delta T^{\min}$



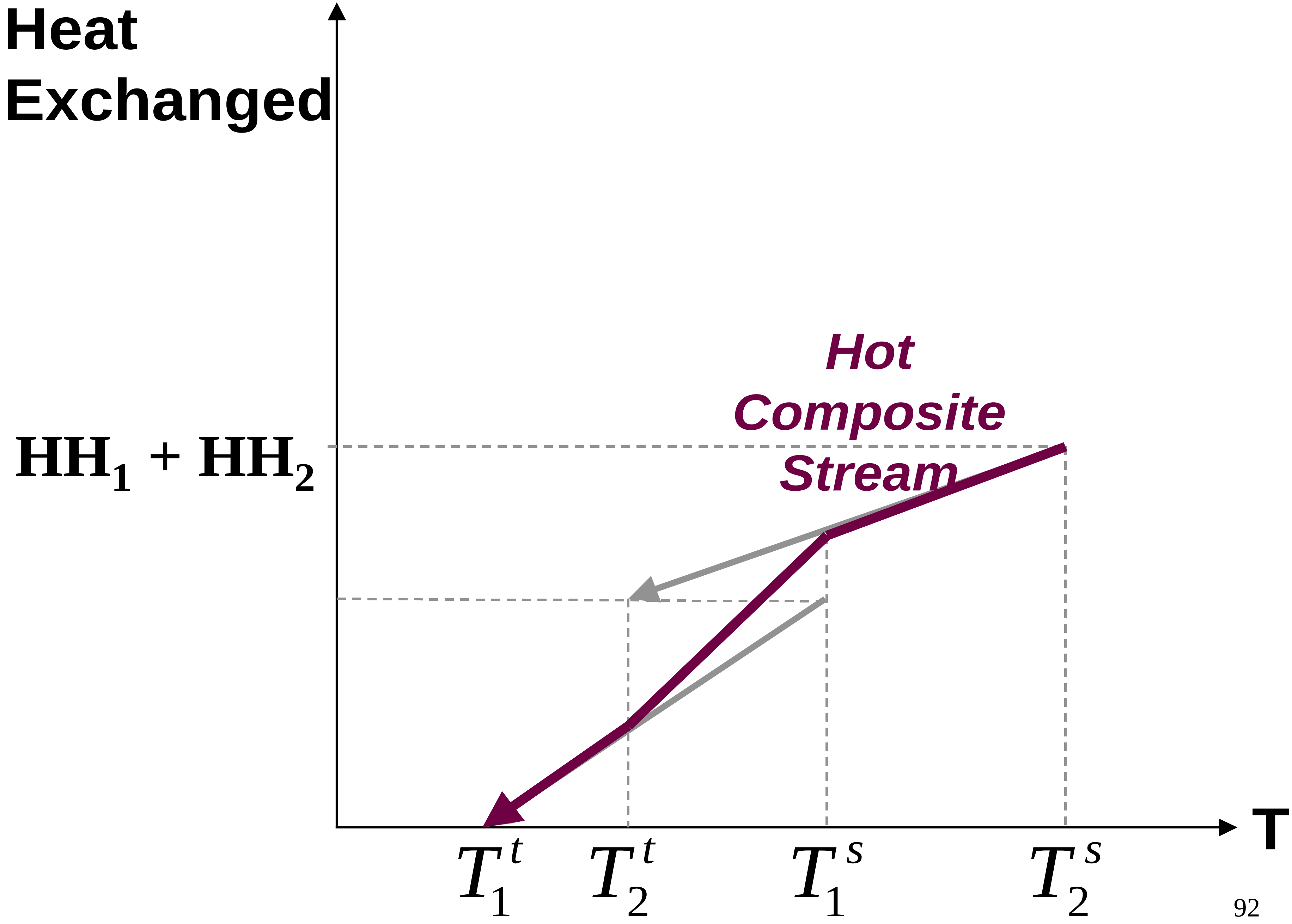
Trading off Fixed vs. Operating Cost

Constructing the Hot Composite Stream (Big Picture for Hot Streams

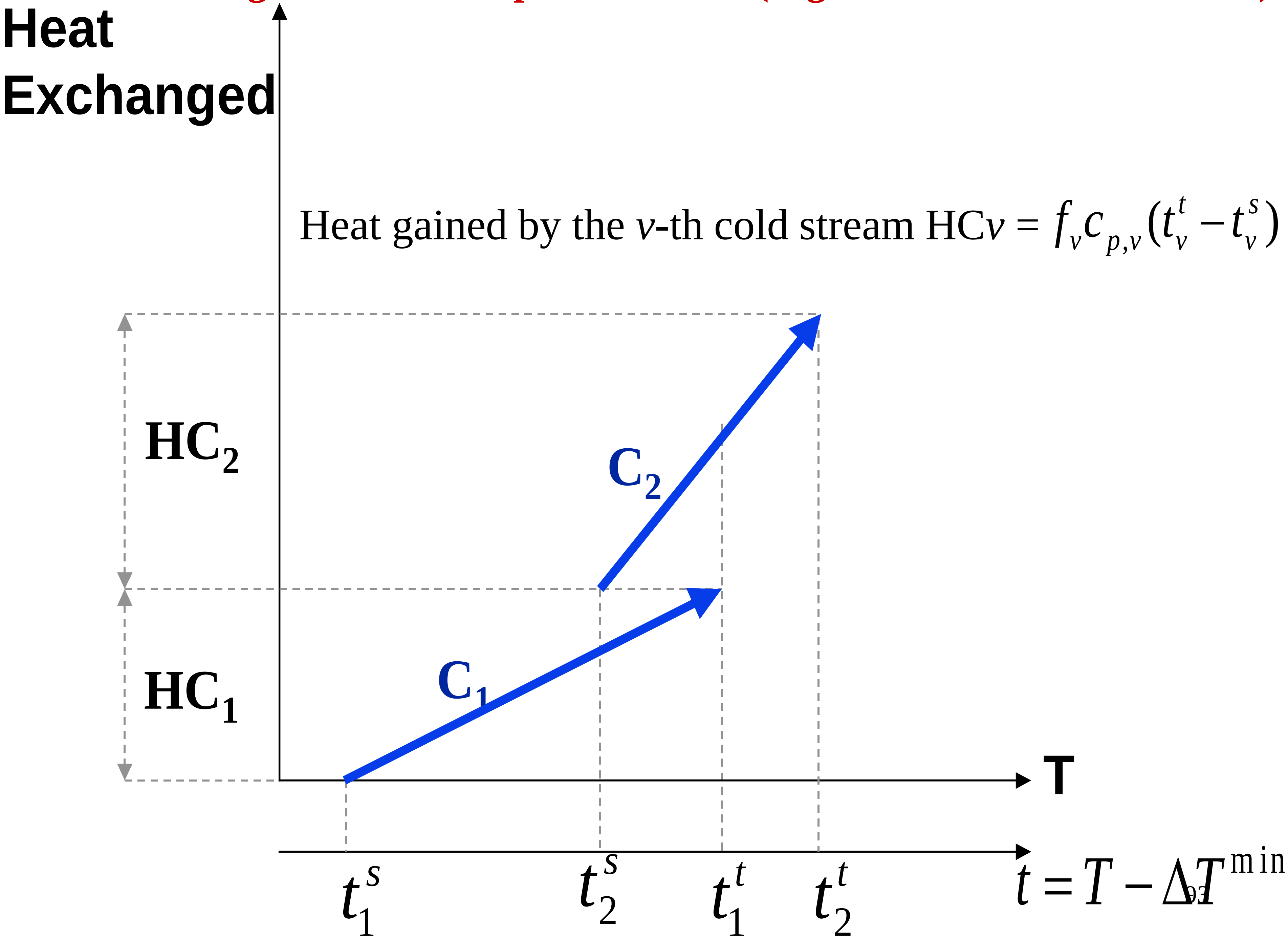
Heat lost from the *u*-th hot stream $HHu = F_u C_{p,u}(T_u^s - T_u^t)$



Using Superposition to Construct the Hot Composite Stream



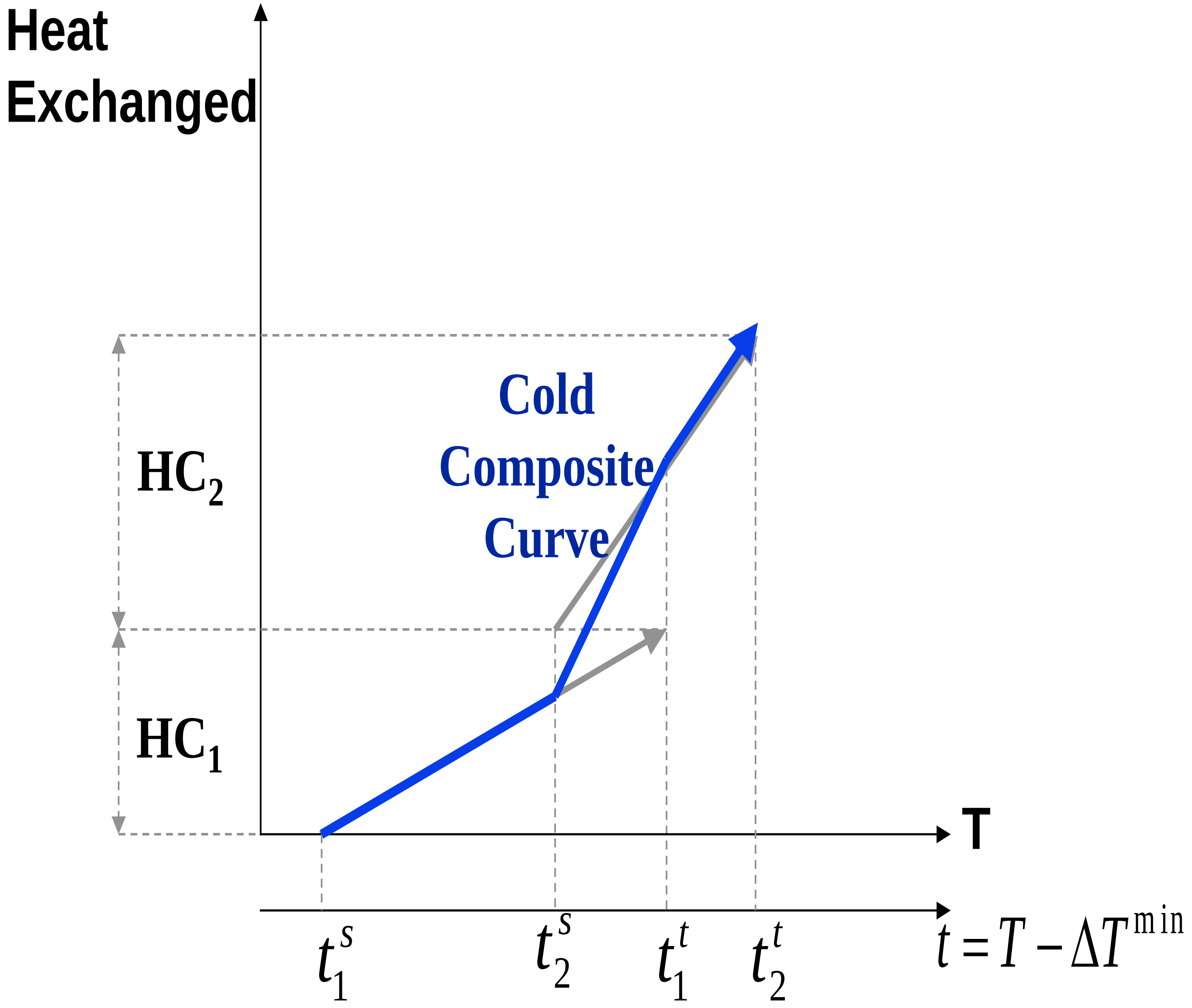
Constructing the Cold Composite Stream (Big Picture for Cold Streams)

