Lecture 4: Sustainable process design

Chemical product centric sustainable process design: Introduction to sustainable process design

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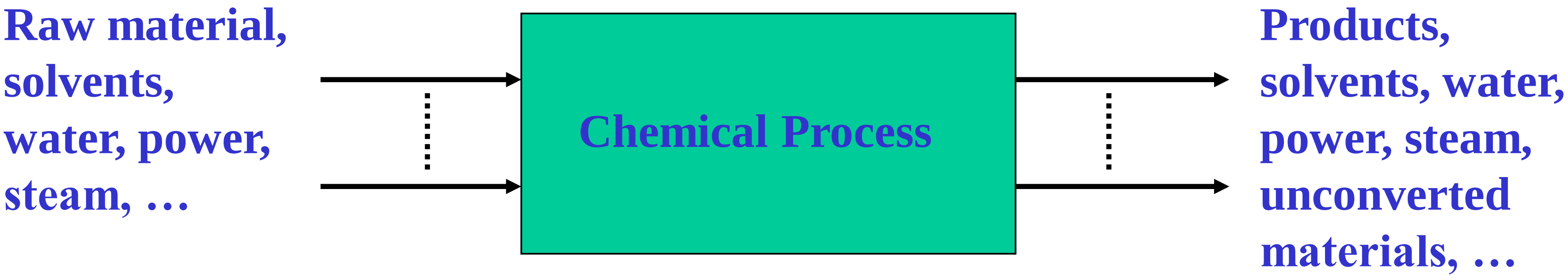
Lecture 4

Problem definition; issues, concepts and definitions

Targeted sustainable process design

Identify design that matches the target



- Start with a reference design
- Calculate sustainability metrics, safety factors plus mass & energy indicators
- Identify attainable design targets
  - Indicator targets (for process improvements)
  - Driving forces targets (for generation of alternatives)
- Apply reverse approach to match design targets
- Order all feasible solutions to find optimal (conflict resolution)

General Problem Definition

$\text{Fobj} = \min \{C^T\underline{y} + f(\underline{x}, \underline{y}, \underline{u}, \underline{d}, \underline{\theta}) + S_e + S_i + S_s + H_c + H_p\}$ **(1)**

$0 = h_1(\underline{x}, \underline{y})$ **process constraints (Eq. 2)**

$0 = P(\underline{f}, \underline{x}, \underline{y}, \underline{d}, \underline{u}, \underline{\theta})$ **process model (Eq. 3)**

$\underline{\theta} = \underline{\theta}(\underline{f}, \underline{x}, \underline{y})$ **property model (Eq. 4)**

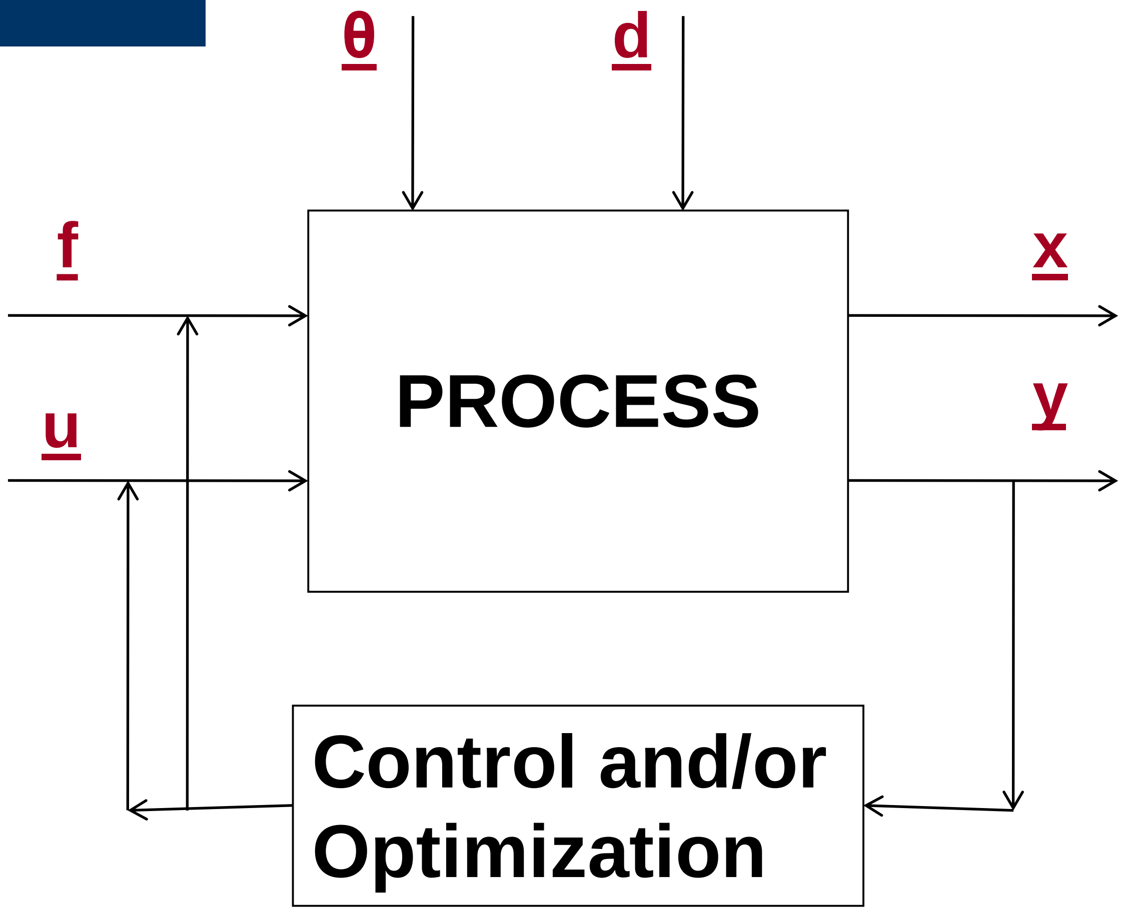
$l_1 \leq g_1(\underline{x}, \underline{u}, \underline{d}) \leq u_1$ **process variable constraints (Eq. 5)**

$l_2 \leq g_2(\underline{x}, \underline{y}) \leq u_2$ **molecular structure constraints (Eq. 6)**

$B\,\underline{x} + C^T\underline{y} \geq D$ **process networks (Eq.7)**

$\underline{x}$: real-process variables; $\underline{y}$ integer-decision variables;
u: process design variables; d: process input variables;
θ: property; B, C, D coefficient matrices

Issues: Models and relationships



$\underline{\theta}$

$\underline{d}$

$\underline{f}$

$\underline{u}$

PROCESS

$\underline{x}$

$\underline{y}$

Control and/or Optimization

Models:

Process/property

$d\underline{x}/dt = f(\underline{f}, \underline{u}, \underline{d}, \underline{\theta}, \underline{x})$

$\underline{y} = g(\underline{x})$

$\underline{\beta} = \beta\,(\underline{C}, \underline{f}, \underline{x})$

Sustainability Metrics

$\underline{S}_e = S_e\,(\underline{f}, \underline{u}, \underline{x}, \underline{y}, \underline{d}, \underline{\theta})$

$\underline{S}_i = S_i\,(\underline{C}, \underline{f}, \underline{x}, \underline{y}, \underline{\theta})$

$\underline{S}_s = S_s\,(\text{size, profit, ?})$

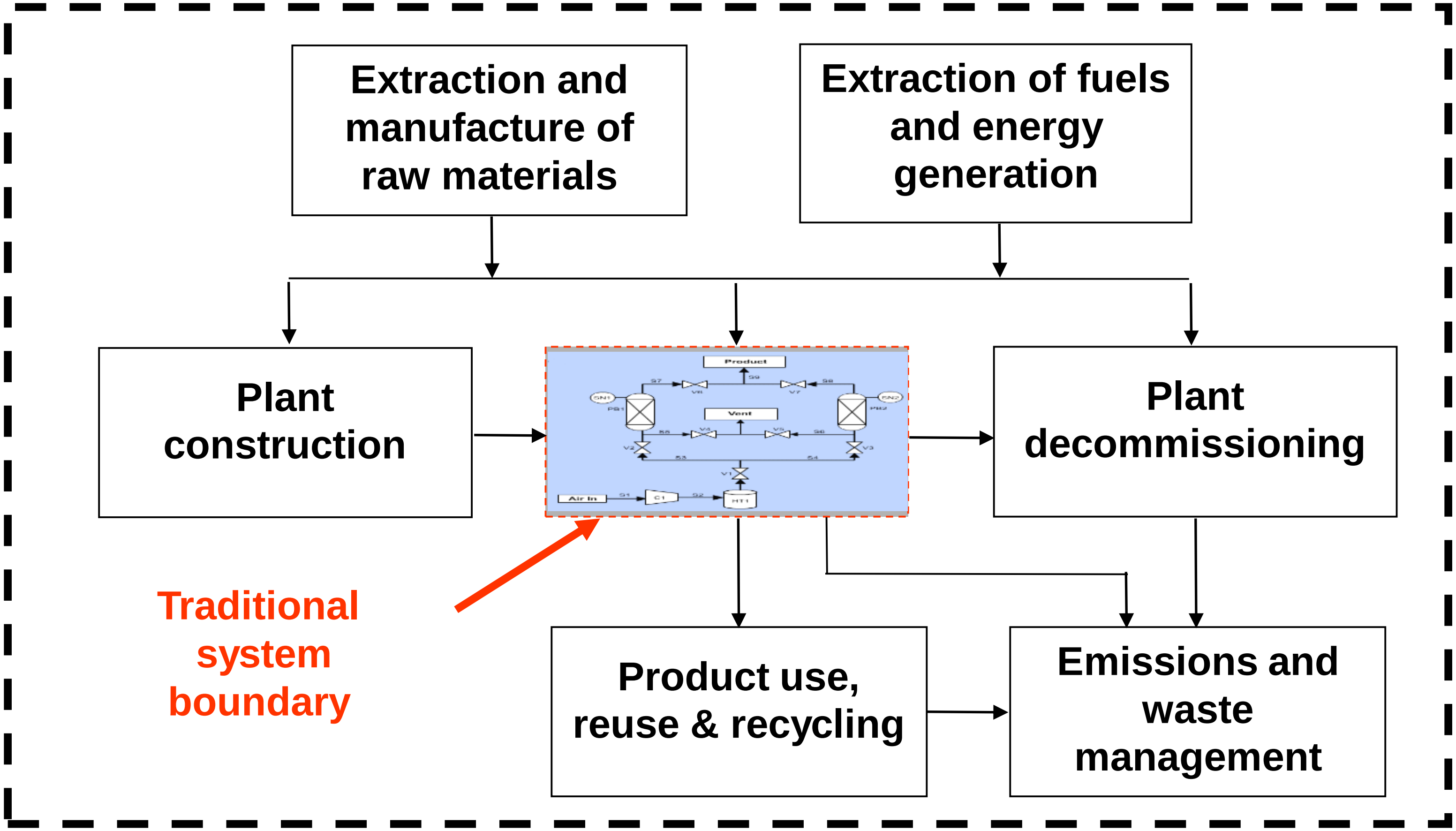
Safety & Hazards

$\underline{H}_c = Hc\,(\underline{C}, \underline{f}, \underline{x}, \underline{y}, \underline{d}, \underline{\theta})$

$\underline{Hp} = H_p\,(\underline{u}, \underline{f}, \underline{x}, \underline{d}, \underline{\theta})$

Issues: System boundary definition

SYSTEM (from ‘cradle to grave’)