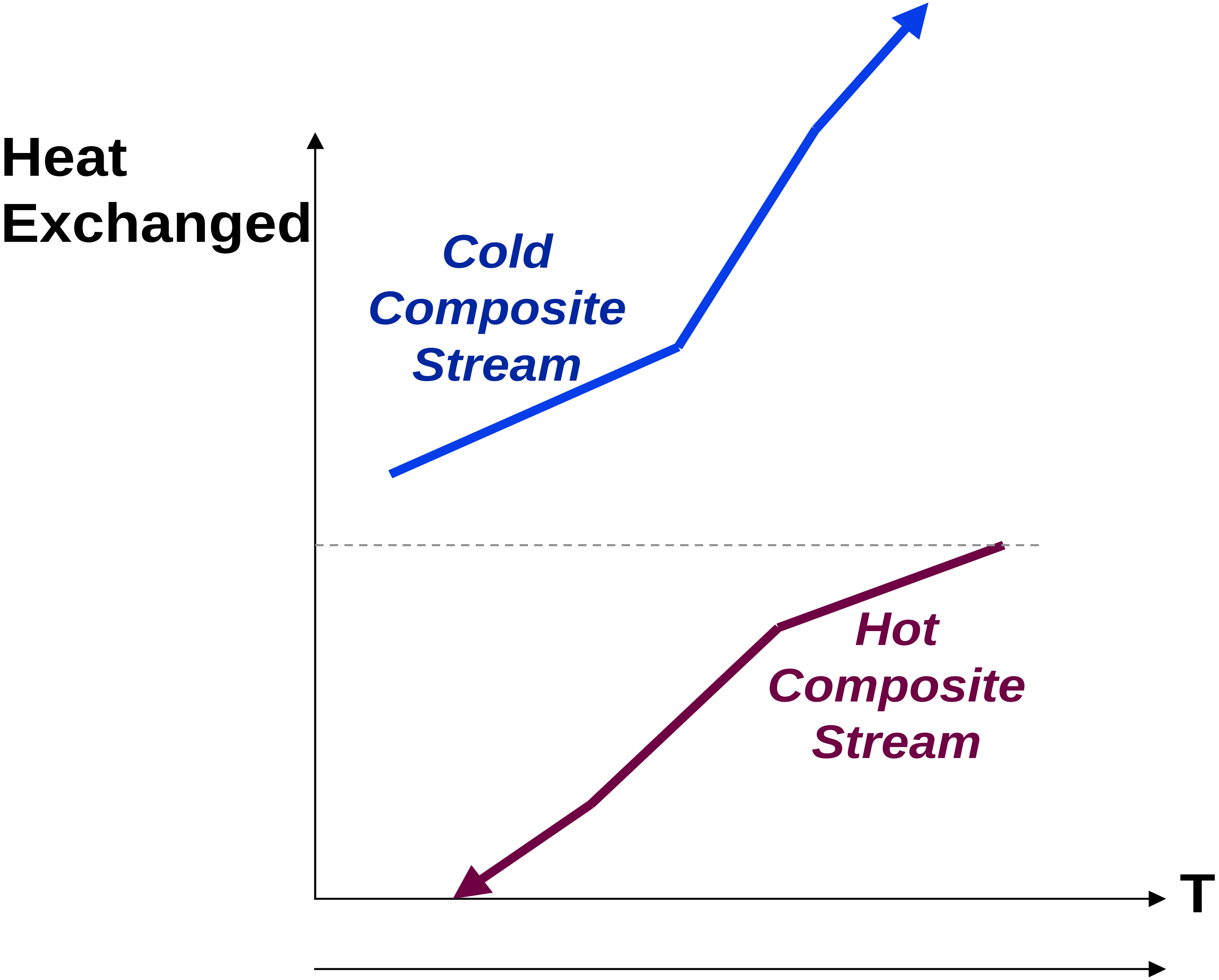


Heat gained by the *v*-th cold stream HC*v* = $f_v c_{p,v}(t_v^t - t_v^s)$

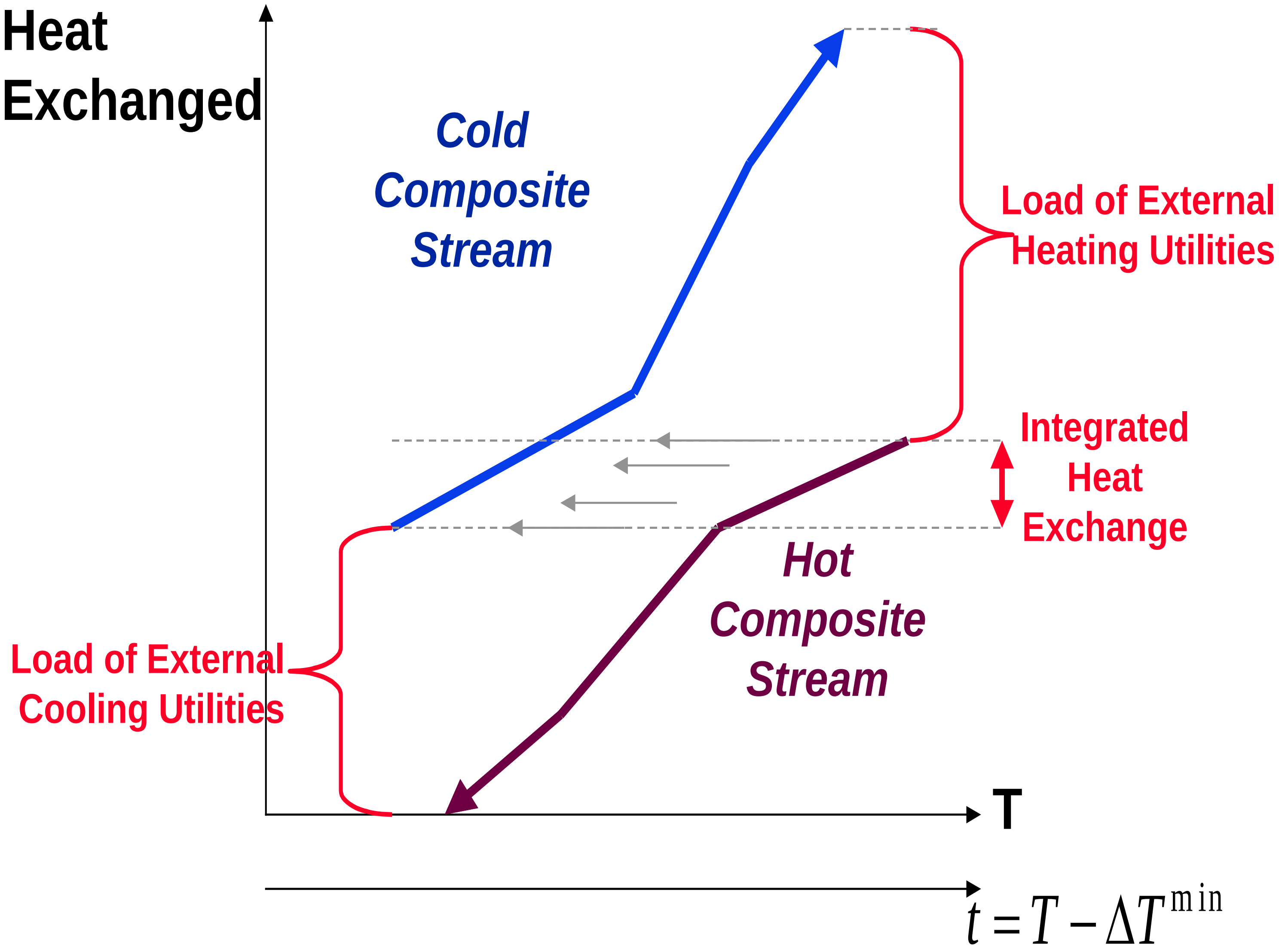
$t = T - \Delta T^{\min}$

Using Superposition to Construct the Cold Composite Stream

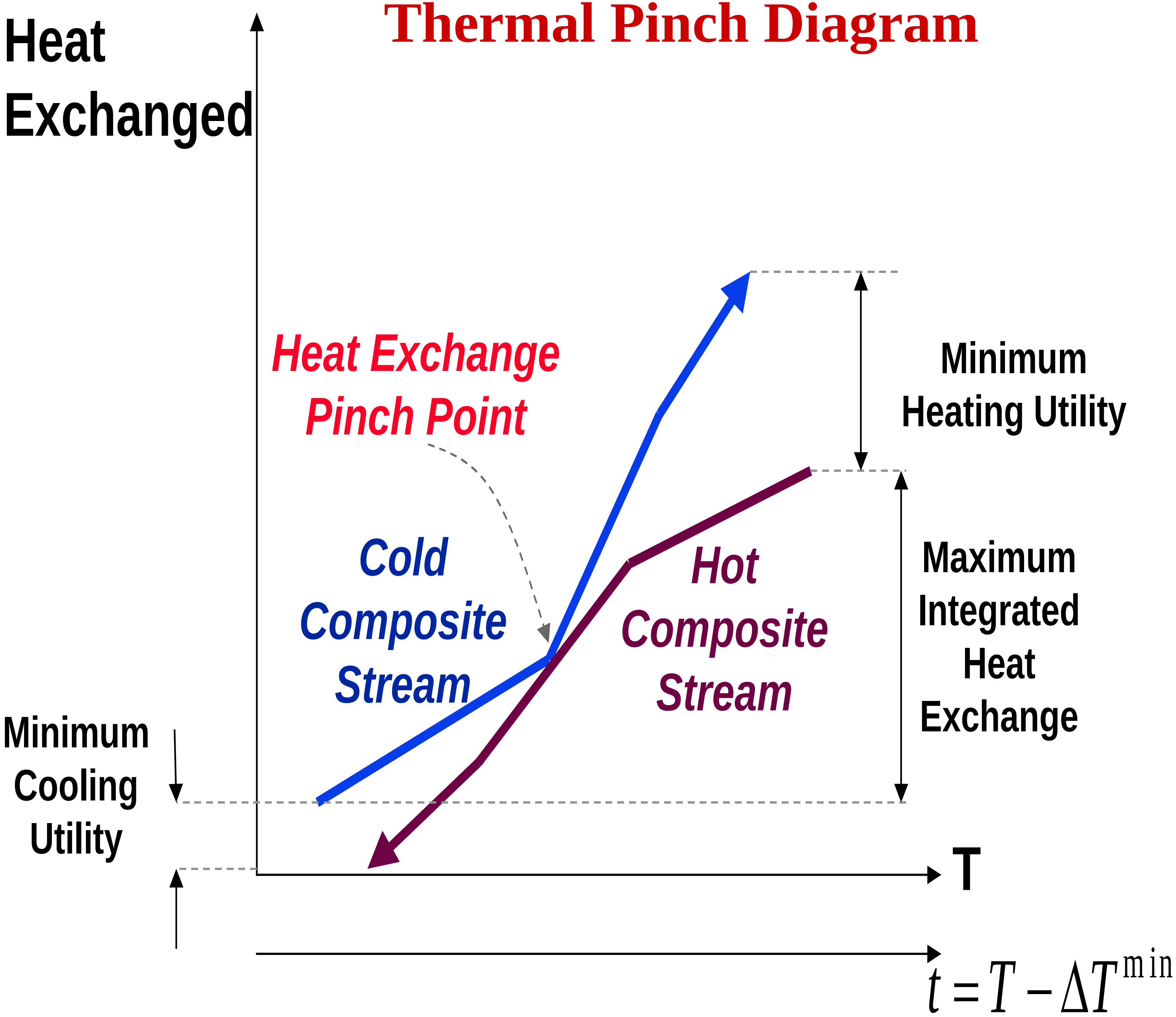




$$t = T - \Delta T^{\min}$$


Heat Exchanged
Cold Composite Stream
Load of External Heating Utilities
Integrated Heat Exchange
Hot Composite Stream
Load of External Cooling Utilities
T
$t = T - \Delta T^{\min}$

Thermal Pinch Diagram



Heat Exchanged

Heat Exchange Pinch Point

Cold Composite Stream

Hot Composite Stream

Minimum Heating Utility

Maximum Integrated Heat Exchange

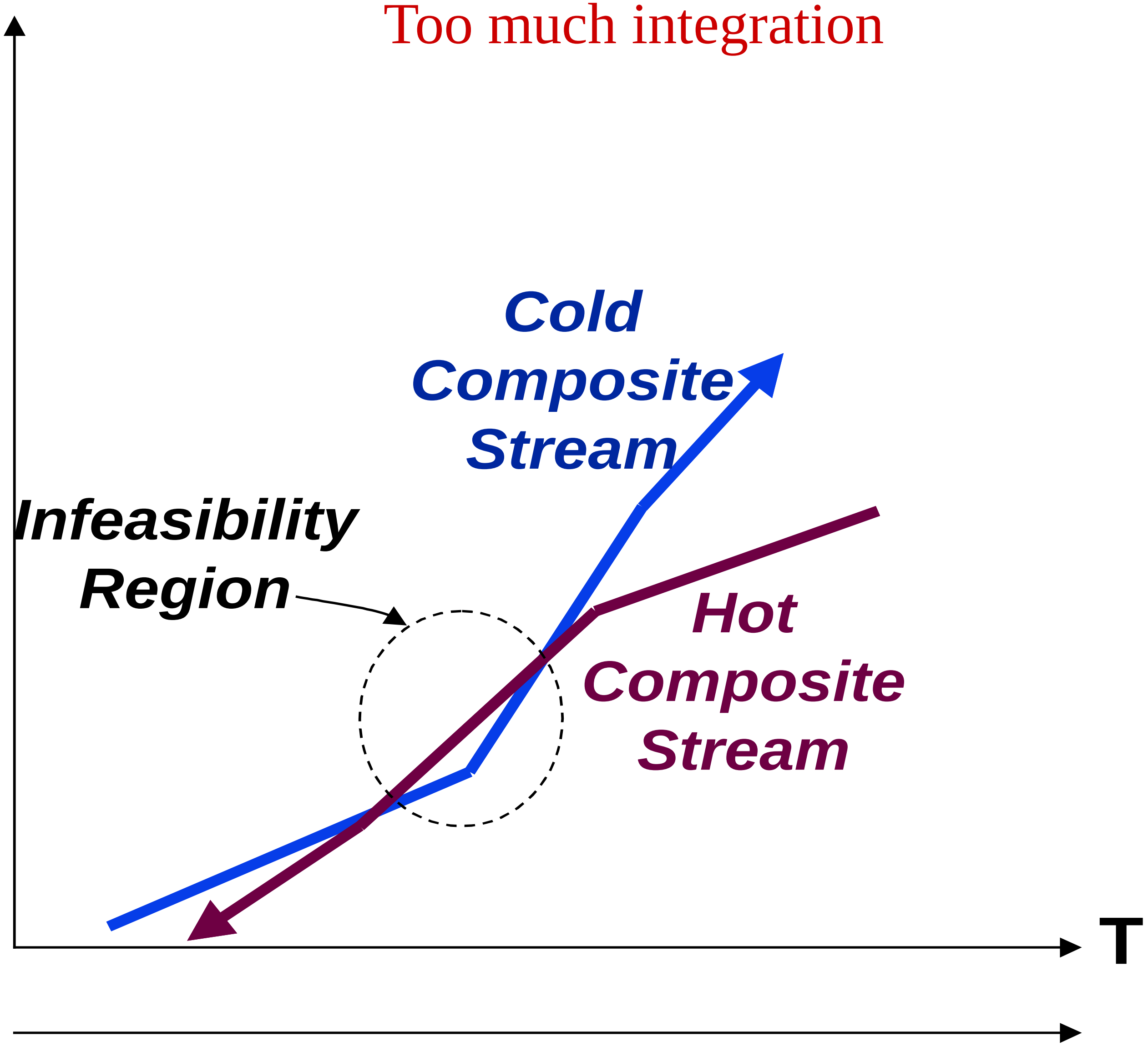
Minimum Cooling Utility

T

$$t = T - \Delta T^{\min}$$

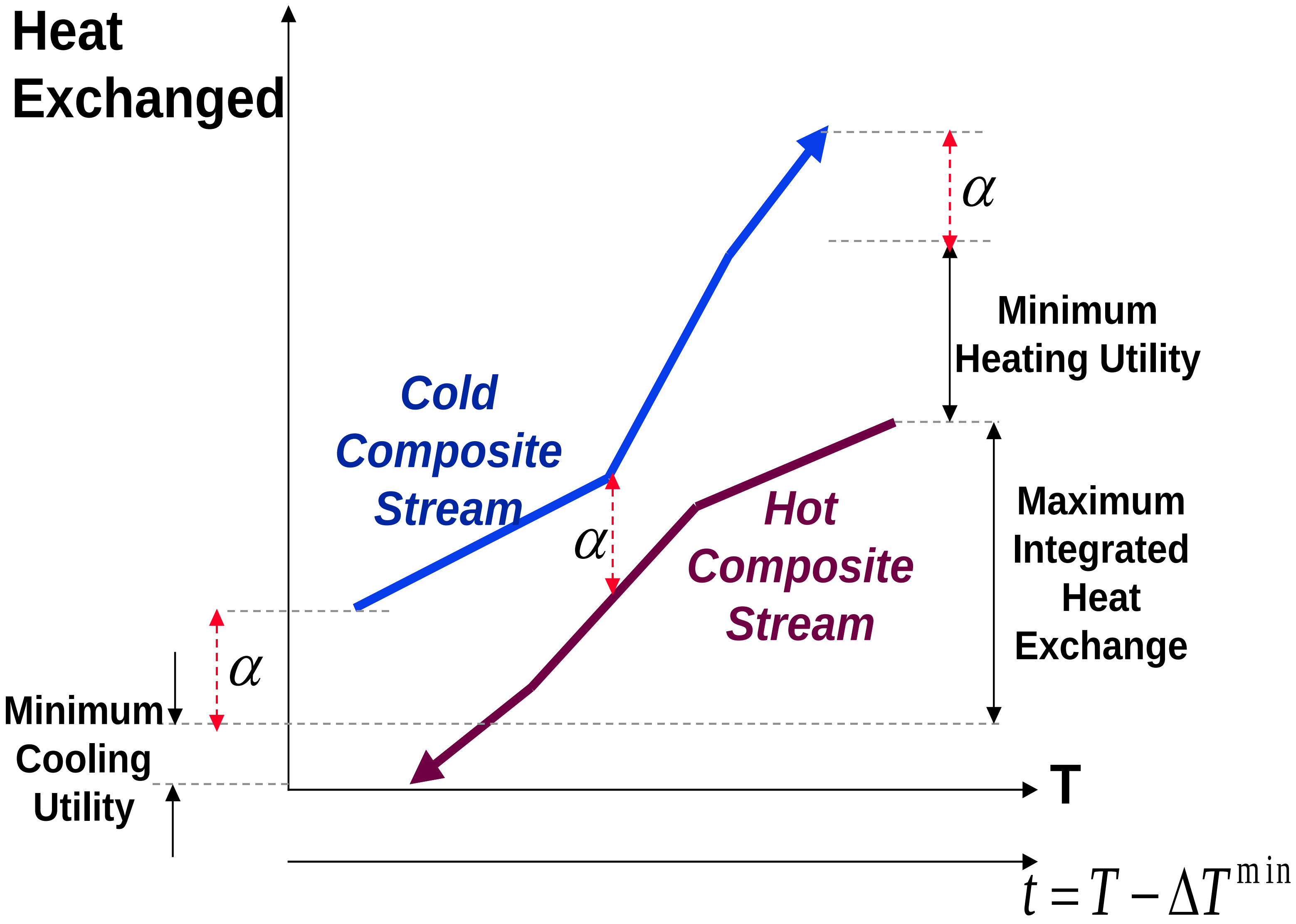
Linnhoff and Hindmarsh (1983)

Too much integration



$$t = T - \Delta T^{\min}$$

Too little integration: Passing heat through the pinch



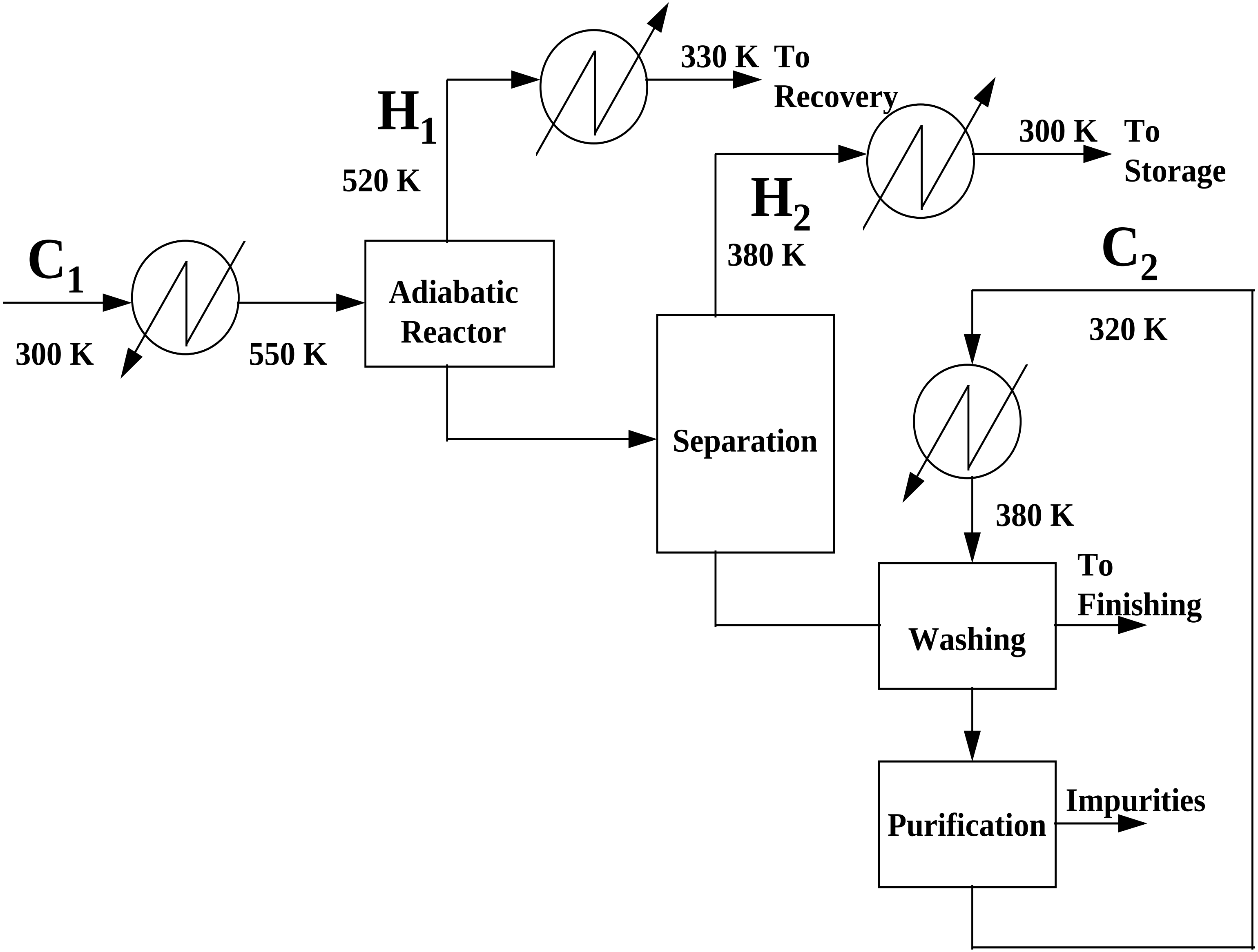
Optimum design rules for thermal pinch analysis:

-No heat should be passed through the pinch

- Above the pinch, no cooling utilities should be used

- Below the pinch, no heating utilities should be used.