Extraction and manufacture of raw materials

Extraction of fuels and energy generation

Plant construction

Plant decommissioning

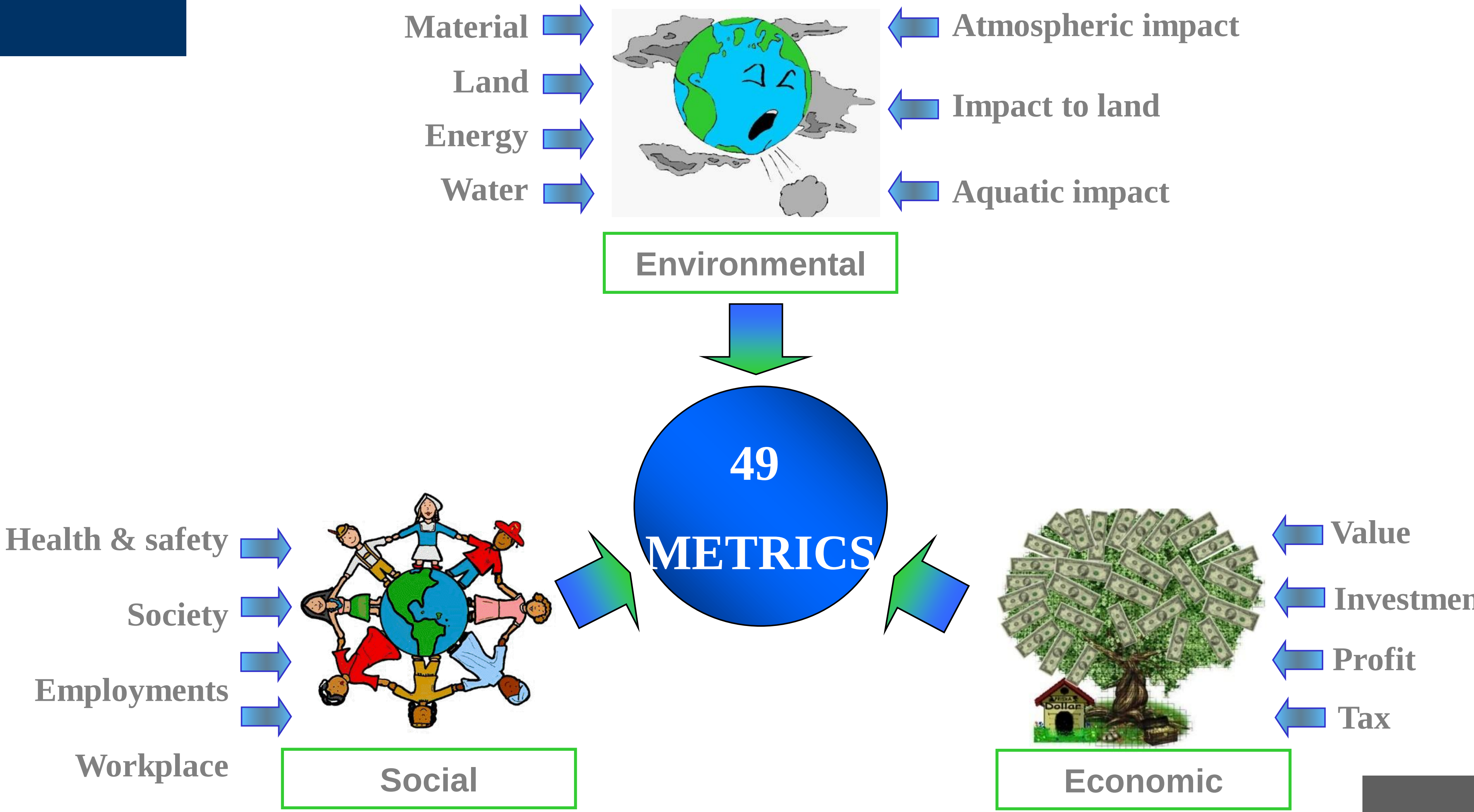
Product use, reuse & recycling

Emissions and waste management

Traditional system boundary

New system boundary

Issues: Measure of sustainability



Material

Land

Energy

Water

Atmospheric impact

Impact to land

Aquatic impact

Environmental

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METRICS

Health & safety

Society

Employments

Workplace

Social

Value

Investmen

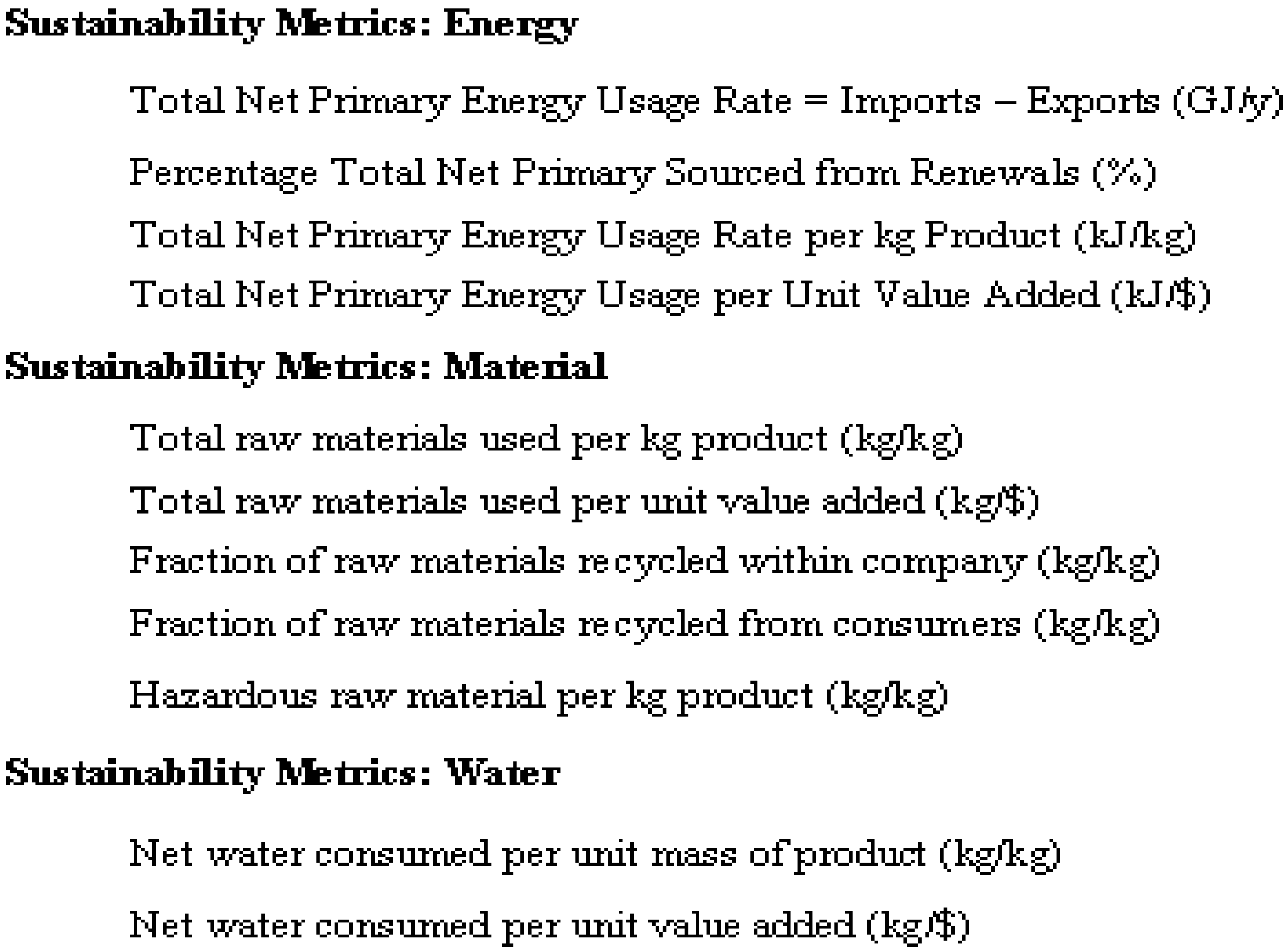
Profit

Tax

Economic

Issues: Measure of sustainability

Example: The IChemE Model



Sustainability Metrics: Energy

Total Net Primary Energy Usage Rate = Imports – Exports (GJ/y)

Percentage Total Net Primary Sourced from Renewals (%)

Total Net Primary Energy Usage Rate per kg Product (kJ/kg)

Total Net Primary Energy Usage per Unit Value Added (kJ/$)

Sustainability Metrics: Material

Total raw materials used per kg product (kg/kg)

Total raw materials used per unit value added (kg/$)

Fraction of raw materials recycled within company (kg/kg)

Fraction of raw materials recycled from consumers (kg/kg)

Hazardous raw material per kg product (kg/kg)

Sustainability Metrics: Water

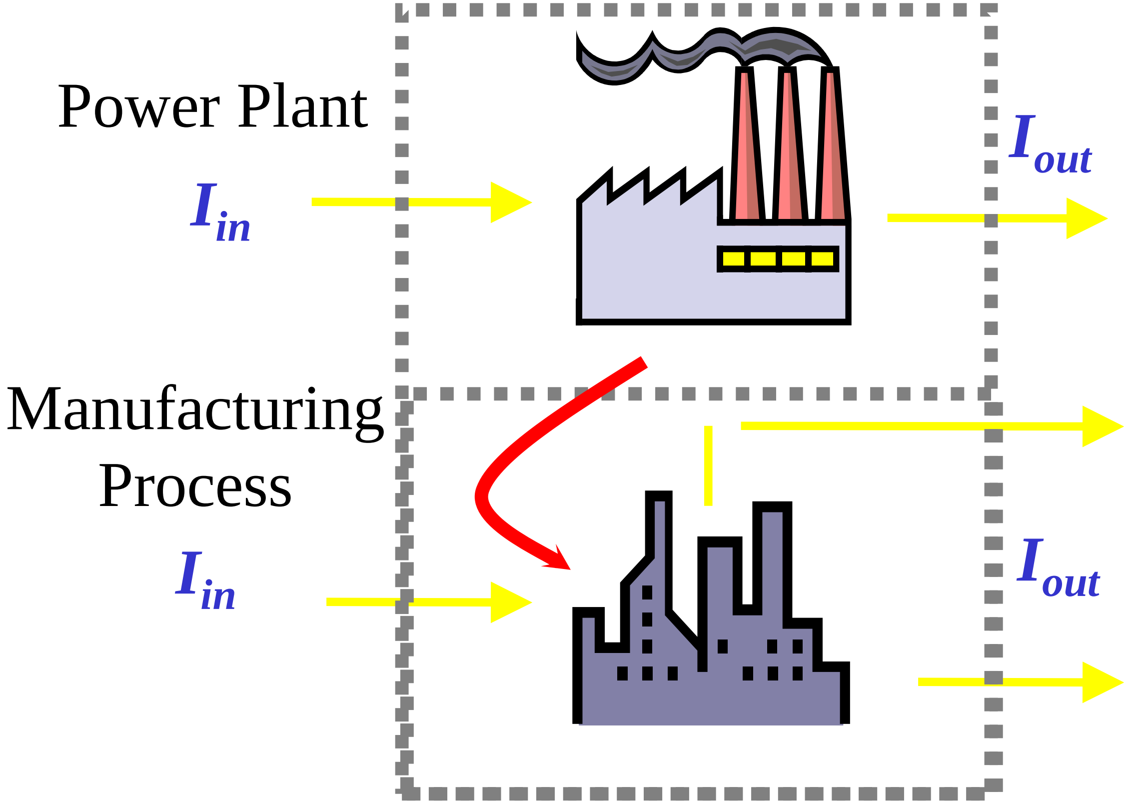
Net water consumed per unit mass of product (kg/kg)

Net water consumed per unit value added (kg/$)

Azapagic , *Sustainable Development Progress Metrics*, IChemE Sustainable Development Working Group, IChemE, Rugby, UK, 2002

Measure of environmental impact - I

US-EPA Model



$$I = \Sigma_i \alpha_i \ \Sigma_j M_j \ \psi_{ij}$$

M_j = mass flow rate of chemical *j* (mass/time)

α_i = weighting factor for impact category *i*

ψ_{ij} = chemical and category specific impact (PEI/mass)

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Measure of environmental impact - II

Atmospheric, Aquatic & Land Impacts

Physical potential impacts (acidification, greenhouse enhancement, ozone depletion and photochemical oxidant depletion)

Human toxicity effects (air, water and soil) and eco-toxicity effects (aquatic and terrestrial)

The important parameters are:

HTPI (Human Toxicity Potential by Ingestion)

HTPE (Human Toxicity Potential by Exposure both Dermal and Inhalation)

TTP (Terrestrial Toxicity Potential)

ATP (Aquatic Toxicity Potential)

GWP (Global Warming Potential)

ODP (Ozone Depletion Potential)

PCOP (Photochemical Oxidation Potential)

AP (Acidification Potential)

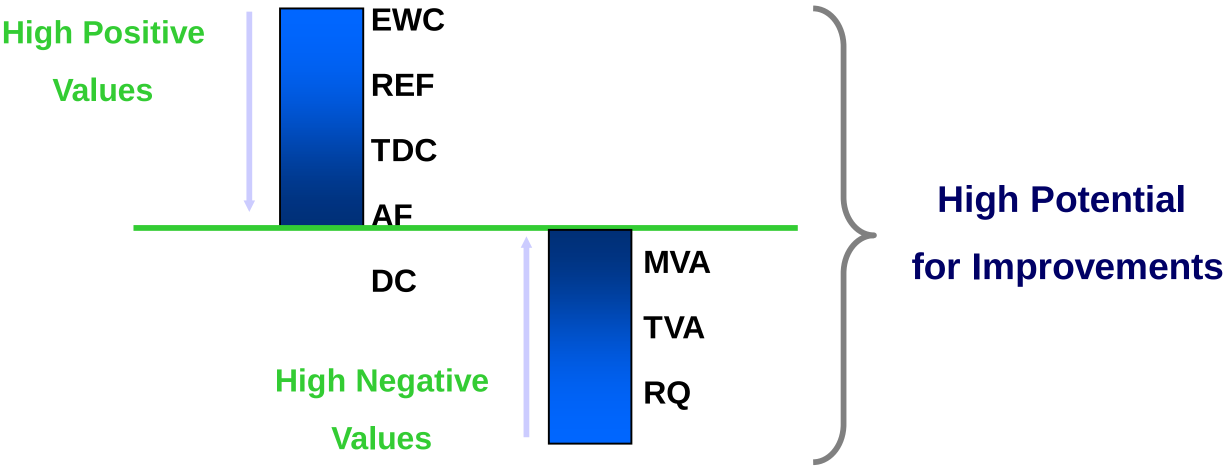
Total PEI Total Potential Environmental Impact), which indicates the unrealised effect or impact that the emission of mass and energy would have on the environment on average

Measure of safety: DOW safety index

Total Inherent Safety Index (ISI)			
Chemical Inherent Safety Index, I_{ci}	**Score**	**Process Inherent Safety Index, Ici**	**Score**
Sub-indices for reactions Hazards		Sub-indices for process conditions	
Heat of the main reaction, I_{rm}	0-4	Inventory, I_i	0-5
Heat of the side reactions, I_{rs}	0-4	Temperature, I_T	0-4
Chemical interactions, I_{int}	0-4	Pressure, I_P	0-4
Sub-indices for Hazards substances		Sub-indices for process conditions	
Flammability, I_{fl}	0-4	Equipment, I_{eq}	
Explosiveness, I_{ex}	0-4	I_{Isbl}	0-4
Toxicity, I_{tox}	0-6	I_{Osbl}	0-3
Corrosivity, I_{cor}	0-2	Process structure, I_{st}	0-5
Maximum, I_{ci} score	28	Maximum, I_{pi} score	25
Maximum, I_{Si} score 53			

Definition: Indicators (mass & energy)

Indicator	Description	Definition
MVA	Material Value Added	$MVA = M_T*(P_{sale}-P_{cost})$
EWC	Energy & Waste Cost	$EWC = E\ P_E\ M_i\ \theta_i/(\Sigma_i\ M_i\ \theta_i)$
TVA	Total Value Added	$TVA = MVA - EWC$
RQ	Reaction Quality	$RQ = R_X\ \theta_R/\ (\Sigma_p\ M_p)$
AF	Accumulation Factor	$AF = M_{i\text{-cycle}}\ /(\Sigma_{k\text{-cycle}}\ M_{k\text{-cycle}})$
REF	Reusable Energy Factor	$REF = E_{used\text{-cycle}}/\ E_{exit\text{-cycle}}$
DC	Demand Cost	$DC = P_{utility}E_{open\text{-path}}$
TDC	Total Demand Cost	$TDC = \Sigma\ DC_k$



High Positive Values

EWC
REF
TDC
AF

DC

MVA
TVA
RQ

High Negative Values

High Potential for Improvements

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Definition: Indicators (batch operations)