Example: Utility Minimization in a Pharmaceutical Plant



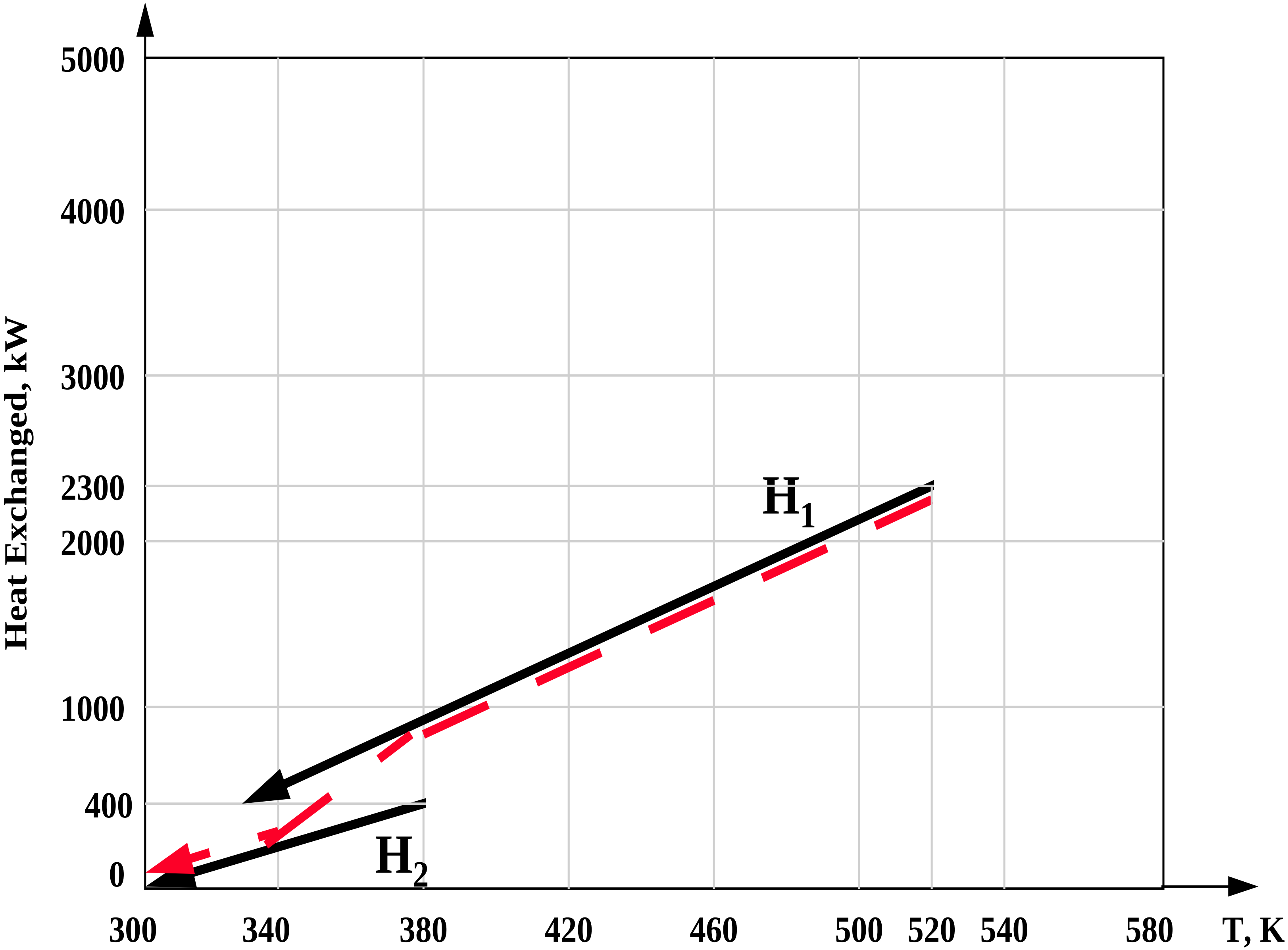
Stream Data

Stream	Flowrate x specific heat kW/^oC	Supply temperature, K	Target temperature, K	Enthalpy change kW
H_1	10	520	330	-1,900
H_2	5	380	300	-400
HU_1	?	560	520	?
C_1	19	300	550	4750
C_2	2	320	380	120
CU_1	?	290	300	?

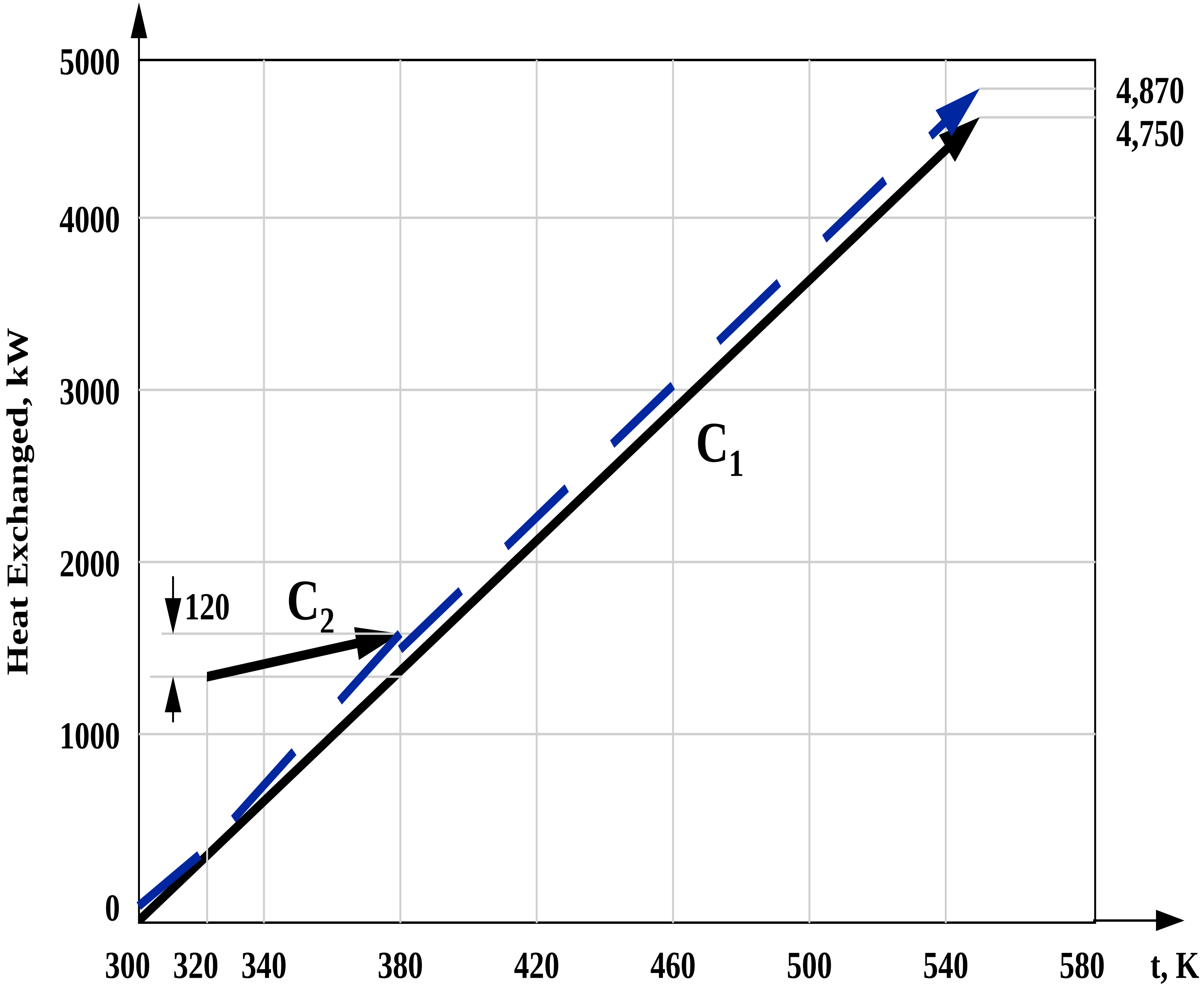
***Current Usage of Cooling Utility*: 2,300 kW**

***Current Usage of Heating Utility*: 4,870 kW**

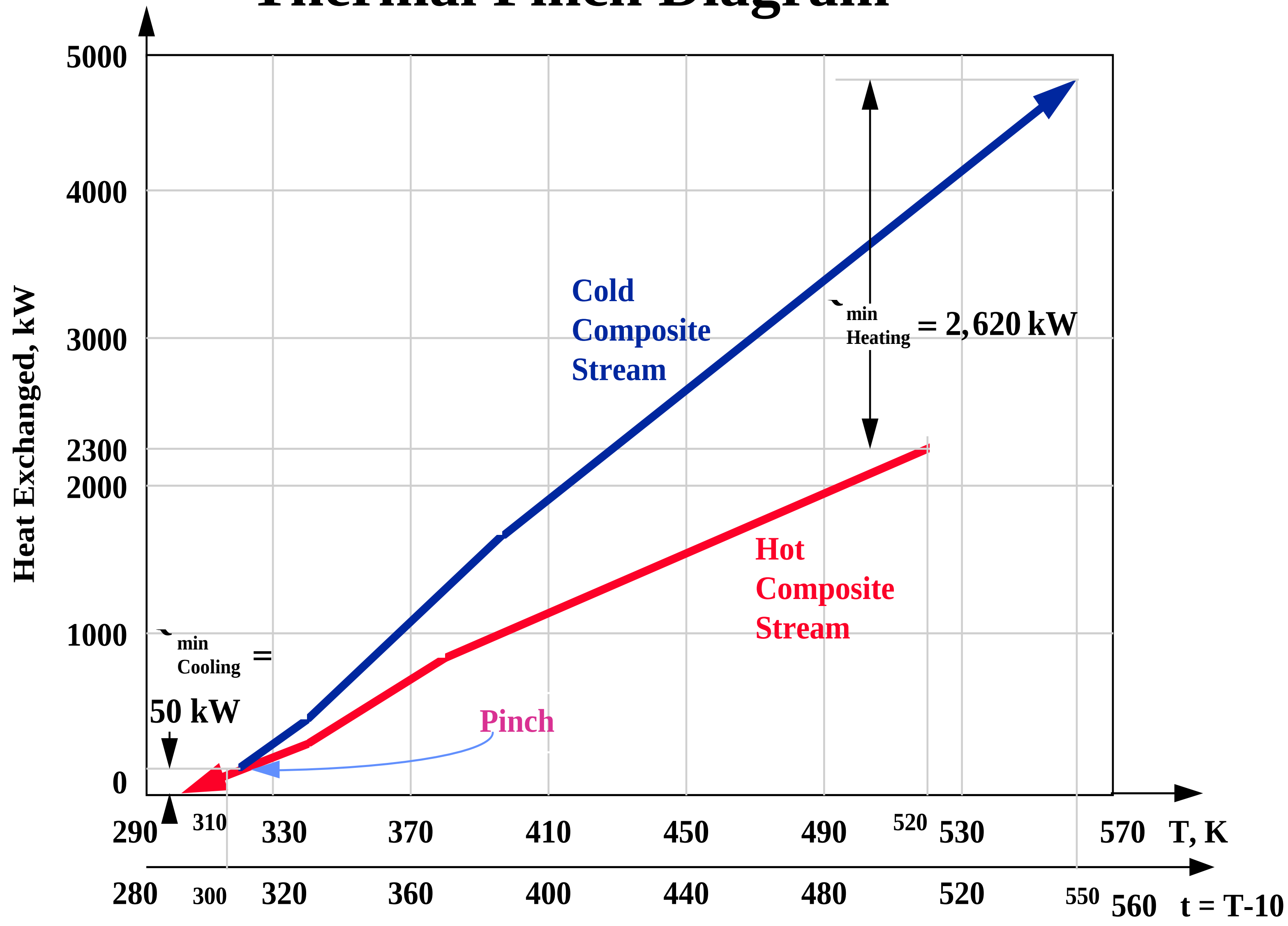
Creating the Hot Composite Curve



Creating the Cold Composite Curve



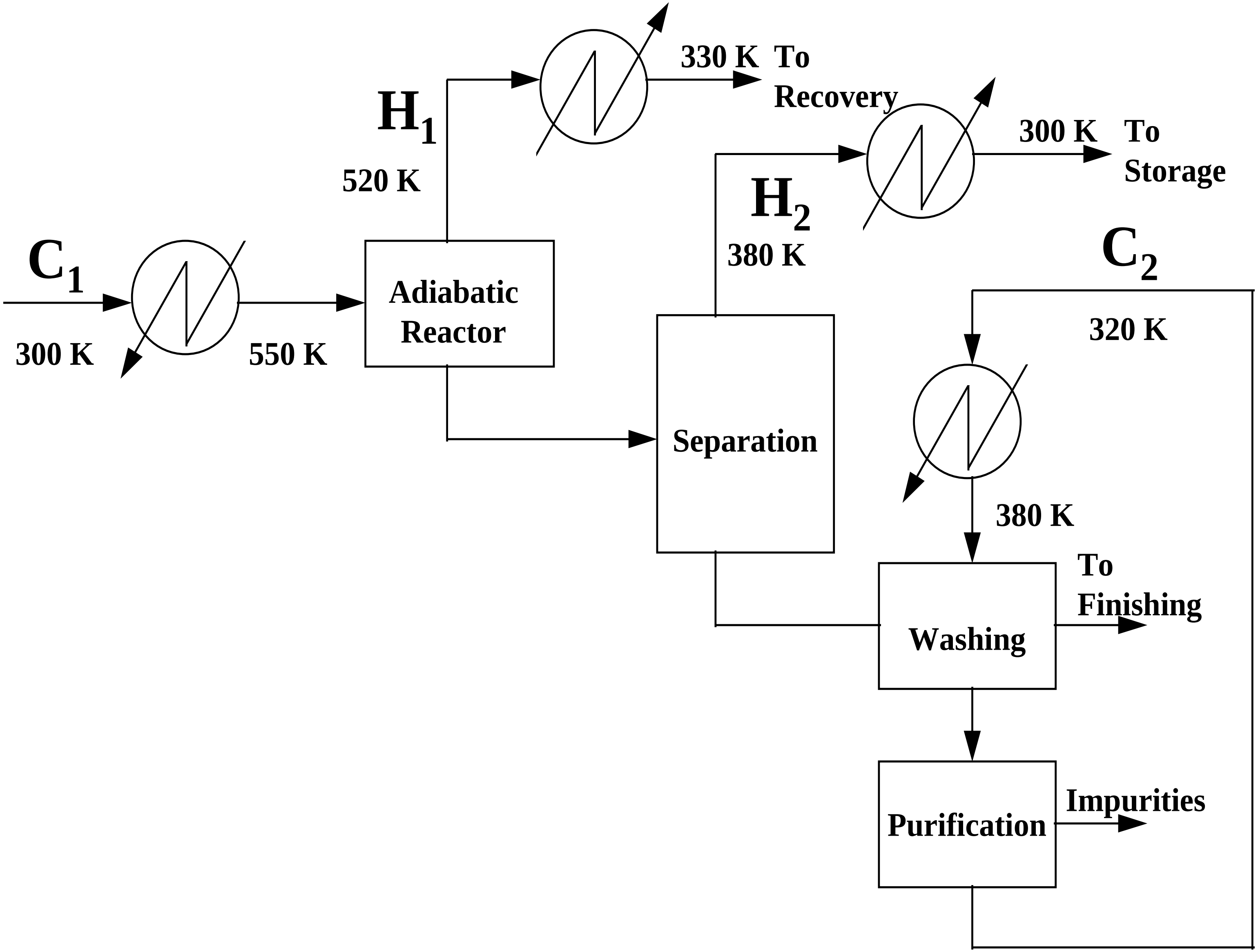
Thermal Pinch Diagram



Target for percentage savings in heating utility $= \dfrac{4{,}870 - 2{,}620}{4{,}870} * 100\% = 46\%$

Target for percentage savings in cooling utility $= \dfrac{2{,}300 - 50}{2{,}300} * 100\% = 98\%$

Example: Utility Minimization in a Pharmaceutical Plant



Stream Data

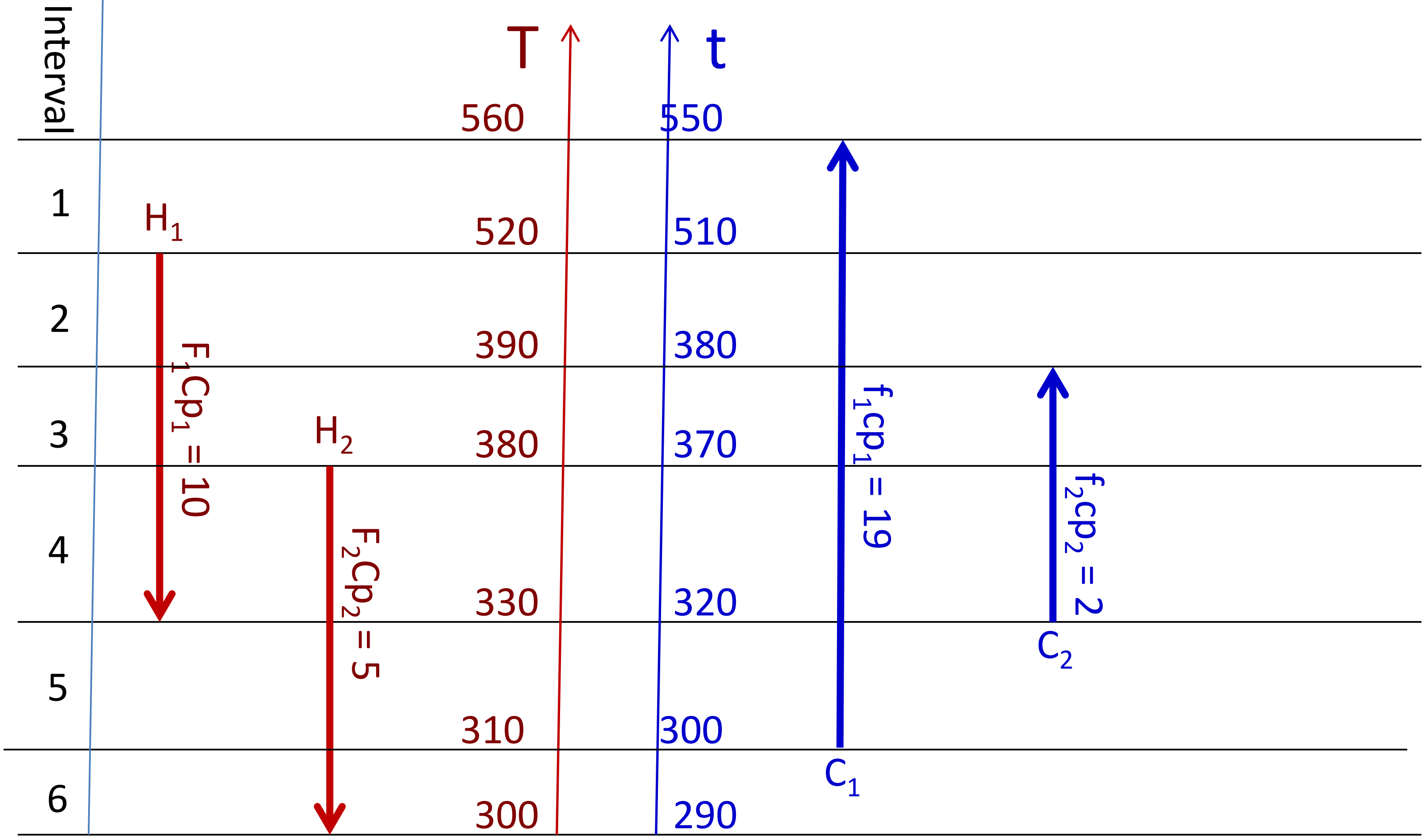
Stream	Flowrate x specific heat kW/^oC	Supply temperature, K	Target temperature, K	Enthalpy change kW
H_1	10	520	330	-1,900
H_2	5	380	300	-400
HU_1	?	560	520	?
C_1	19	300	550	4750
C_2	2	320	380	120
CU_1	?	290	300	?

***Current Usage of Cooling Utility*: 2,300 kW**

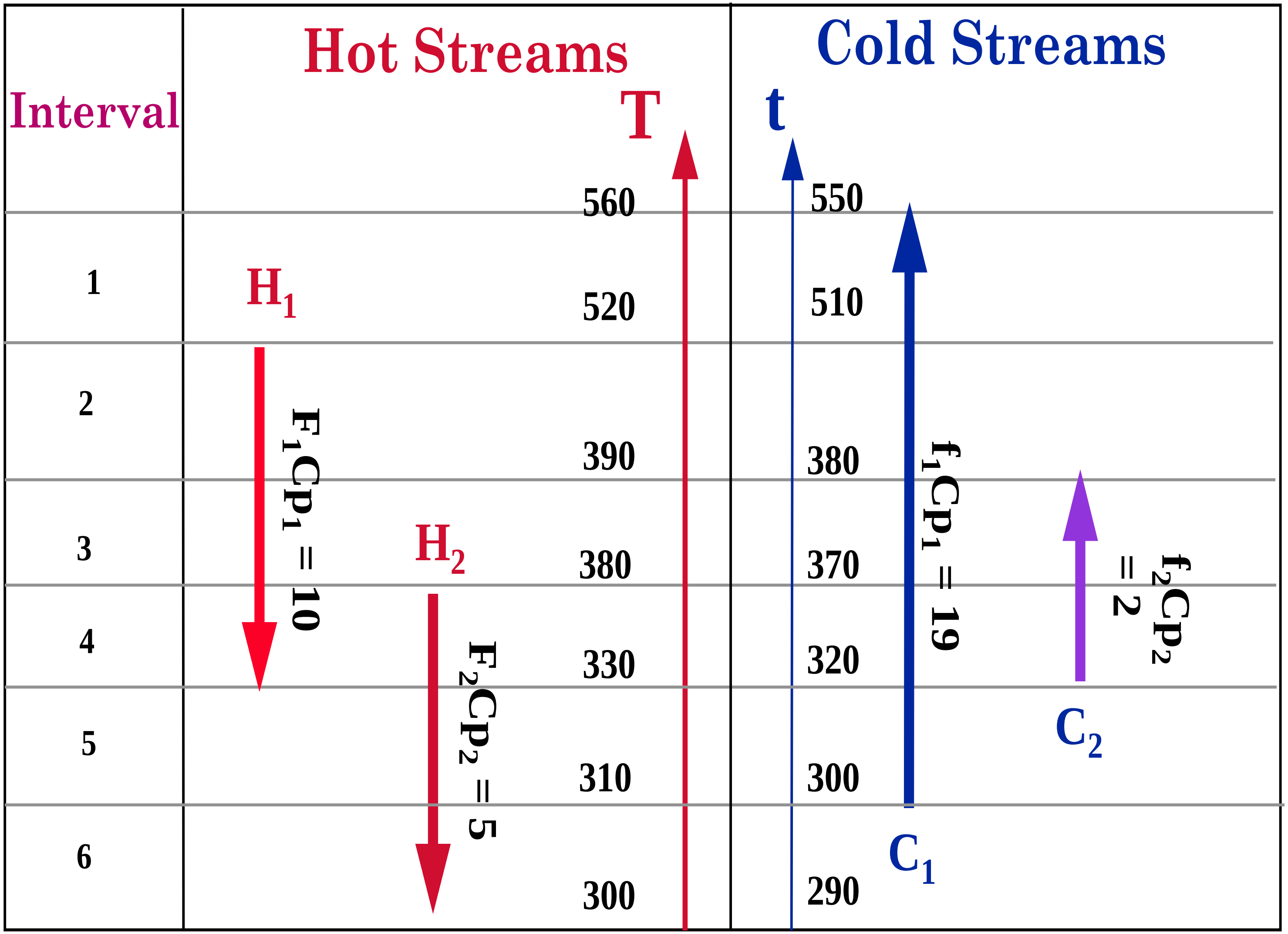
***Current Usage of Heating Utility*: 4,870 kW**