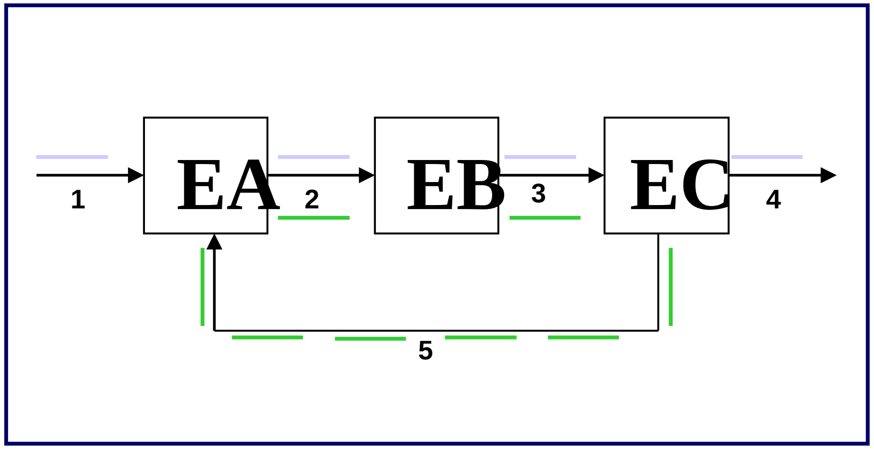
Indicator	Description	Operation	Definition
FVF	Free Volume Fraction	All	$FVF=\frac{V_{equi}-\sum_{i}^{I}\frac{F_{AP}^{(i)}}{\rho(i)}}{V_{equi}}$
TF	Time Factor	Mixer	$TF_{j,i}=\frac{1}{\frac{F_{AP}^{(c)}}{\sum_{co}^{CO}F_{AP}^{(co)}}}\times\frac{t_j}{t_{total}}$
		Reactor	$TF_{j,i}=x\left(\frac{1}{\frac{F_{AP}^{(c)}}{\upsilon^{(c)}}}\times\frac{t_j}{t_{total}}\right)+(1-x)\left((1-z)\frac{1}{\frac{F_{AP}^{(c)}}{\upsilon^{(c)}}}\times\frac{t_j}{t_{total}}\right)$
		Heat Exchanger	$TF_{j,i}=\frac{F_{AP}^{(c)}\times cp^{(c)}}{\sum_{co}^{CO}F_{AP}^{(co)}\times cp^{(co)}}\times\frac{t_j}{t_{total}}$
		Separation	$TF_{j,i}=\frac{F_{AP}^{(c)}}{\lvert \Pr operty^{R}-\Pr operty^{C}\rvert}\times\frac{t_j}{t_{total}}$
EF	Energy Factor	Mixer	$EF_{j,i}=\frac{F_{AP}^{(c)}\sum_{h}^{H}\Delta\rho_{i}^{(c)}}{\sum_{n}^{N}F_{AP}^{(c)}\sum_{h}^{H}\Delta\rho_{h}^{(c)}}\times\frac{E_j}{\sum_{j}^{J}E_j}$
		Reactor	$EF_{j,i}=F_{AP}^{(c)}\times\Delta H_R\left(y\times\left(x\times\frac{\Delta H_f}{\sum_{co}^{CO}\Delta H_f^{(co)}}+(1-x)\left(1-\frac{\Delta H_f}{\sum_{co}^{CO}\Delta H_f^{(co)}}\right)\right)+(1-y)\left(x\times\frac{\Delta H_f}{\sum_{co}^{CO}\Delta H_f^{(co)}}\left(1-\frac{\Delta H_f}{\sum_{co}^{CO}\Delta H_f^{(co)}}\right)+(1-x)\frac{\Delta H_f}{\sum_{co}^{CO}\Delta H_f^{(co)}}\right)\right)\times\frac{E_j}{\sum_{j}^{J}E_j}$
		Heat Exchanger	$EF_{j,i}=\frac{F_{AP}^{(c)}\times cp^{(c)}}{\sum_{co}^{CO}F_{AP}^{(co)}\times cp^{(co)}}\times\frac{E_j}{\sum_{j}^{J}E_j}$
		Separation	$EF_{j,i}=\frac{F_{AP}^{(c)}\times\Pr operty^{(c)}}{\sum_{co}^{CO}F_{AP}^{(co)}\times\Pr operty^{(co)}}\times\frac{E_j}{\sum_{j}^{J}E_j}$

Definition: Open & closed paths

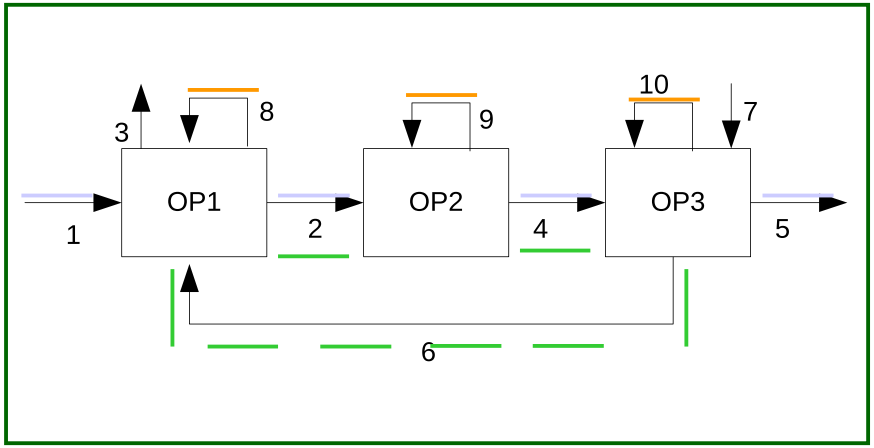
Data

OR

Simulators



Continuous Process

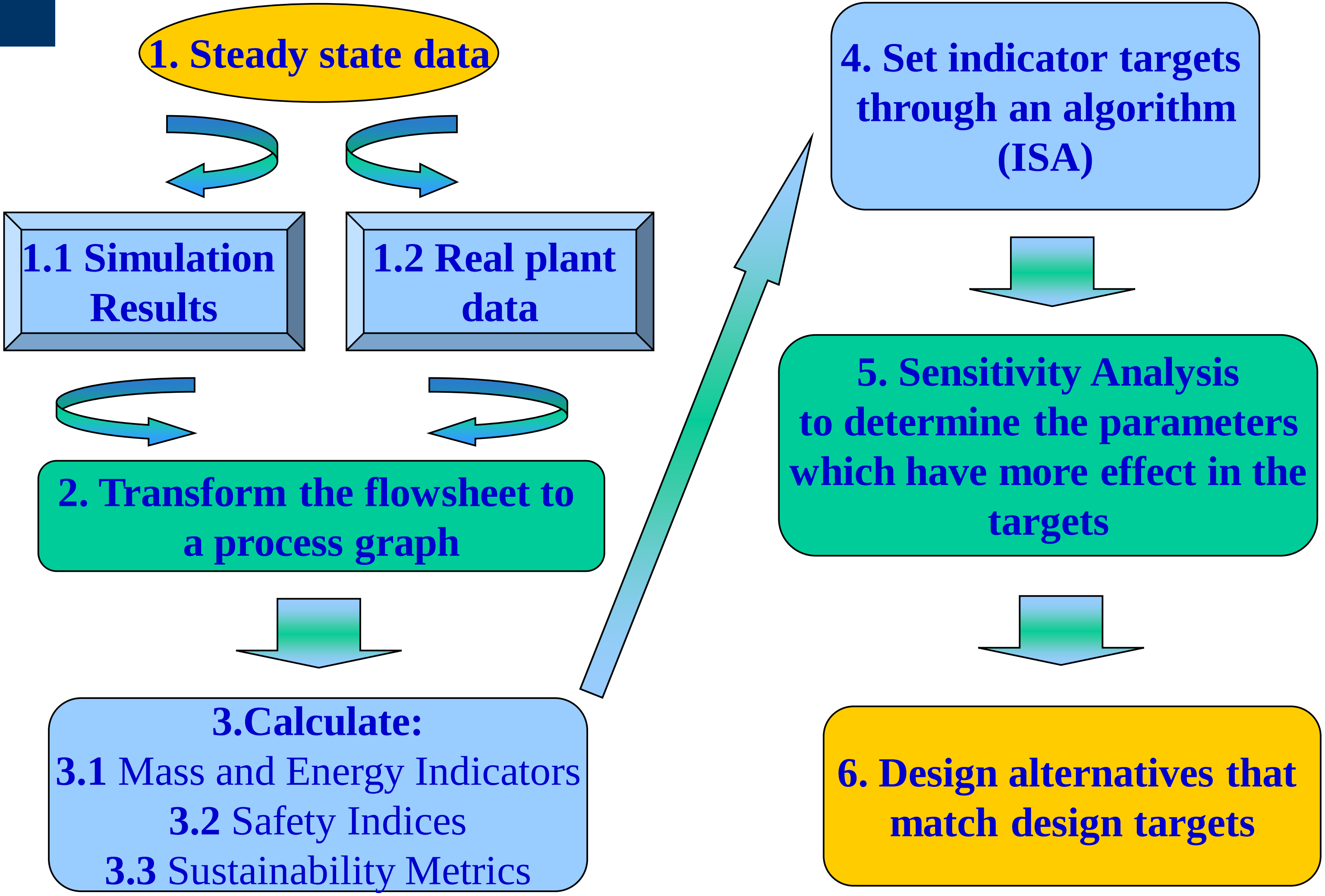


Batch Process

🟩 Closed-path 🟪 Open-path 🟧 Accumulation-path

Indicator Based Method for Generation of Sustainable Process Alternatives

Overview of the Methodology



1. Steady state data

1.1 Simulation Results

1.2 Real plant data

2. Transform the flowsheet to a process graph

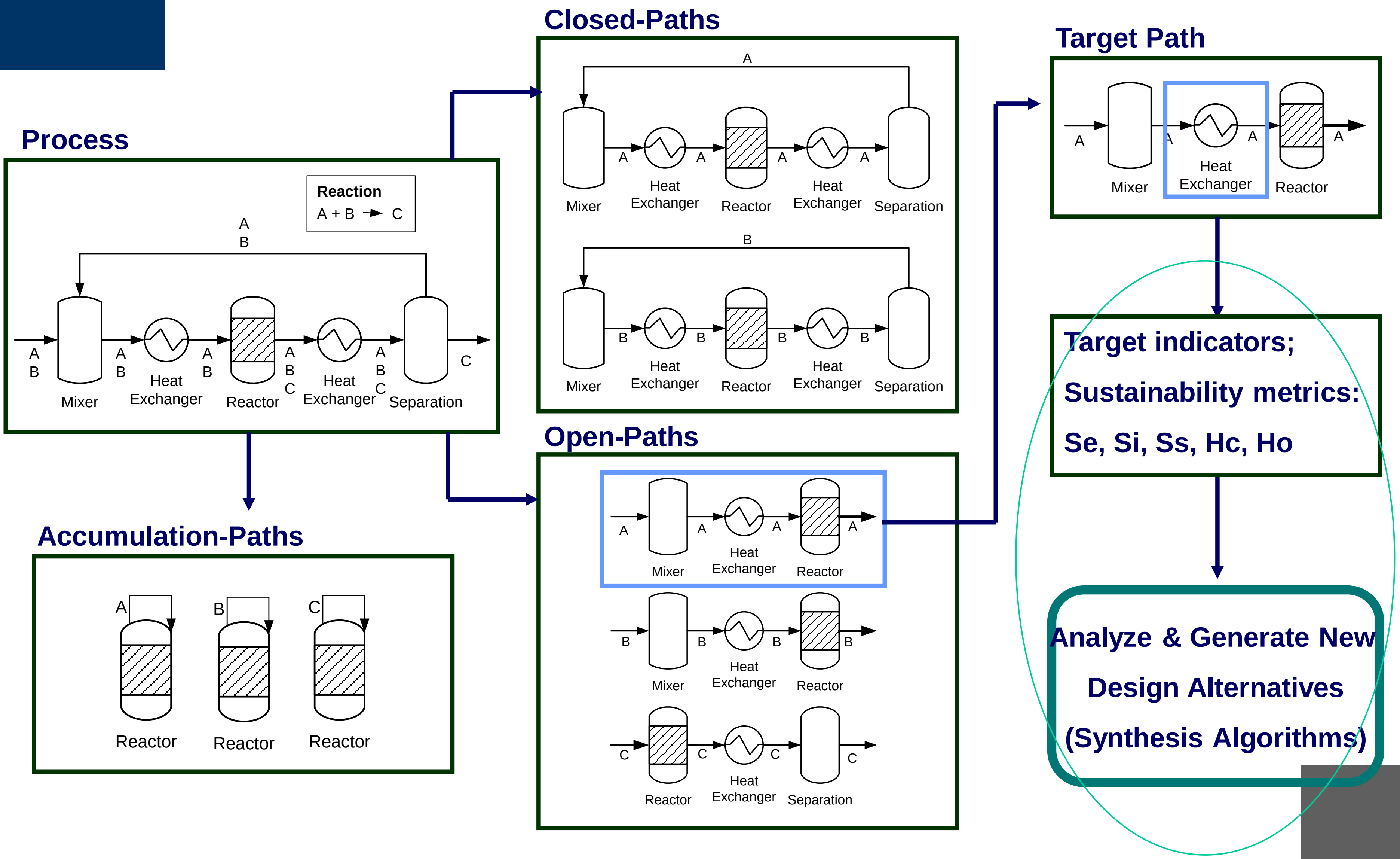
3.Calculate:
3.1 Mass and Energy Indicators
3.2 Safety Indices
3.3 Sustainability Metrics

4. Set indicator targets through an algorithm (ISA)

5. Sensitivity Analysis to determine the parameters which have more effect in the targets

6. Design alternatives that match design targets

Methodology: Overview



Target indicators;

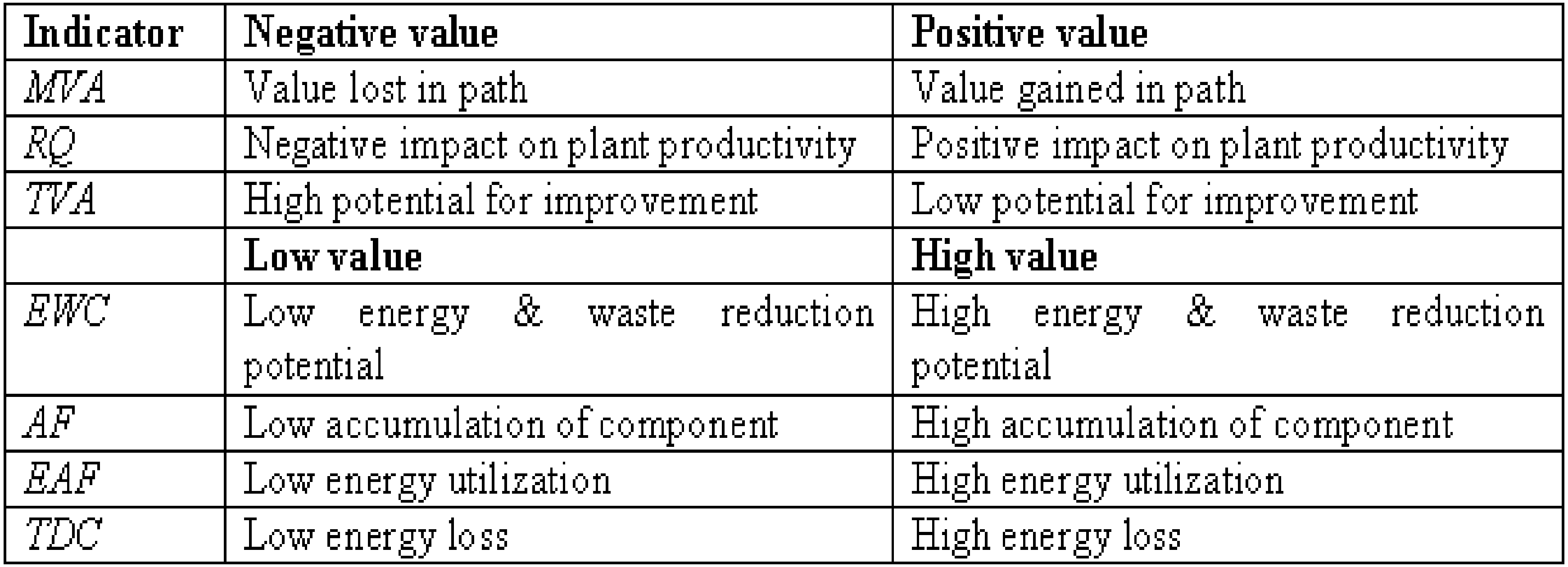
Sustainability metrics:

Se, Si, Ss, Hc, Ho

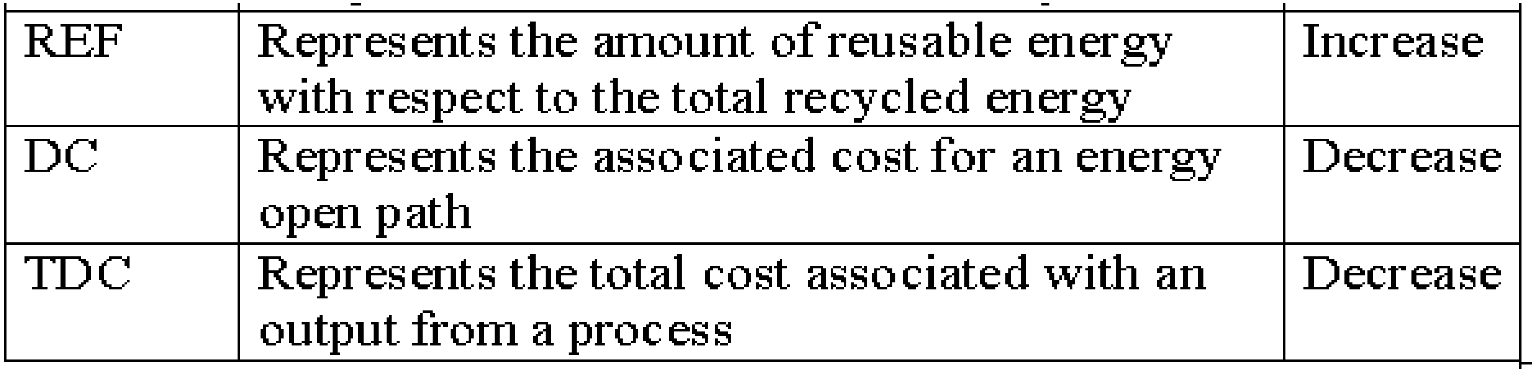
Analyze & Generate New Design Alternatives (Synthesis Algorithms)

Analysis of Indicators

Identify the target indicators



Indicator	**Negative value**	**Positive value**
MVA	Value lost in path	Value gained in path
RQ	Negative impact on plant productivity	Positive impact on plant productivity
TVA	High potential for improvement	Low potential for improvement
	Low value	**High value**
EWC	Low energy & waste reduction potential	High energy & waste reduction potential
AF	Low accumulation of component	High accumulation of component
EAF	Low energy utilization	High energy utilization
TDC	Low energy loss	High energy loss



REF	Represents the amount of reusable energy with respect to the total recycled energy	Increase
DC	Represents the associated cost for an energy open path	Decrease
TDC	Represents the total cost associated with an output from a process	Decrease

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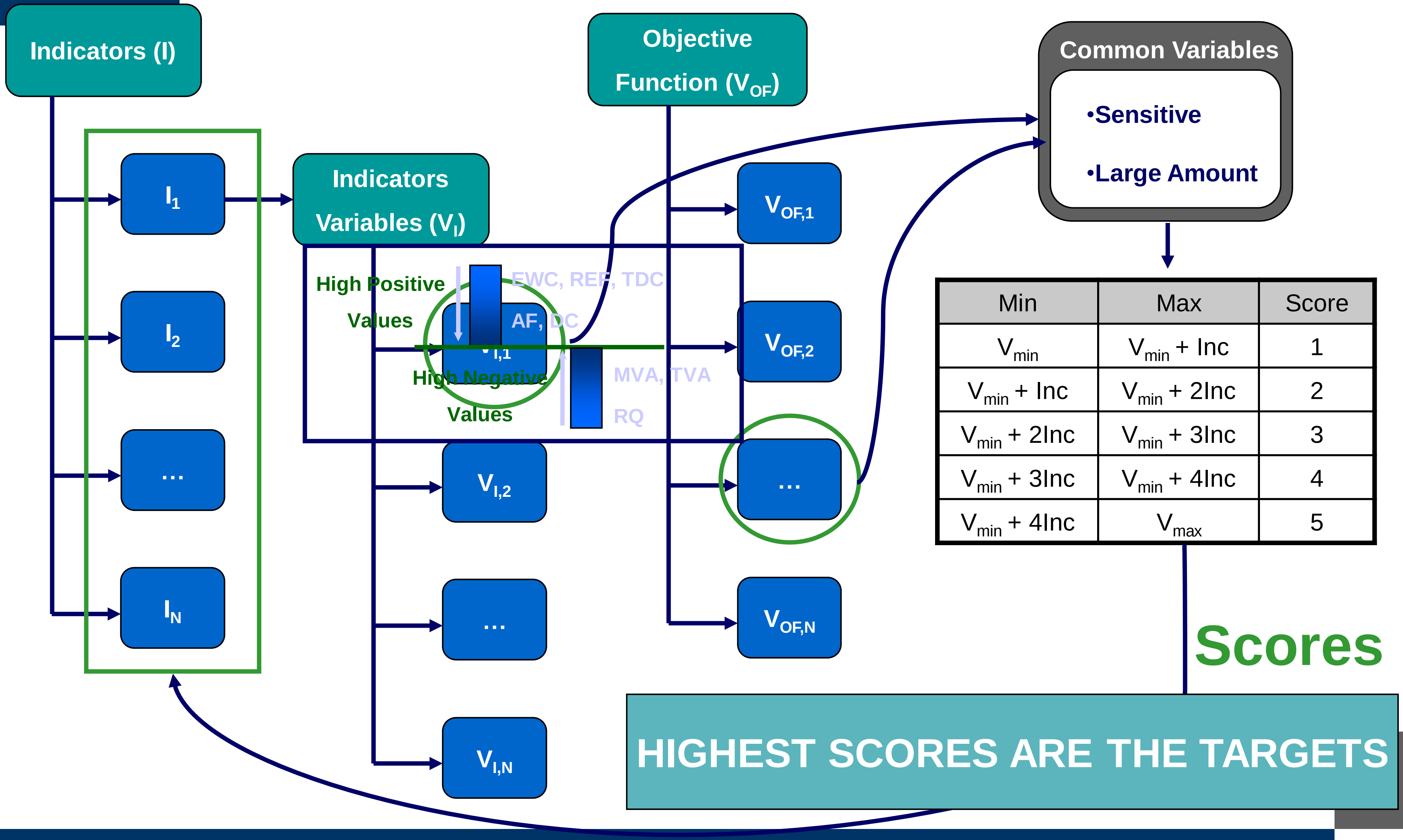
Defining targets for improvement

Indicators – variables - objective

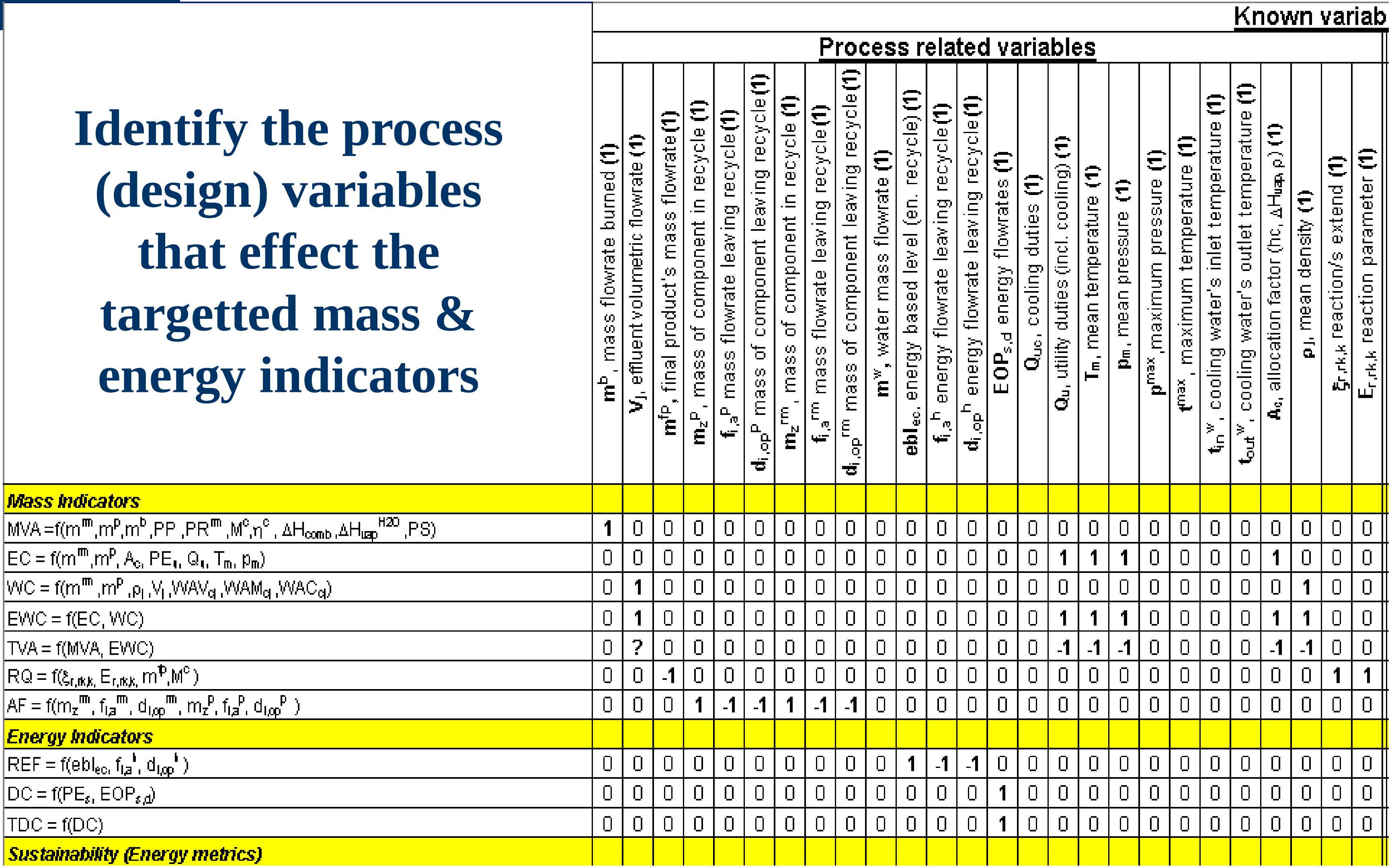


Min	Max	Score
V_{min}	V_{min} + Inc	1
V_{min} + Inc	V_{min} + 2Inc	2
V_{min} + 2Inc	V_{min} + 3Inc	3
V_{min} + 3Inc	V_{min} + 4Inc	4
V_{min} + 4Inc	V_{max}	5

HIGHEST SCORES ARE THE TARGETS

Model Structural & Sensitivity Analysis - 1

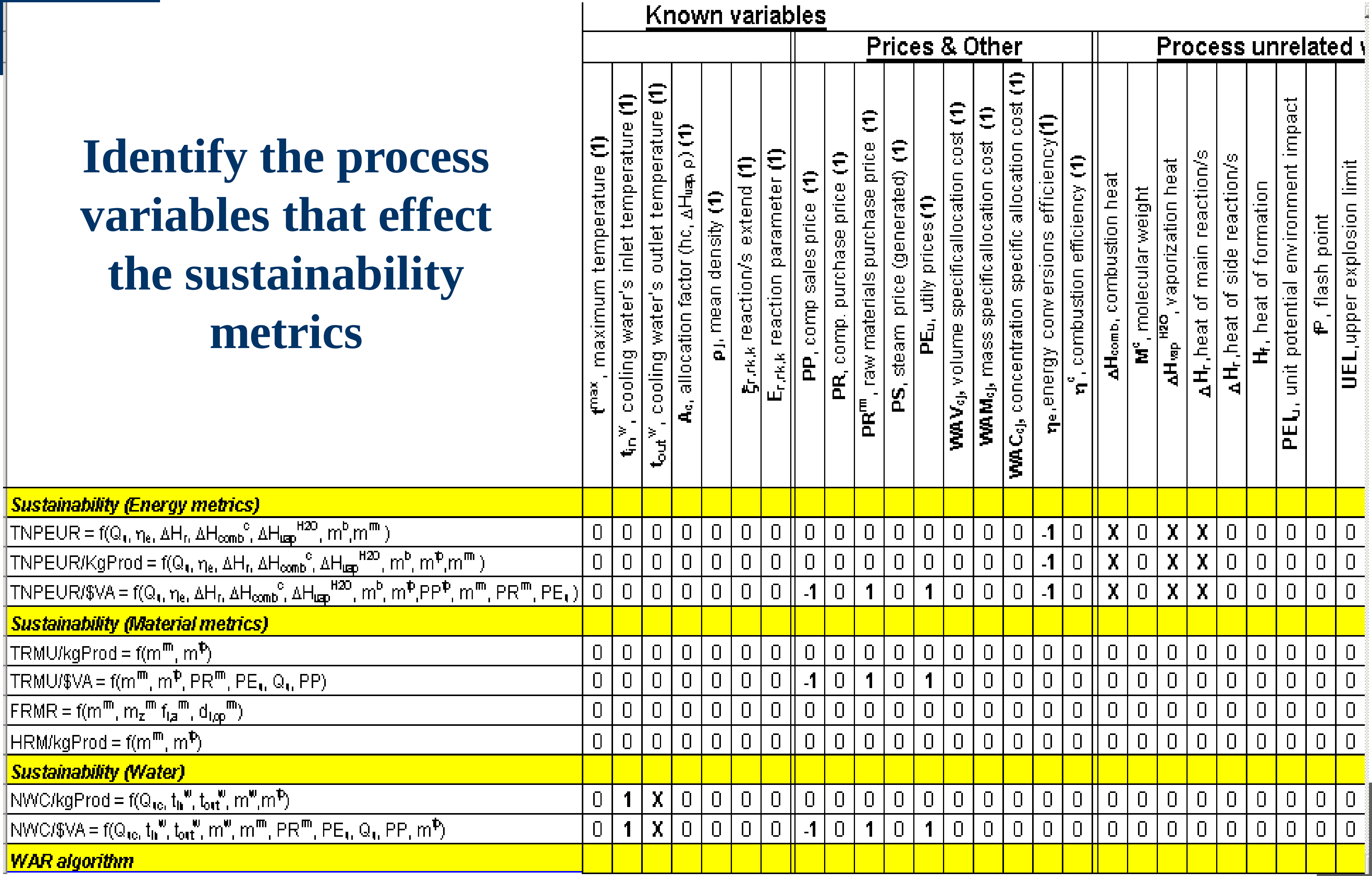
Identify the process (design) variables that effect the targetted mass & energy indicators