	FCp kW/ºC	T_s	T_t
H_1	10	520	330
H_2	5	380	300
C_1	19	300	550
C_2	2	320	380

Temperature Interval Diagram (TID)



Temperature Interval Diagram (TID)



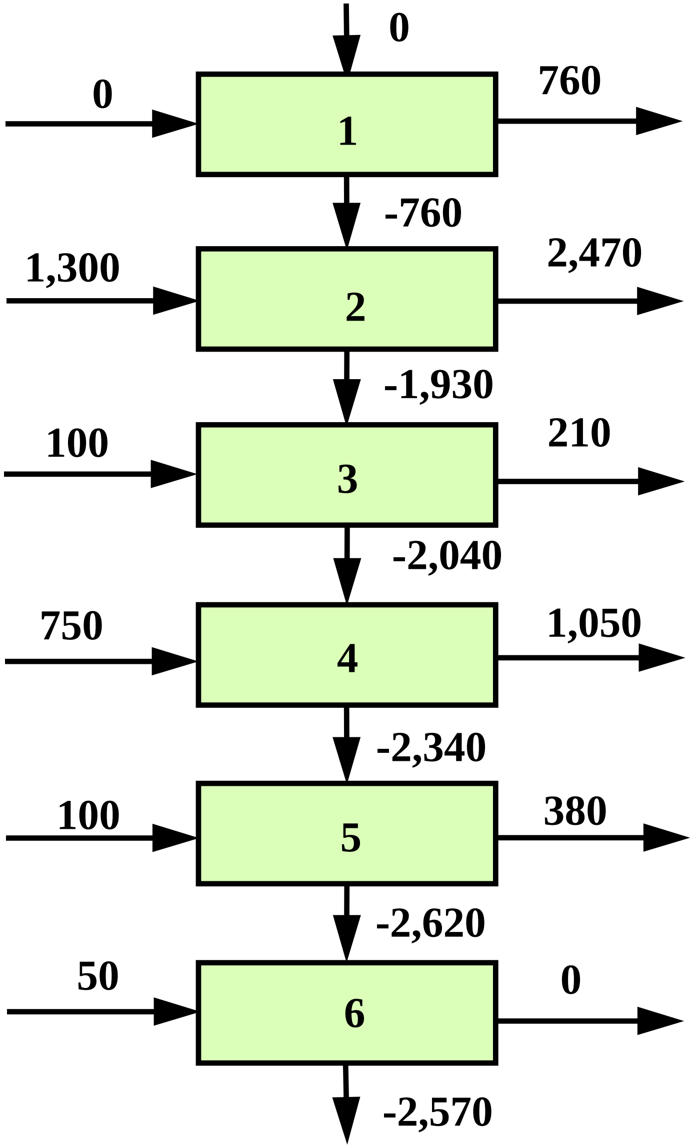
TEHL for Process Hot Streams

Interval	Load of H_1 (kW)	Load of H_2 (kW)	Total Load (kW)
1	-	-	-
2	1300	-	1300
3	100	-	100
4	500	250	750
5	-	100	100
6	-	50	50

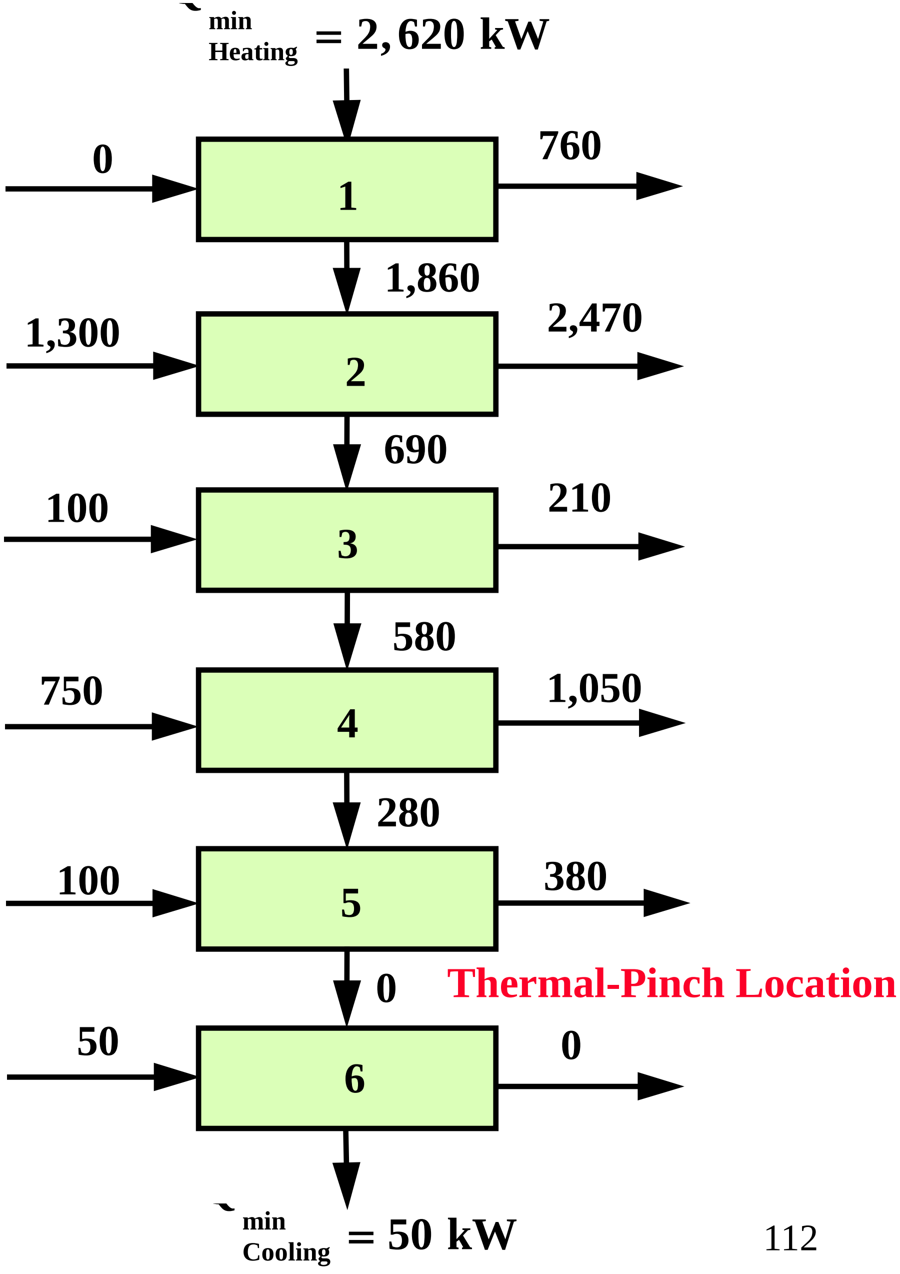
TEHL for Process Cold Streams

Interval	Capacity of C_1 (kW)	Capacity of C_2 (kW)	Total capacity (kW)
1	760	-	760
2	2470	-	2470
3	190	20	210
4	950	100	1050
5	380	-	380
6	-	-	-

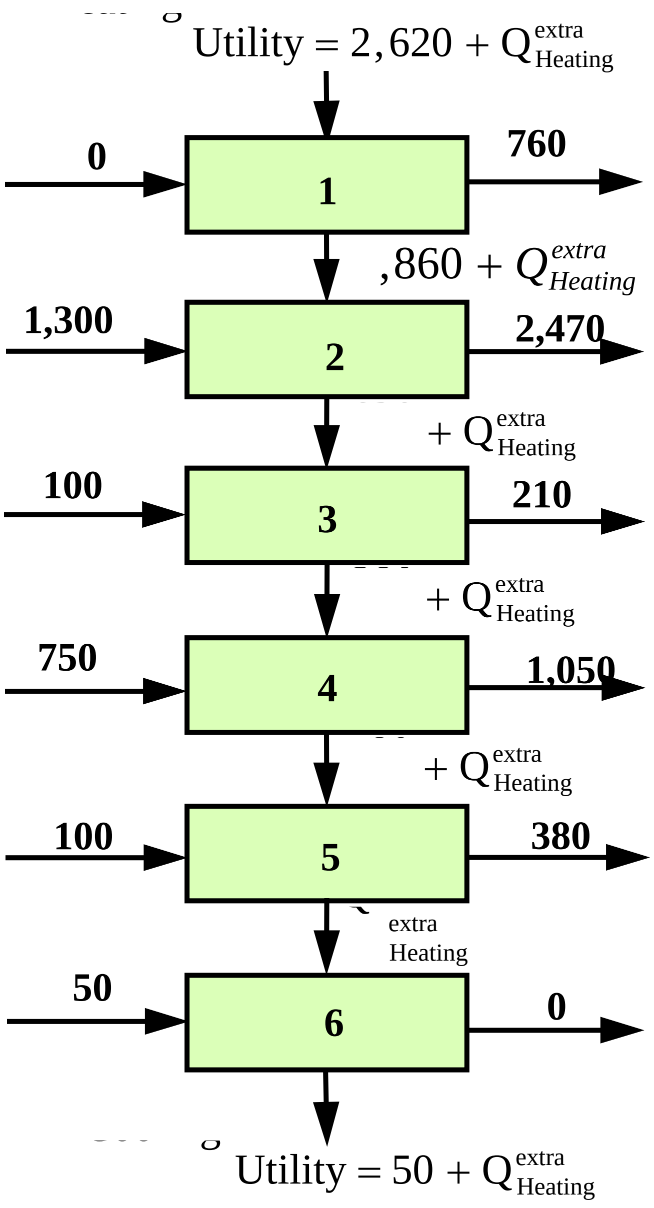
Cascade Diagram



Revised Cascade Diagram



Passing Heat Through the Pinch?



$\text{Utility} = 2{,}620 + Q^{extra}_{Heating}$

0

1

760

$,860 + Q^{extra}_{Heating}$

1,300

2

2,470

$+ Q^{extra}_{Heating}$

100

3

210

$+ Q^{extra}_{Heating}$

750

4

1,050

$+ Q^{extra}_{Heating}$

100

5

380

extra
Heating

50

6

0

$\text{Utility} = 50 + Q^{extra}_{Heating}$

Increase in the Heating and Cooling Utilities

INCORPORATING SUSTAINABILITY AND TARGETING IN PROFITABILITY CALCULATIONS

- Process improvement projects are typically driven/assessed by profitability criteria (e.g., return on investment, payback period, net present value)
- Sustainability goals are well aligned with process integration activities (natural-resource conservation, process-efficiency enhancement, pollution prevention, etc.)
- Targeting approaches can set goals for sustainability
- Sustainability considerations are best included in the early stages of decision making

How to use a consistent platform for including sustainability in development and assessment of process integration and improvement projects?

ECONOMIC RETURN ON INVESTMENT "*ROI*":

$$ROI = \frac{\text{Annual Economic Profit } (AEP)}{\text{Capital Investment}}$$

Units: fraction per year
or % per year

Most common definition:

$$ROI = \frac{\text{Annual Net (After Tax) Profit}}{\text{Total Capital Investment}}$$

For Project *p*:

$$ROI_P = \frac{AEP_P}{TCI_P}$$

ROI: the higher, the better

Each company has **a minimum "threshold" ROI** to recommend a project (relative to inflation rate and alternative investments including financial investment (bank, bonds, etc.)

Calculation of Annual Net Profit:

Annual net (after-tax) profit = Net income per year = Annual after-tax cash flow
How to calculate annual net profit?

Annual net (after-tax) profit = Annual gross profit – Annual income taxes

Annual gross profit = Annual income (or savings) – Annual operating cost

How to calculate taxes?
Remember: depreciation is tax shielded (write-off)
➔ Taxable annual gross profit = Annual gross profit - Depreciation

➔ Annual income taxes = Taxable annual gross profit*Tax rate

➔Annual net (after-tax) profit = Annual gross profit – (Annual gross profit – Depreciation)*Tax rate
Let’s subtract and add Depreciation
➔Annual net (after-tax) profit = (Annual gross profit - Depreciation)
+ Depreciation - (Annual gross profit – Depreciation)*Tax rate
= (Annual gross profit – Depreciation)*(1 – Tax rate) + Depreciation

Annual net (after-tax) profit = Net income per year = Annual after-tax cash flow
= (Annual income – Annual operating cost – Depreciation)*(1-Tax rate) +Depreciation
= (Annual income – Total annualized cost)*(1-Tax rate) + Depreciation

INCREMENTAL RETURN ON INVESTMENT "*IROI*"

- For project that are incremental in nature (build on one another)
- Start with the base project then evaluate IROI for incremental addition *p*

$$IROI_p = \frac{\Delta AEP_p}{\Delta TCI_p}$$

ΔAEP_p : additional annual net economic profit resulting from incremental project p

ΔTCI_p : additional *TCI* associated with the incremental project

IROI must meet the company's minimum hurdle rate

SUSTAINABILITY WEIGHTED RETURN ON INVESTMENT METRIC “SWROIM”

- consider a set of process integration project alternatives: $p = 1,2,\ldots, N_{Projects}$.
- For the p^{th} project, a new term called the ***Annual Sustainability Profit “ASP”*** is defined as follows

$$ASP_p = AEP_P\left[1+\sum_{i=1}^{N_{Indicators}} w_i\left(\frac{Indicator_{p,i}}{Indicator_i^{\text{Target}}}\right)\right]$$

Value of the i^{th} sustainability indicator for the p^{th} project: may be positive, 0, or negative

Annual Economic Profit

Index for sustainability indicators

weighing factor: a ratio representing the relative importance of the i^{th} sustainability indicator compared to the annual net economic profit

Target value of the i^{th} sustainability indicator (obtained from process integration benchmarking or taken as the largest value from all projects, or set by the company as a goal): always positive indicating improvement

Source: El-Halwagi, M. M., “A Return on Investment Metric for Incorporating Sustainability in Process Integration and Improvement Projects”, Clean Technologies and Environmental Policy (DOI 10.1007/s10098-016-1280-2, 2017)

Annual Sustainability Profit "ASP"

$$ASP_p = AEP_P\left[1+\sum_{i=1}^{N_{Indicators}} w_i\left(\frac{Indicator_{p,i}}{Indicator_i^{\text{Target}}}\right)\right]$$

Extended
form of AEP

Relative
importance of the
i^{th} sustainability
indicator
compared to the
annual net
economic profit

Fractional contribution of project
p towards meeting the
desired/targeted performance for
the i^{th} sustainability metric (+ive,
0, or –ive)

SUSTAINABILITY WEIGHTED RETURN ON INVESTMENT METRIC *“SWROIM”*

$$SWROIM_p = \frac{ASP_p}{TCI_p}$$

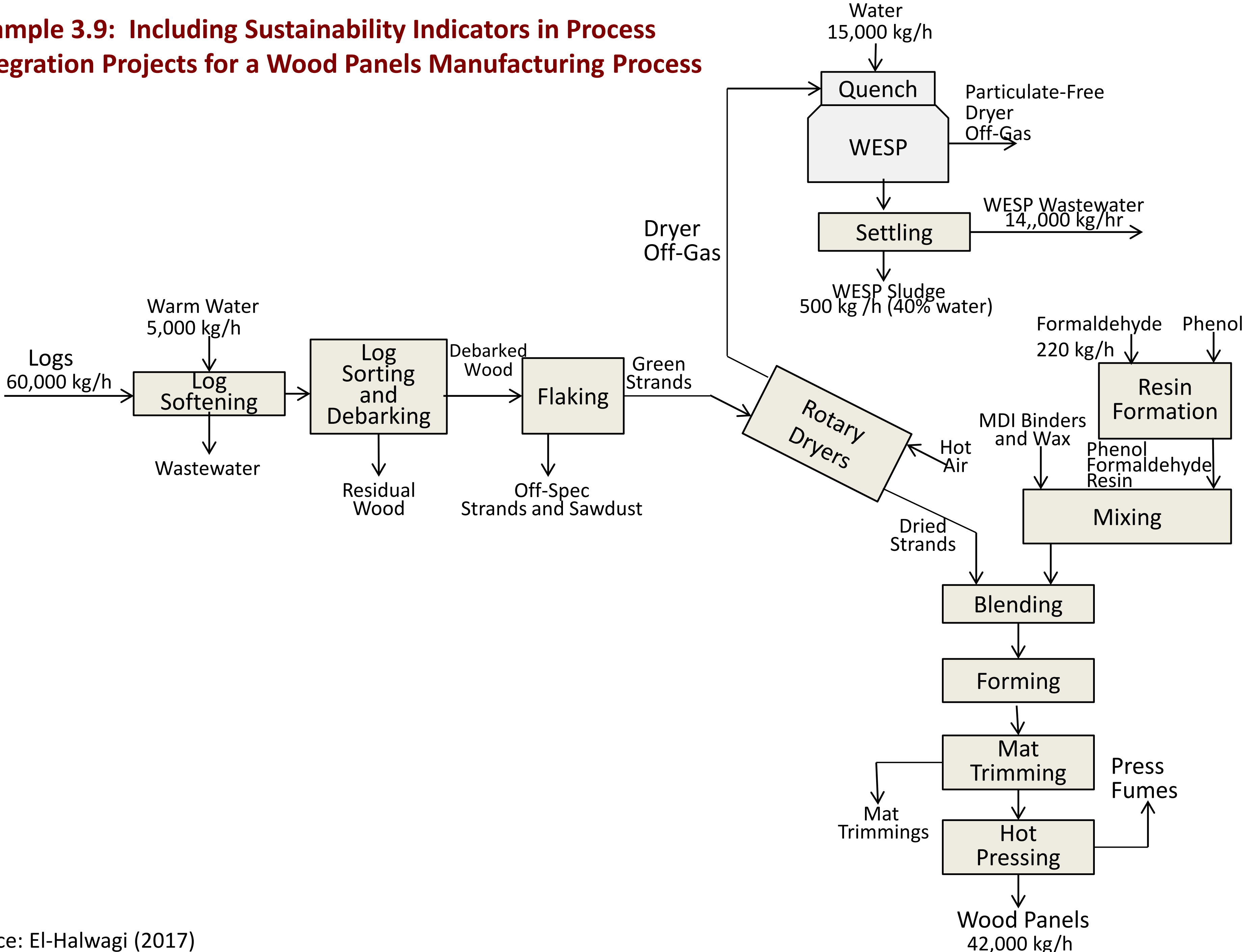
$$ASP_p = AEP_P \left[1 + \sum_{i=1}^{N_{Indicators}} w_i \left(\frac{Indicator_{p,i}}{Indicator_i^{\text{Target}}} \right) \right]$$

- *SWROIM* may be >, =, or < *ROI*
- For a project to be recommended, *SWROIM* > threshold *ROI*
- If all w_i’s are set to zero, $SWROIM_p$ reverts to the economic ROI_p
- For incremental projects: incremental sustainability return on investment “*ISWROIM*”:

$$ISWROIM_p = \frac{\Delta ASP_p}{\Delta TCI_p}$$

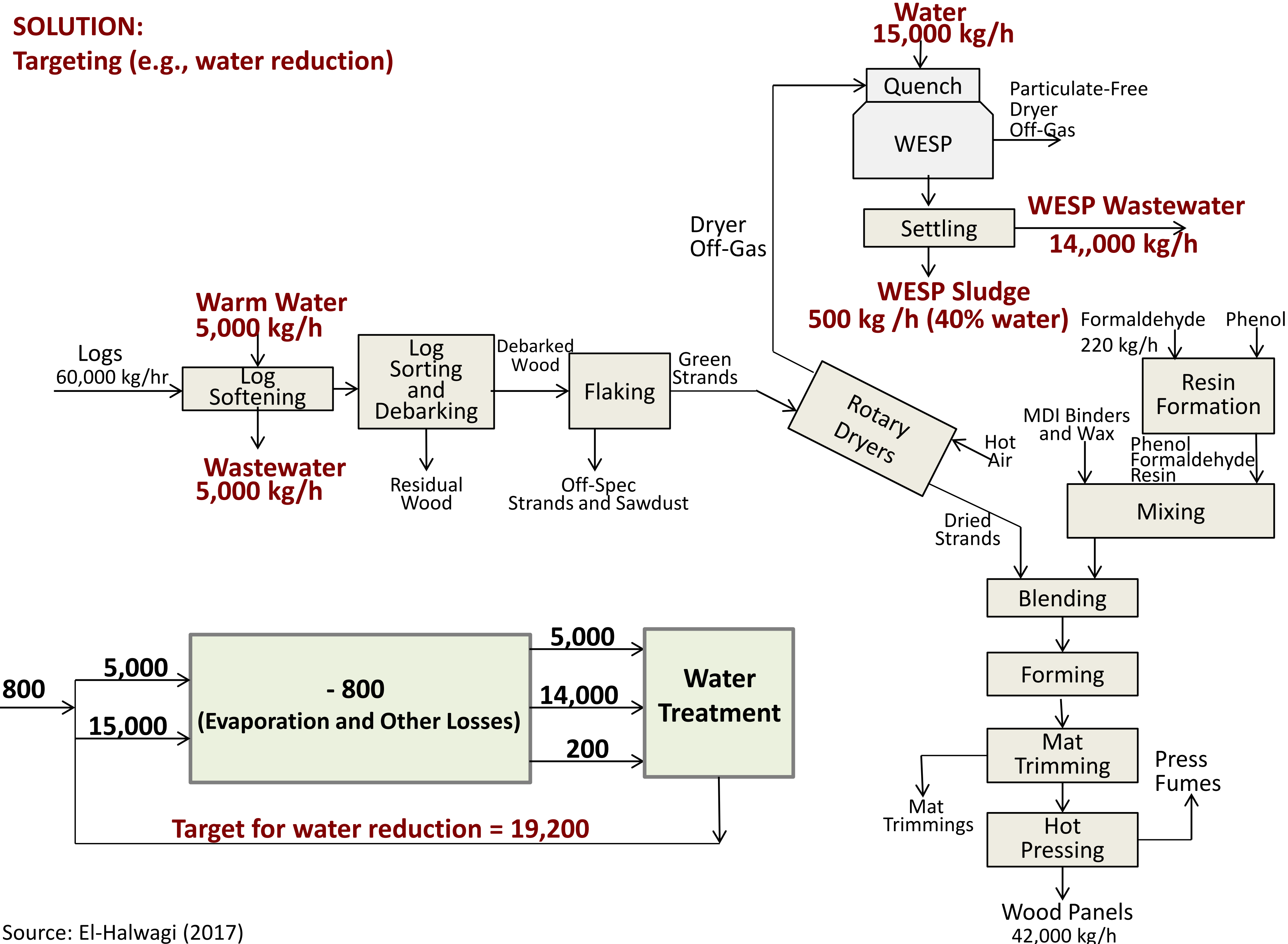
Source: El-Halwagi, M. M., “A Return on Investment Metric for Incorporating Sustainability in Process Integration and Improvement Projects”, Clean Technologies and Environmental Policy 19:611-617 (2017)