																										Known variab
	Process related variables																								
	m^b, mass flowrate burned (1)	V_j, effluent volumetric flowrate (1)	m^{fP}, final product's mass flowrate (1)	m_z^P, mass of component in recycle (1)	$f_{i,a}^P$ mass flowrate leaving recycle (1)	$d_{i,op}^P$ mass of component leaving recycle (1)	m_z^{rm}, mass of component in recycle (1)	$f_{i,a}^{rm}$ mass flowrate leaving recycle (1)	$d_{i,op}^{rm}$ mass of component leaving recycle (1)	m^w, water mass flowrate (1)	ebl_{ec}, energy based level (en. recycle) (1)	$f_{i,a}^h$ energy flowrate leaving recycle (1)	$d_{i,op}^h$ energy flowrate leaving recycle (1)	$EOP_{s,d}$ energy flowrates (1)	Q_{uc}, cooling duties (1)	Q_u, utility duties (incl. cooling) (1)	T_m, mean temperature (1)	p_m, mean pressure (1)	p^{max}, maximum pressure (1)	t^{max}, maximum temperature (1)	t_{in}^w, cooling water's inlet temperature (1)	t_{out}^w, cooling water's outlet temperature (1)	A_c, allocation factor (hc, ΔH_{vap}, ρ) (1)	ρ_j, mean density (1)	$\xi_{r,rk,k}$ reaction/s extend (1)	$E_{r,rk,k}$ reaction parameter (1)
Mass Indicators																										
MVA =f(m^{rm}, m^p, m^b, PP, PR^{rm}, M^c, η^c, ΔH_{comb}, ΔH_{vap}^{H2O}, PS)	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
EC = f(m^{rm}, m^p, A_c, PE_I, Q_I, T_m, p_m)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	1	0	0	0
WC = f(m^{rm}, m^p, ρ_j, V_j, WAV_q, WAM_q, WAC_q)	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
EWC = f(EC, WC)	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	1	1	0	0
TVA = f(MVA, EWC)	0	?	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	-1	0	0	0	0	-1	-1	0	0
RQ = f($\xi_{r,rk,k}$, $E_{r,rk,k}$, m^p, M^c)	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
AF = f(m_z^{rm}, $f_{i,a}^{rm}$, $d_{i,op}^{rm}$, m_z^p, $f_{i,a}^p$, $d_{i,op}^p$)	0	0	0	1	-1	-1	1	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Energy Indicators																										
REF = f(ebl_{ec}, $f_{i,a}^h$, $d_{i,op}^h$)	0	0	0	0	0	0	0	0	0	0	1	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
DC = f(PE_s, $EOP_{s,d}$)	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
TDC = f(DC)	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
Sustainability (Energy metrics)																										

Model Structural & Sensitivity Analysis - 2

Identify the process variables that effect the sustainability metrics



	Known variables																									
								Prices & Other										Process unrelated								
	t^{max}, maximum temperature (1)	t_{in}^{w}, cooling water's inlet temperature (1)	t_{out}^{w}, cooling water's outlet temperature (1)	A_c, allocation factor (hc, ΔH_{vap}, ρ) (1)	ρ_J, mean density (1)	$\xi_{r,rk,k}$ reaction/s extend (1)	$E_{r,rk,k}$ reaction parameter (1)	PP, comp sales price (1)	PR, comp. purchase price (1)	PR^{m}, raw materials purchase price (1)	PS, steam price (generated) (1)	PE_u, utily prices (1)	WAV_{cj}, volume specificallocation cost (1)	WAM_{cj}, mass specificallocation cost (1)	WAC_{cj}, concentration specific allocation cost (1)	η_e, energy conversions efficiency (1)	η^{c}, combustion efficiency (1)	ΔH_{comb}, combustion heat	M^{c}, molecular weight	ΔH_{vap}^{H2O}, vaporization heat	ΔH_r, heat of main reaction/s	ΔH_r, heat of side reaction/s	H_f, heat of formation	PEI_J, unit potential environment impact	F_P, flash point	UEL, upper explosion limit
Sustainability (Energy metrics)																										
TNPEUR = f(Q_I, η_e, ΔH_r, ΔH_{comb}^{c}, ΔH_{vap}^{H2O}, m^{b},m^{m})	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	X	0	X	X	0	0	0	0	0
TNPEUR/KgProd = f(Q_I, η_e, ΔH_r, ΔH_{comb}^{c}, ΔH_{vap}^{H2O}, m^{b}, m^{P},m^{m})	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	X	0	X	X	0	0	0	0	0
TNPEUR/$VA = f($Q_I$, η_e, ΔH_r, ΔH_{comb}^{c}, ΔH_{vap}^{H2O}, m^{b}, m^{P},PP^{P}, m^{m}, PR^{m}, PE_I)	0	0	0	0	0	0	0	-1	0	1	0	1	0	0	0	-1	0	X	0	X	X	0	0	0	0	0
Sustainability (Material metrics)																										
TRMU/kgProd = f(m^{m}, m^{P})	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRMU/$VA = f($m^{m}$, m^{P}, PR^{m}, PE_I, Q_I, PP)	0	0	0	0	0	0	0	-1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
FRMR = f(m^{m}, m_z^{m} $f_{I,a}^{m}$, $d_{I,op}^{m}$)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HRM/kgProd = f(m^{m}, m^{P})	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sustainability (Water)																										
NWC/kgProd = f(Q_{Ic}, t_{in}^{w}, t_{out}^{w}, m^{w},m^{P})	0	1	X	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NWC/$VA = f($Q_{Ic}$, t_{in}^{w}, t_{out}^{w}, m^{w}, m^{m}, PR^{m}, PE_I, Q_I, PP, m^{P})	0	1	X	0	0	0	0	-1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
WAR algorithm																										

Model Structural & Sensitivity Analysis - 3

Identify the process variables that effect the environmental impact factors

$$I = \Sigma_i \alpha_i \; \Sigma_j M_j \, \psi_{ij}$$

M_j = mass flow rate of chemical *j* (mass/time)

α_i = weighting factor for impact category *i*

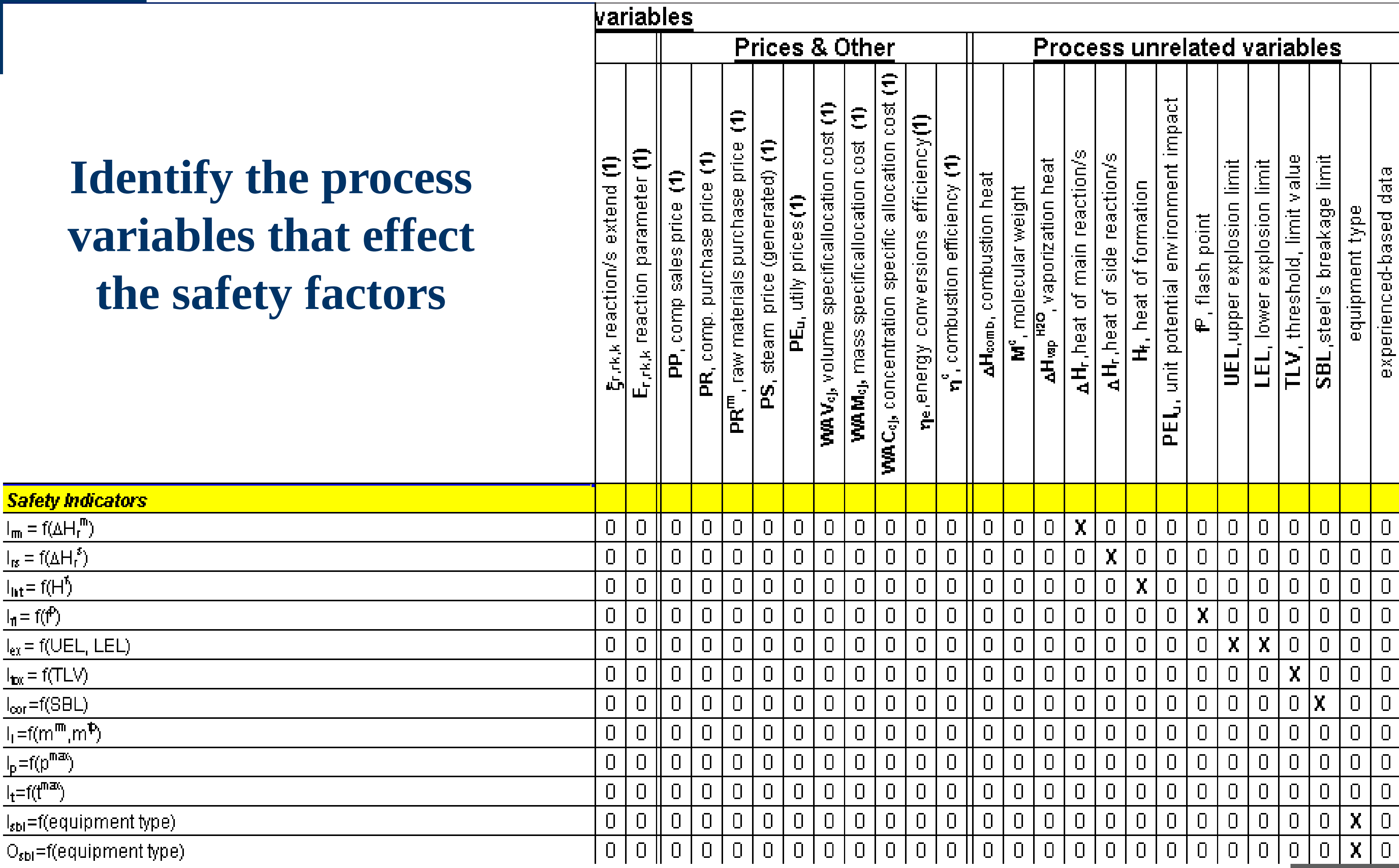
ψ_{ij} = chemical and category specific impact (PEI/mass)

Identify: Chemicals that cause the impact I to be high

Solution: Replace the chemical or reduce the flowrate

Model Structural & Sensitivity Analysis - 4

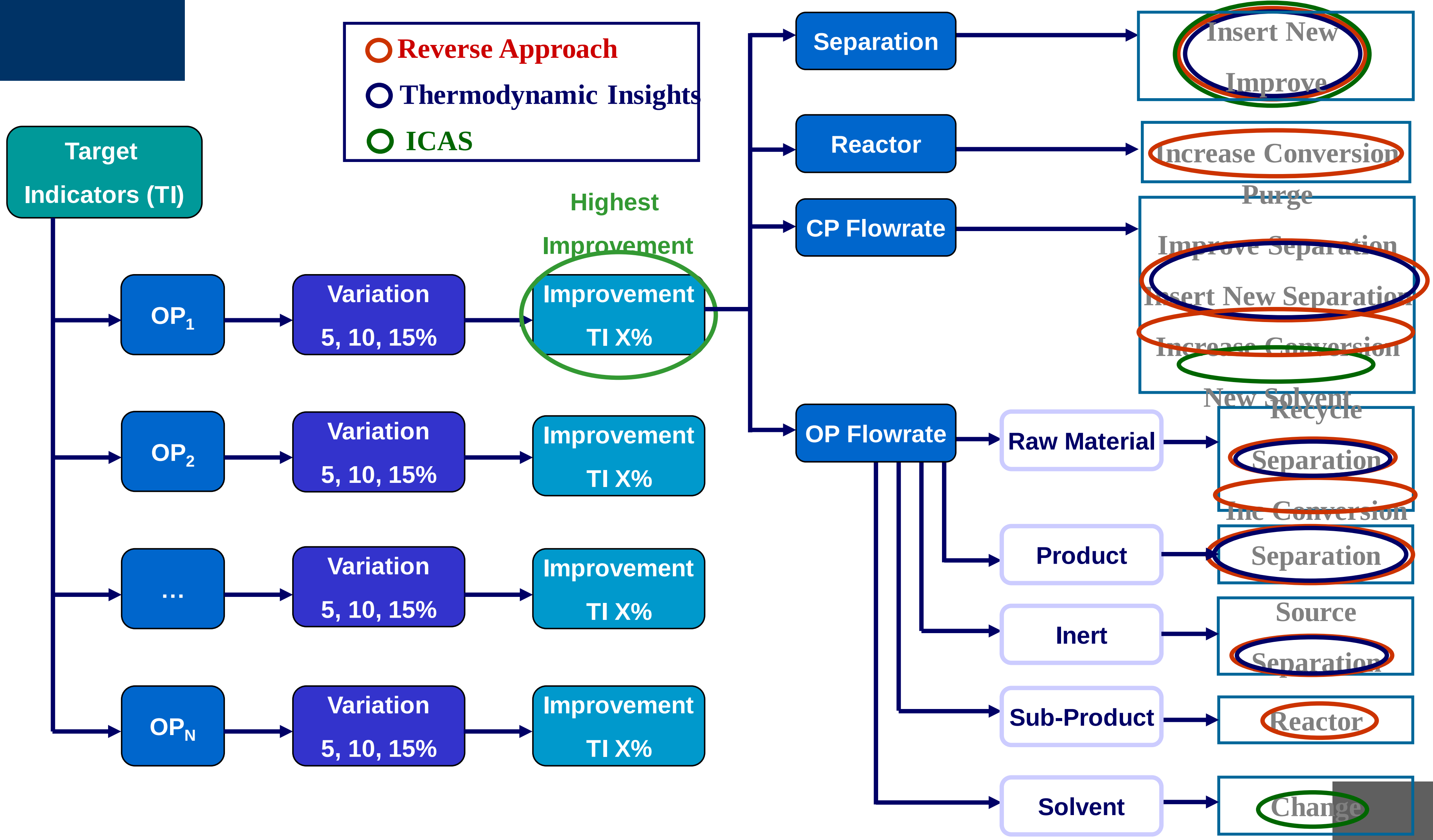
Identify the process variables that effect the safety factors



variables

			Prices & Other									Process unrelated variables													
	$\xi_{r,rk,k}$ reaction/s extend **(1)**	$E_{r,rk,k}$ reaction parameter **(1)**	**PP**, comp sales price **(1)**	**PR**, comp. purchase price **(1)**	**PR^{rm}**, raw materials purchase price **(1)**	**PS**, steam price (generated) **(1)**	**PE_u**, utily prices **(1)**	**WAV_{cj}**, volume specificallocation cost **(1)**	**WAM_{cj}**, mass specificallocation cost **(1)**	**WAC_{cj}**, concentration specific allocation cost **(1)**	η_e,energy conversions efficiency**(1)**	η^c, combustion efficiency **(1)**	**ΔH_{comb}**, combustion heat	**M^c**, molecular weight	**ΔH_{vap}^{H2O}**, vaporization heat	**ΔH_r**,heat of main reaction/s	**ΔH_r**,heat of side reaction/s	**H_f**, heat of formation	**PEL_i**, unit potential environment impact	**f^P**, flash point	**UEL**,upper explosion limit	**LEL**, lower explosion limit	**TLV**, threshold, limit value	**SBL**,steel's breakage limit	equipment type	experienced-based data
Safety Indicators																										
$I_m = f(\Delta H_r^m)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	X	0	0	0	0	0	0	0	0	0	0
$I_{rs} = f(\Delta H_r^s)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	X	0	0	0	0	0	0	0	0	0
$I_{int} = f(H^f)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	X	0	0	0	0	0	0	0	0
$I_{fl} = f(f^P)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	X	0	0	0	0	0	0
$I_{ex} = f(UEL, LEL)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	X	X	0	0	0	0
$I_{tox} = f(TLV)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	X	0	0	0
$I_{cor}=f(SBL)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	X	0	0
$I_l=f(m^{m},m^{fP})$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$I_p=f(p^{max})$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$I_t=f(t^{max})$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
I_{sbl}=f(equipment type)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	X	0
O_{sbl}=f(equipment type)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	X	0

Generate sustainable design alternatives



Reverse Approach
Thermodynamic Insights
ICAS

Target Indicators (TI)

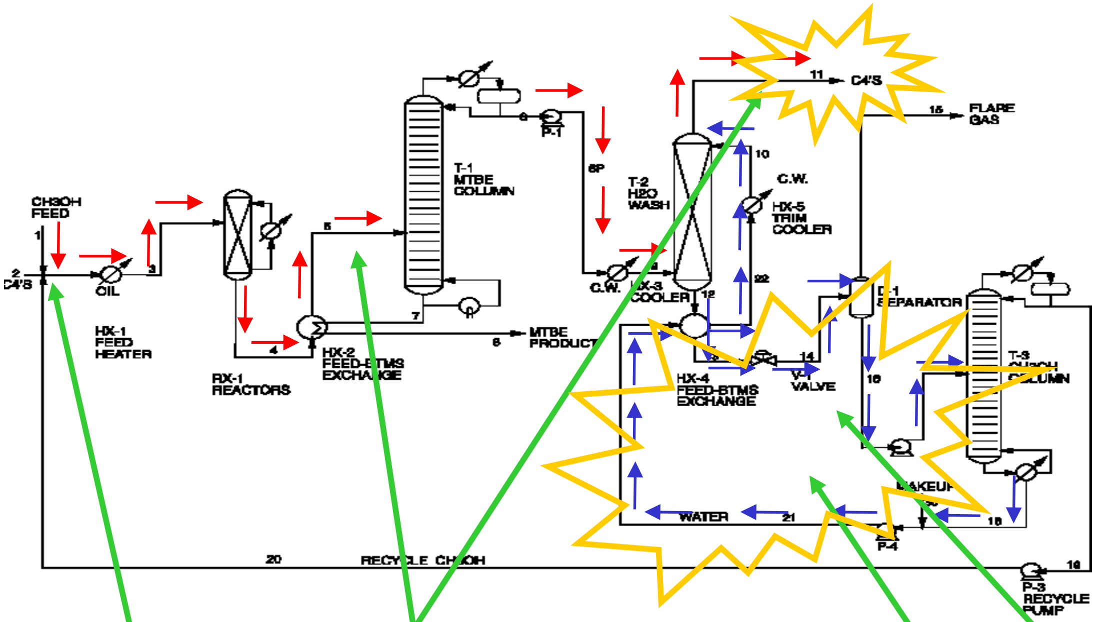
OP$_1$ → Variation 5, 10, 15% → Improvement TI X%
OP$_2$ → Variation 5, 10, 15% → Improvement TI X%
… → Variation 5, 10, 15% → Improvement TI X%
OP$_N$ → Variation 5, 10, 15% → Improvement TI X%

Highest Improvement

Separation → Insert New / Improve
Reactor → Increase Conversion
CP Flowrate → Purge / Improve Separation / Insert New Separation / Increase Conversion / New Solvent
OP Flowrate

Raw Material → Recycle / Separation / Inc Conversion
Product → Separation
Inert → Source / Separation
Sub-Product → Reactor
Solvent → Change

Application Example: MTBE Process

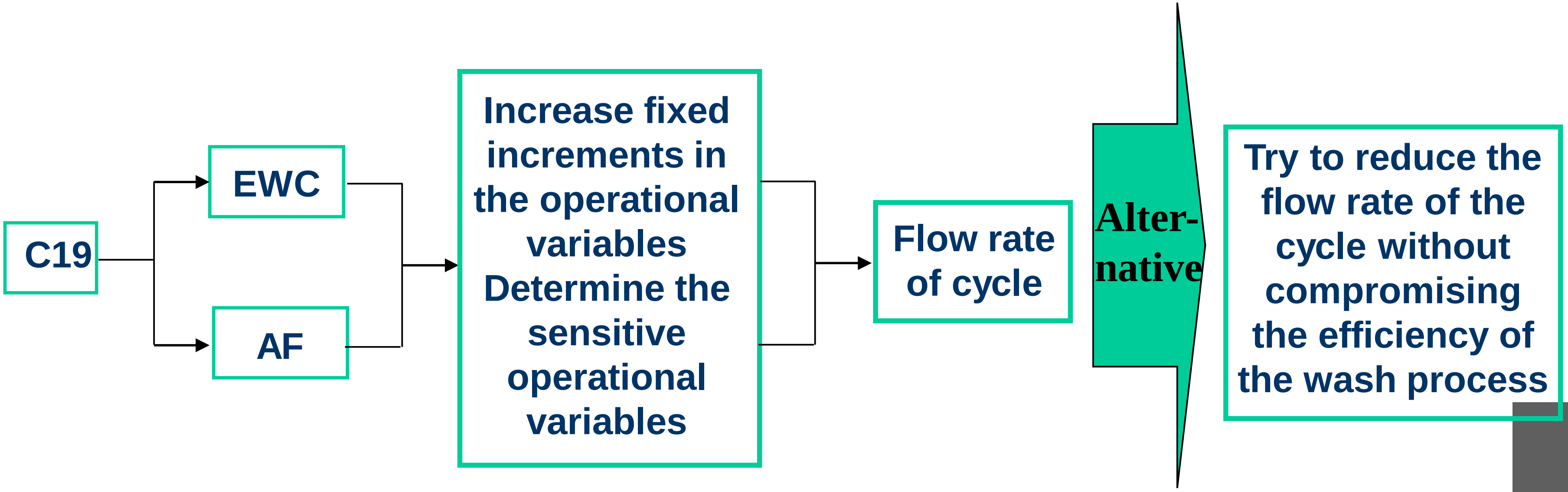


Open path	Component	MVA $(10^3\ \$/y)$	EWC $(10^3\ \$/y)$
O7	n-butane	-376.41	9.07
O9	Isobutane	-1714.78	260.70
O11	1 Butene	-282.62	43.41
O14	BTC2/BTT2	-403.74	63.91

Closed path	Component	AF	EWC $(10^3\ \$/y)$
C19	Water	626.51	313.35

Application Example: MTBE Process

- Energy, water, material, environmental impact and economic metrics
  Total metrics= 23
- Safety index = 30
- Through an algorithm determinations of the indicators which have more influence in the profit- Cycle path C19



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Generate (design) process alternatives

Results of the sensitivity analysis

A set of indicators; their target values; the process variables that can be changed to achieve the target; the sustainability metrics that would be affected; the environmental impact factors that would be affected; the safety factors that would be affected

Each set of changed process variables corresponds to a generated sustainable process alternative

SPEED

Compare measures of sustainability

Reduce 20% water in recycle

↔ Constant efficiency 99.9 % (methanol, water)

↑ 14.4 % and 20.0 % reduction of AF, and EWC

↓ Insignificant increase MVA values for paths O3, O4, O5, O9, O13 and O18

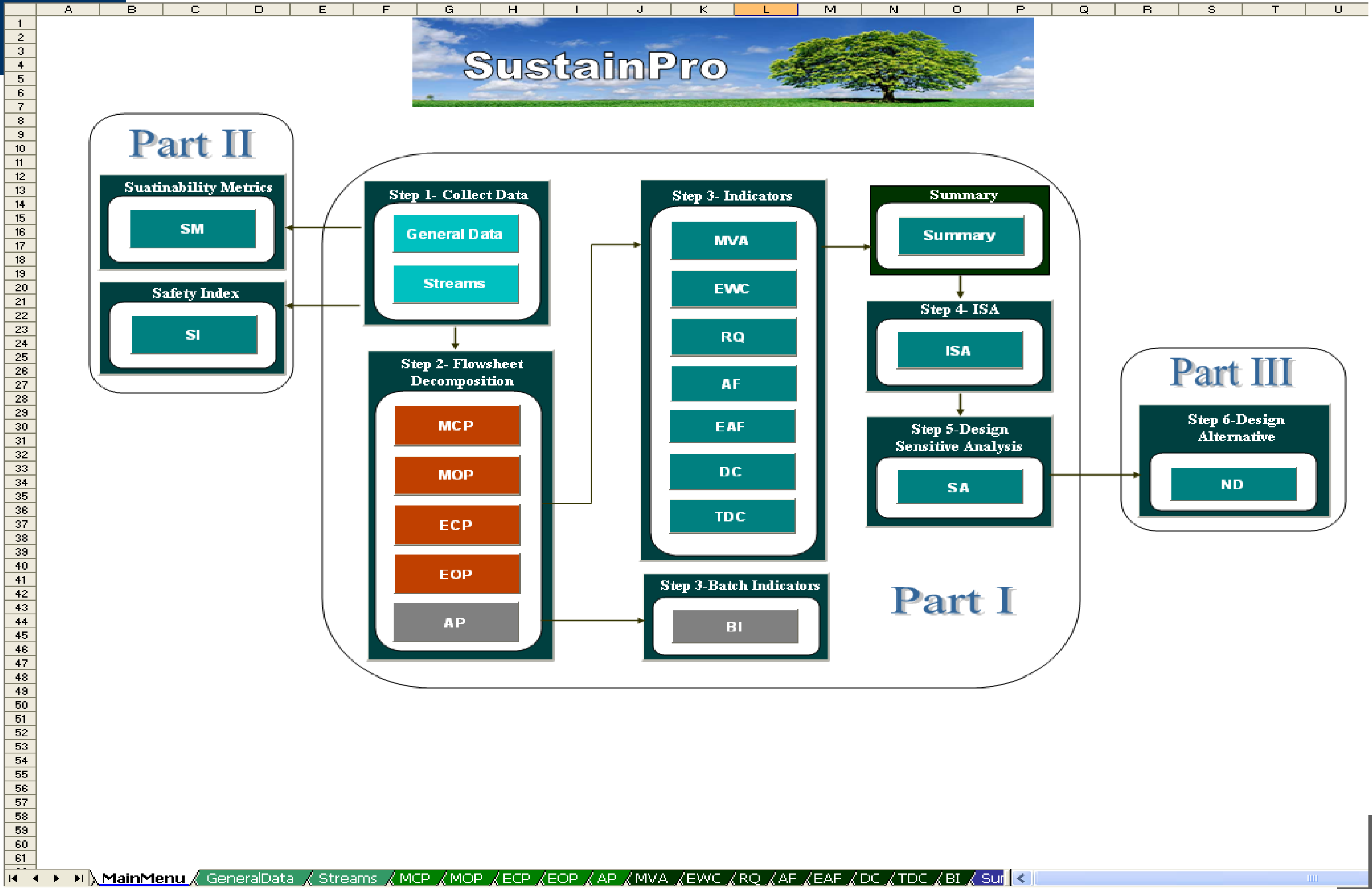
↔ Safety Index constant

↑ Energy and water sustainability metrics decrease 3% and 4 %

↔ Global impact almost constant

↑ **Gross margin increase 1.6%, but the increase in the profit will be greater due to the reduction in investment costs**

Software: SustainPro



Software issues: Supply of needed data (θ)

- Cost data (prices of materials, chemicals, ..)
- Equipment sizing & costing data
- Utility availability, cost, ...
- Property model parameters
- Kinetic model parameters
- Reconciliation of data (comes from different sources)