Example 3.9: Including Sustainability Indicators in Process Integration Projects for a Wood Panels Manufacturing Process



Source: El-Halwagi (2017)

SOLUTION:
Targeting (e.g., water reduction)



Water
15,000 kg/h

Quench

WESP

Particulate-Free
Dryer
Off-Gas

Settling

WESP Wastewater
14,,000 kg/h

Dryer
Off-Gas

WESP Sludge
500 kg /h (40% water)

Formaldehyde
220 kg/h

Phenol

Warm Water
5,000 kg/h

Logs
60,000 kg/hr

Log
Softening

Wastewater
5,000 kg/h

Log
Sorting
and
Debarking

Residual
Wood

Debarked
Wood

Flaking

Off-Spec
Strands and Sawdust

Green
Strands

Rotary
Dryers

Hot
Air

Resin
Formation

MDI Binders
and Wax

Phenol
Formaldehyde
Resin

Mixing

Dried
Strands

Blending

Forming

Mat
Trimming

Mat
Trimmings

Press
Fumes

Hot
Pressing

Wood Panels
42,000 kg/h

800

5,000

15,000

- 800
(Evaporation and Other Losses)

5,000

14,000

200

Water
Treatment

Target for water reduction = 19,200

Source: El-Halwagi (2017)

Targets and Relative Importance of Sustainability Indicators for the Wood Panels Case Study

Sustainability Indicator (i)	Target $Indicator_i^{\text{Target}}$	Unit	Relative Importance as a Ratio to Economic Profit (w_i)
Reduction in Water Footprint	19,200	kg/h	0.10
Hazardous Waste Reduction	500	kg/h	0.10
Thermal Energy Savings (via Heat Integration)	2.8	MW	0.07
Fuel Savings (Excluding Heat Integration Projects)	41.5	MW	0.07
VOC Emission Reduction	89	kg/h	0.05
CO_2 Emission Reduction	856	tonne/yr	0.25

Summary of Process Improvement Projects with Relevant Indicators

#	Project Description	*AEP* $(10^3\$/yr)$	*TCI* $(10^3\$)$	Water Reduction (kg/h)	Hazardous Waste Reduction (kg/h)	Thermal Energy Savings (via Heat Integration) (MW)	Fuel Savings (Excluding Heat Integration Projects) (MW)	VOC Emission Reduction (kg/h)	CO_2 Emission Reduction (tonne/yr)
I	Utilization of 17,000 kg/h of wood waste (barks, sawdust, and off-spec strands) as fuel in retrofitted and expanded boilers	3,642	9,600				40.8		789
II	Heat integration of dryer outlet stream with incoming air stream	249.9	1,450			2.8			54
III	Usage of a process mass separating agent “MSA” to remove VOCs from the dryers off-gas and combustion of spent MSA	9.3	100				9	76	145
IV	VOC recovery from the dryers to substitute fresh formaldehyde and sell methanol and acetaldehyde (this project is mutually exclusive with Project III)	54	526				**-39 (additional fuel usage)**	89	**-710 (additional emissions)**

Summary of Process Improvement Projects with Relevant Indicators (Continued)

#	Project Description	*AEP* (10^3\$/yr)	*TCI* (10^3\$)	Water Reduction (kg/h)	Hazardous Waste Reduction (kg/h)	Thermal Energy Savings (via Heat Integration) (MW)	Fuel Savings (Excluding Heat Integration Projects) (MW)	VOC Emission Reduction (kg/h)	CO_2 Emission Reduction (tonne/yr)
V.1	Treatment and recycle of wastewater from log softening and WESP	49	420	18,800			0.03		1
V.2	WESP sludge dewatering then treatment of separated wastewater with log softening wastewater and the rest of the WESP wastewater for recycle (**this project is an incremental addition to Project V.1**)	98 (Incremental AEP)	610 (Incremental TCI)	200	280		-0.06 (additional fuel usage)		-2 (additional emissions)
V.3	Combustion of dewatered sludge in a retrofitted boiler (**this project is an incremental addition to Project V.2**)	164 (Incremental AEP)	780 (Incremental TCI)		420		0.6		11

Illustration for Project I

#	Project Description	*AEP* (10^3\$/yr)	*TCI* (10^3\$)	Water Reduction (kg/h)	Hazardous Waste Reduction (kg/h)	Thermal Energy Savings (via Heat Integration) (MW)	Fuel Savings (Excluding Heat Integration Projects) (MW)	VOC Emission Reduction (kg/h)	CO_2 Emission Reduction (tonne/yr)
I	Utilization of 17,000 kg/h of wood waste (barks, sawdust, and off-spec strands) as fuel in retrofitted and expanded boilers	3,642	9,600				40.8		789

$$ROI_{\text{Project I}} = \frac{3{,}642{,}000}{9{,}600{,}000} * 100\% = 37.9\%$$

$$SWROIM_{\text{Project I}} = \frac{3{,}642{,}000\left[1 + 0.07 * \left(\frac{40.8}{41.5}\right) + 0.25 * \left(\frac{789}{856}\right)\right]}{9{,}600{,}000} * 100\%$$

$$= 49.3\%$$

Sustainability Indicator (*i*)	Target	Unit	Relative Importance as a Ratio to Economic Profit (w_i)
Fuel Savings (Excluding Heat Integration Projects)	**41.5**	MW	**0.07**
CO_2 Emission Reduction	**856**	tonne/yr	**0.25**

Results Summary: Economic and Sustainability-Weighted Returns on Investments

(Threshold ROI = 10%)

Project #	**ROI%**	**SWROIM%**
I	37.9	49.3
II	17.2	18.7
III	**9.3**	**10.2**
IV	**10.3**	**8.0**
V.1	11.7	12.8
V.2	16.1 (IROI)	17.0 (ISWROIM)
V.3	21.0 (IROI)	22.9 (ISWROIM)

I–II: Aligned economic and sustainability objectives

III →Recommended after sustainability inclusion

IV →Not recommended after sustainability inclusion

Concluding Thoughts

- Systematic tools for sustainable design through process integration
- Benchmarking sets targets ahead of detailed design
- Ideal for inclusion in process design course(s) or electives on sustainability

BIG Picture first, details later

Additional Problems

Source: El-Halwagi, M. M., “Sustainable Design through Process Integration: Fundamentals and Applications to Industrial Pollution Prevention, Resource Conservation, and Profitability Enhancement”, Second Edition, Elsevier (2017)

Problem 1. Stoichio-nomic Targeting for CO_2 Methanation

Carbon dioxide is one of the primary greenhouse gases (GHG) resulting from industrial processes. Laboratory experiments have shown that CO_2 can be converted to methane by hydrogenation over a composite catalyst via the following methanation reaction:

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$

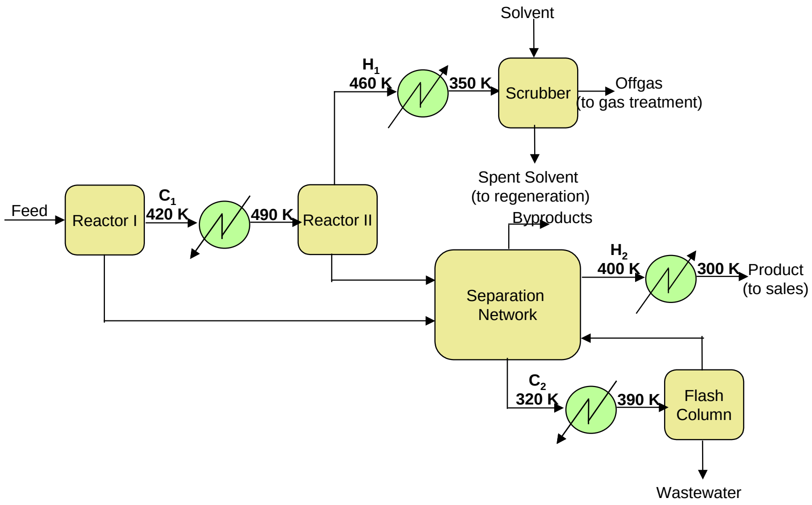
A new catalyst has been recently developed to induce high conversion of CO_2 and selectivity to CH4 under reasonably mild conditions. A group of investors, interested in reducing GHG emissions while making a profit, are considering the use of this methanation approach to convert CO_2 from industrial emissions to methane. Since CO2 will be extracted from an industrial waste streams, it will be supplied free of charge. Hydrogen is available at $1.60/kg. The value of methane is $3.50/1000 SCF (at 60 ^{o}F and 1 atm). The value of produced water is negligible compared to the value of methane.

Part a. How would you advise the group of investors?

Part b. you were advising the government to offer a GHG-reduction incentive for this technology, what you recommend as the minimum acceptable subsidy ($/tonne CO_2)?

Problem 2. Heat Integration

Consider the chemical processing facility illustrated in the figure below. The process has two adiabatic reactors. The intermediate product leaving the first reactor (C_1) is heated from 420 to 490 K before being fed to the second reactor. The off-gases leaving the reactor (H_1) at 460 K are cooled to 350 K prior to being forwarded to the gas-treatment unit. The product leaving the bottom of the reactor is fed to a separation network. The product stream leaving the separation network (H_2) is cooled from 400 to 300 prior to sales. A byproduct stream (C_2) is heated from 320 to 390 K before being fed to a flash column. Stream data are given in the Table below.



Stream	Flowrate x Specific Heat kW/K	Supply temperature, K	Target temperature, K	Enthalpy change kW
H_1	300	460	350	-33,000
H_2	500	400	300	-50,000
C_1	600	420	490	42,000
C_2	200	320	390	14,000

In the current operation, the heat exchange duties of H_1, H_2, C_1, and C_2 are fulfilled using the cooling and heating utilities. Therefore, the current usage of cooling and heating utilities are 83,000 and 56,000 kW, respectively. The objective of this problem is to identify the target for minimum heating and cooling utilities and. A value of 10 K is used as the minimum driving force.

Problem 3. Sustainability Weighted Return on Investment

A company is considering a number of process integration projects. A summary of the key characteristics of these projects is given by the Table below. The desired targets and the relative weights of four indicators are shown by the second Table below. If the projects are mutually exclusive, how would you rank the proposed projects?

Project #	*AEP* (10^3\$/yr)	*TCI* (10^3\$)	Reduction in Water Usage (kg/h) $Indicator_i^{\text{Target}}$	Reduction in Hazardous Air Pollutants (HAPs) Discharge (kg/h)	Reduction in Energy Consumption (MW)	Greenhouse Gas Emission (GHG) Reduction (tonne $CO_{2\ eq.}$/yr)
I	7,046	48,985	23,400	50	1.3	220
II	239	1,450	-19,400	900	4.9	750
III	12	100	3,980	470	-6.0	-1,100
IV	54	526	11,990	830	5.1	830

Sustainability Indicator (*i*)	Target Indicator $Indicator_i^{\text{Target}}$	Relative Importance as a Ratio to Economic Profit (w_i)
Reduction in Water Footprint (kg/h)	23,400	0.10
Reduction in HAPs Discharge (kg/h)	900	0.10
Reduction in Energy Consumption (MW)	6.1	0.05
Reduction in GHG Emissions (tonne $CO_{2\ eq}$/yr)	1,200	0.05