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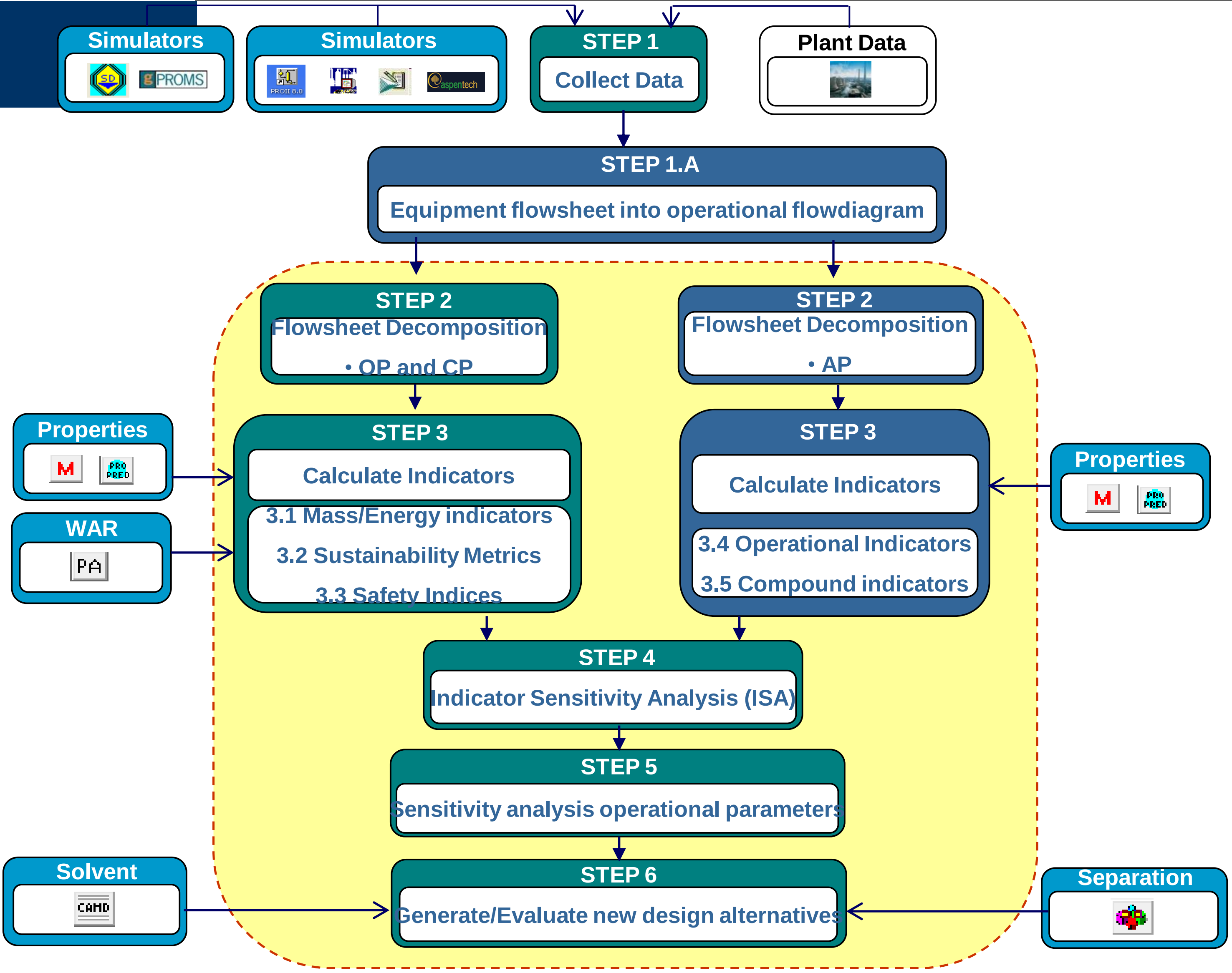
Software issues: Availability & accuracy of models

- Property prediction models
- Enviornmental impact calculations
- Reaction rates/conversion calculations
- Energy estimates
- Cost models
- Planning models
- Operation models
- ....

SPEED SustainPro Software



Simulators

Simulators

STEP 1
Collect Data

Plant Data

STEP 1.A
Equipment flowsheet into operational flowdiagram

STEP 2
Flowsheet Decomposition
- OP and CP

STEP 2
Flowsheet Decomposition
- AP

Properties

WAR

STEP 3
Calculate Indicators
3.1 Mass/Energy indicators
3.2 Sustainability Metrics
3.3 Safety Indices

STEP 3
Calculate Indicators
3.4 Operational Indicators
3.5 Compound indicators

Properties

STEP 4
Indicator Sensitivity Analysis (ISA)

STEP 5
Sensitivity analysis operational parameters

STEP 6
Generate/Evaluate new design alternatives

Solvent

Separation

Labels

- ▬ Continuous & Batch
- ▬ Batch
- ▬ Tools
- – – SustainPro
- Super Pro Designer
- Gproms
- Aspen Tech
- Pro II
- ICAS 11
- HYSYS
- CAPEC Database
- ICAS - ProPred
- ICAS – WAR algorithm
- ICAS - ProCamd
- Thermodynamic insights

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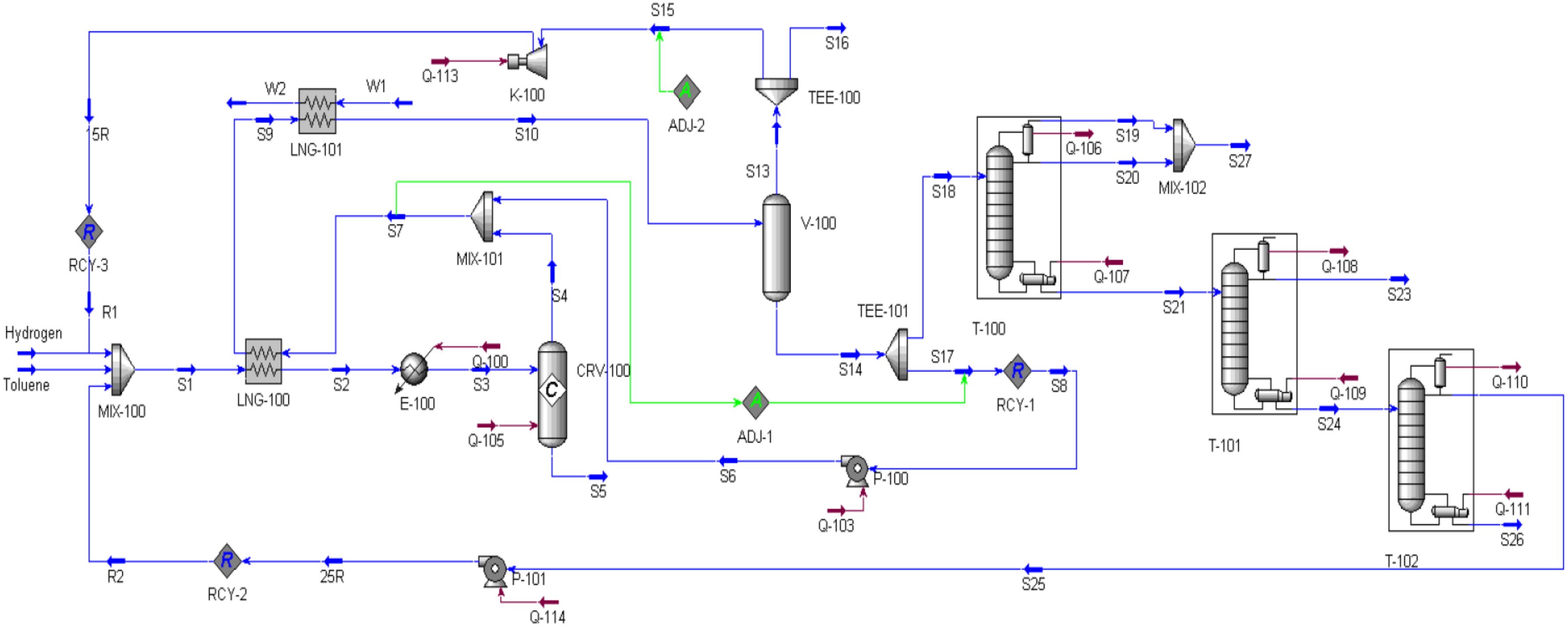
Case Study: HDA Process (step 1)

Hydrogen reacts with Toluene to produce Benzene. Methane is present as impurity and Biphenyl is produced as a by-product



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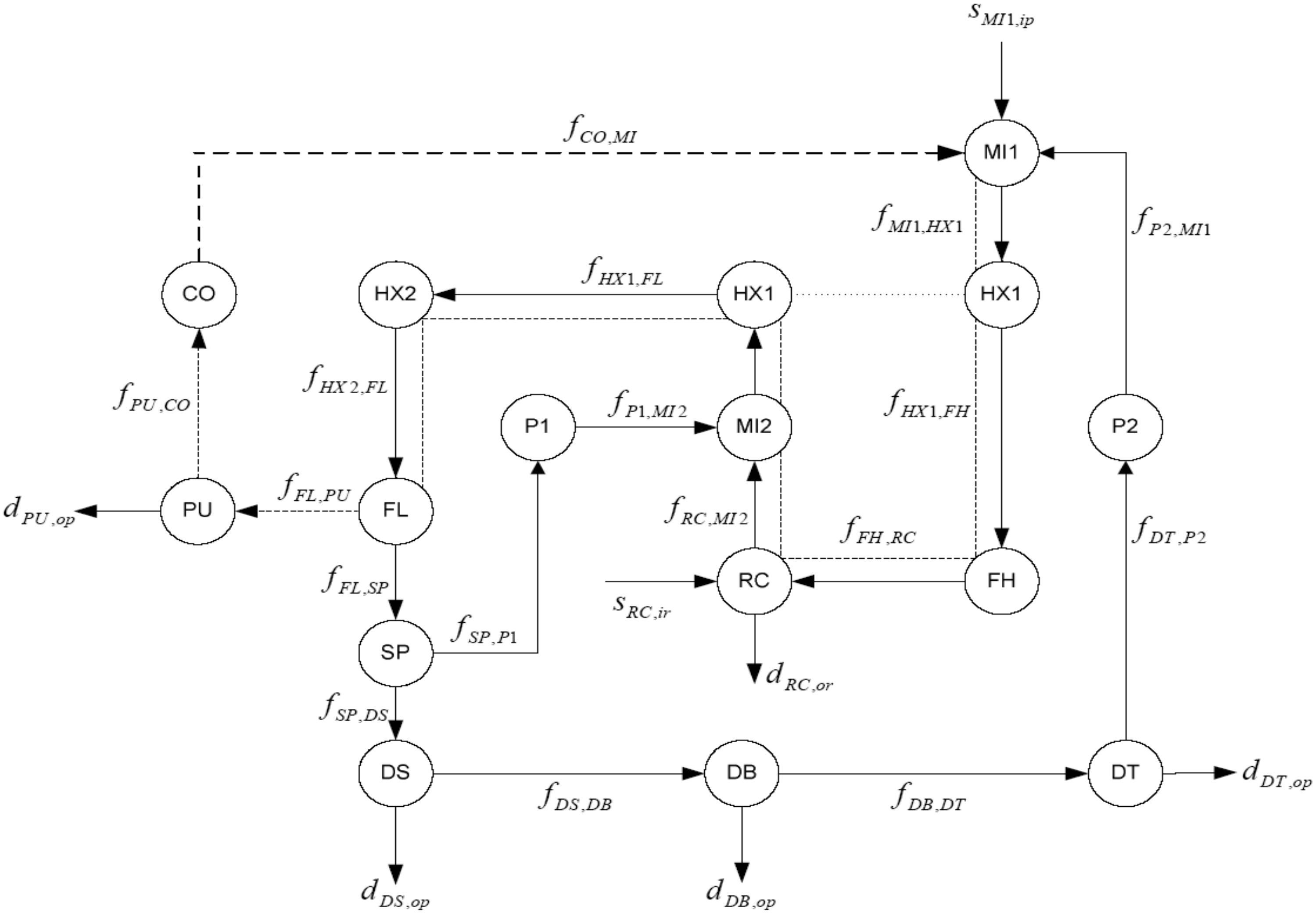
HDA process: Step 2

Process flowsheet: Open & closed paths



HDA process: Step 3

Mass Indicators

Indicators for open paths

Open path #	Component	Path	Flowrate (kg	RQ	MVA (10^3 $	EWC (10^3 $	TVA (10^3 $/yr)
O1	Methane	sMI1,ip-dPU,op	195.72	0.000	321.30	7.19	314.10
O2	Hydrogen	sMI1,ip-dPU,op	244.30	1.037	-2947.75	33.99	-2981.74
O3	Benzene	sRC,ir-dPU,op	134.57	0.000	-78.43	0.30	-78.72
O4	Biphenyl	sRC,ir-dPU,op	0.00	0.000	0.00	0.00	0.00
O5	Toluene	sMI1,ip-dPU,op	18.33	1.037	-18.50	0.43	-18.93
O6	Methane	sRC,ir-dPU,op	1887.71	0.000	-8747.91	7.78	-8755.70
O7	Methane	sMI1,ip-dDS,op	10.78	0.000	17.70	0.40	17.30
O8	Hydrogen	sMI1,ip-dDS,op	1.35	1.060	-16.31	0.19	-16.49
O9	Benzene	sRC,ir-dDS,op	3.80	0.000	-2.22	0.44	-2.66
O10	Biphenyl	sRC,ir-dDS,op	0.00	0.000	0.00	0.00	0.00
O11	Toluene	sMI1,ip-dDS,op	0.00	1.011	0.00	0.00	0.00
O12	Methane	sRC,ir-dDS,op	103.99	0.000	-481.88	0.43	-482.31
O13	Benzene	sRC,ir-dDB,op	9348.60	0.000	14629.37	626.29	14003.08
O14	Biphenyl	sRC,ir-dDB,op	0.00	0.000	0.00	0.00	0.00
O15	Toluene	sMI1,ip-dDB,op	2.68	1.037	-6.42	0.20	-6.62
O16	Benzene	sRC,ir-dDT,op	0.00	0.000	0.00	0.00	0.00
O17	Biphenyl	sRC,ir-dDT,op	207.23	0.000	-13.41	266.80	-280.21
O18	Toluene	sRC,ir-dDT,op	0.38	1.037	-0.38	0.58	-0.96
O19	Hydrogen	sMI1,ip-dRC,or	247.66	1.037	not defined	28.83	-28.83
O20	Toluene	sMI1,ip-dRC,or	11442.91	1.037	not defined	243.07	-243.07

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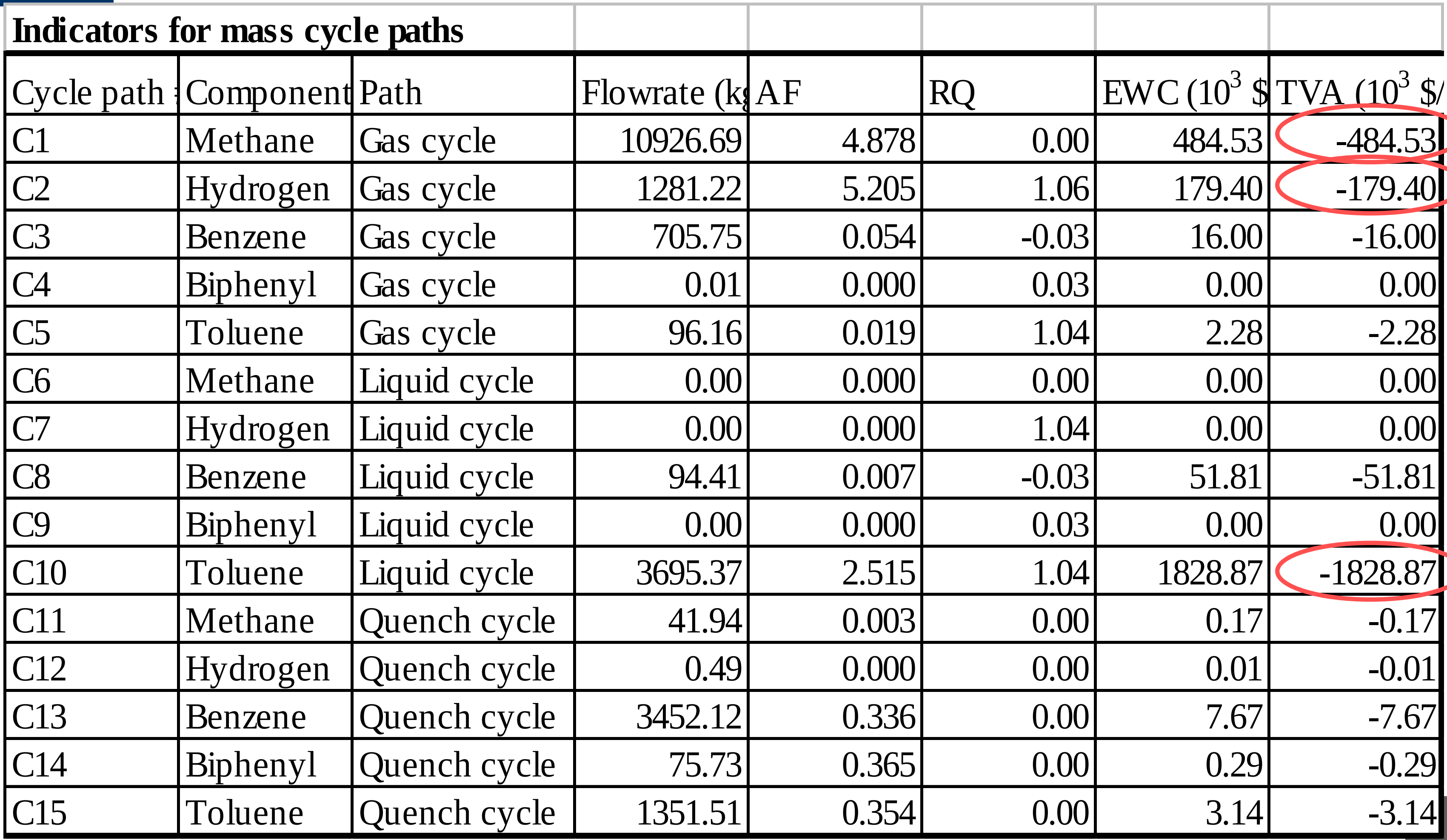
HDA process: Step 3

Mass Indicators



Indicators for mass cycle paths

Cycle path :	Component	Path	Flowrate (kg	AF	RQ	EWC (10^3 $	TVA (10^3 $/
C1	Methane	Gas cycle	10926.69	4.878	0.00	484.53	-484.53
C2	Hydrogen	Gas cycle	1281.22	5.205	1.06	179.40	-179.40
C3	Benzene	Gas cycle	705.75	0.054	-0.03	16.00	-16.00
C4	Biphenyl	Gas cycle	0.01	0.000	0.03	0.00	0.00
C5	Toluene	Gas cycle	96.16	0.019	1.04	2.28	-2.28
C6	Methane	Liquid cycle	0.00	0.000	0.00	0.00	0.00
C7	Hydrogen	Liquid cycle	0.00	0.000	1.04	0.00	0.00
C8	Benzene	Liquid cycle	94.41	0.007	-0.03	51.81	-51.81
C9	Biphenyl	Liquid cycle	0.00	0.000	0.03	0.00	0.00
C10	Toluene	Liquid cycle	3695.37	2.515	1.04	1828.87	-1828.87
C11	Methane	Quench cycle	41.94	0.003	0.00	0.17	-0.17
C12	Hydrogen	Quench cycle	0.49	0.000	0.00	0.01	-0.01
C13	Benzene	Quench cycle	3452.12	0.336	0.00	7.67	-7.67
C14	Biphenyl	Quench cycle	75.73	0.365	0.00	0.29	-0.29
C15	Toluene	Quench cycle	1351.51	0.354	0.00	3.14	-3.14

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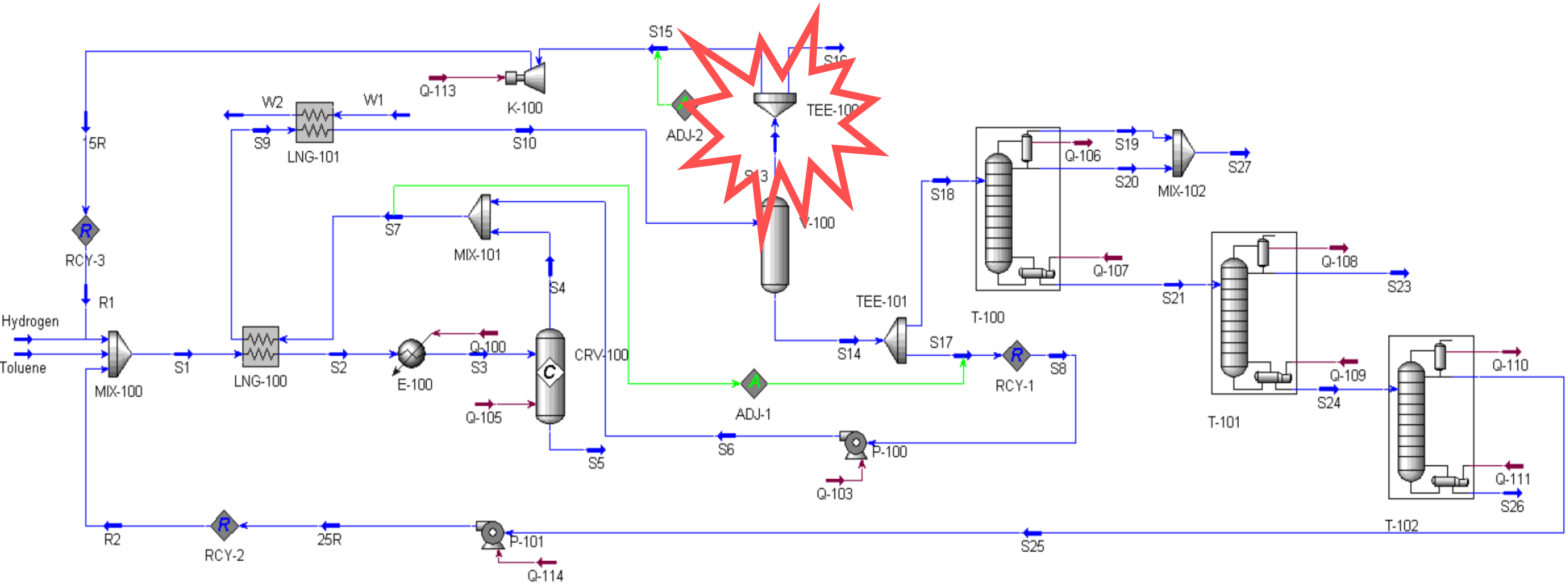
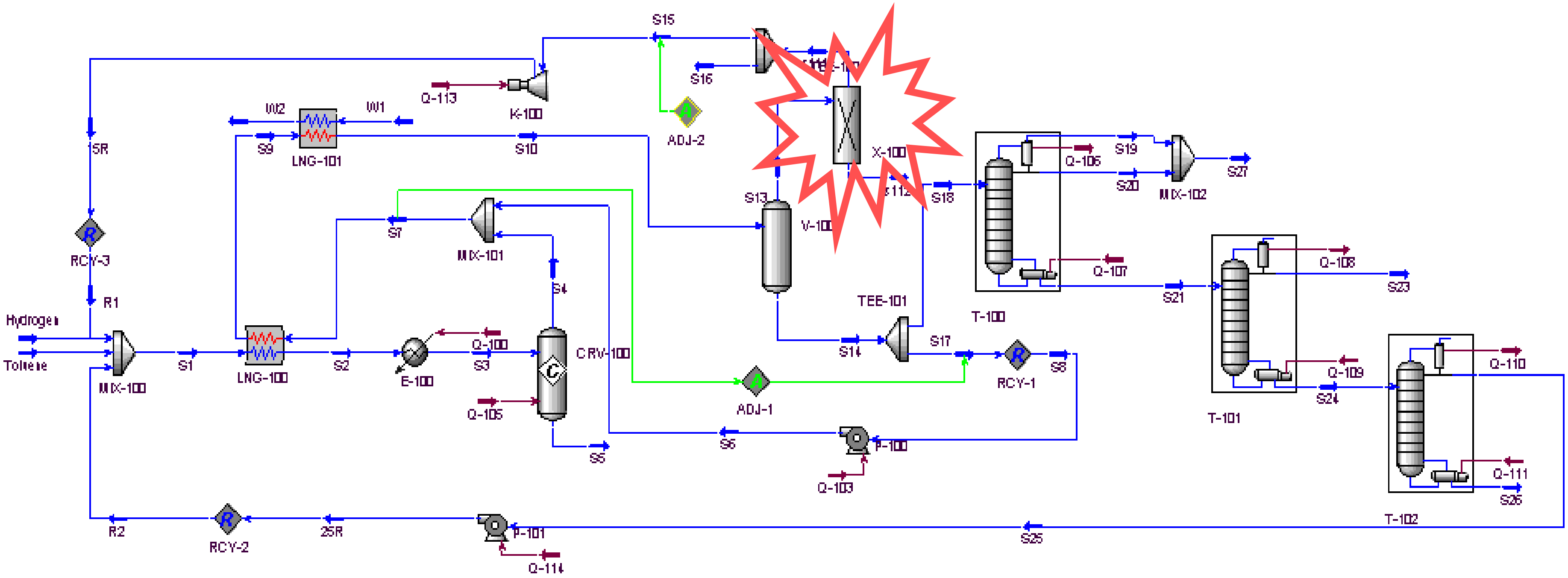
HDA process: Steps 4-5

Locate the process variable that can satisfy the target indicators

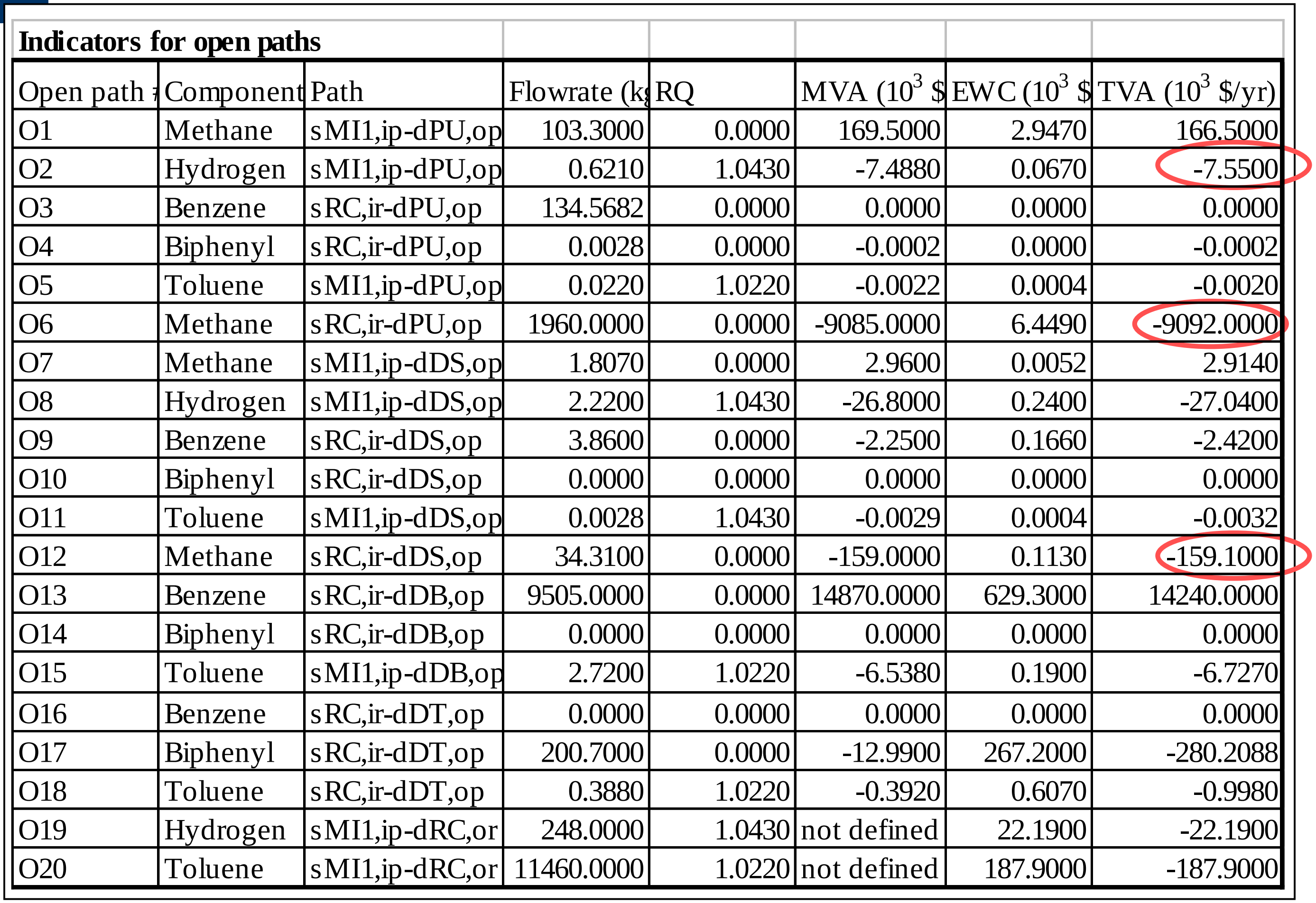


HDA process: Step 6

Generated sustainable design alternative



HDA process: Evaluate new alternative



Indicators for open paths

Open path	Component	Path	Flowrate (k	RQ	MVA (10^3 $	EWC (10^3 $	TVA (10^3 $/yr)
O1	Methane	sMI1,ip-dPU,op	103.3000	0.0000	169.5000	2.9470	166.5000
O2	Hydrogen	sMI1,ip-dPU,op	0.6210	1.0430	-7.4880	0.0670	-7.5500
O3	Benzene	sRC,ir-dPU,op	134.5682	0.0000	0.0000	0.0000	0.0000
O4	Biphenyl	sRC,ir-dPU,op	0.0028	0.0000	-0.0002	0.0000	-0.0002
O5	Toluene	sMI1,ip-dPU,op	0.0220	1.0220	-0.0022	0.0004	-0.0020
O6	Methane	sRC,ir-dPU,op	1960.0000	0.0000	-9085.0000	6.4490	-9092.0000
O7	Methane	sMI1,ip-dDS,op	1.8070	0.0000	2.9600	0.0052	2.9140
O8	Hydrogen	sMI1,ip-dDS,op	2.2200	1.0430	-26.8000	0.2400	-27.0400
O9	Benzene	sRC,ir-dDS,op	3.8600	0.0000	-2.2500	0.1660	-2.4200
O10	Biphenyl	sRC,ir-dDS,op	0.0000	0.0000	0.0000	0.0000	0.0000
O11	Toluene	sMI1,ip-dDS,op	0.0028	1.0430	-0.0029	0.0004	-0.0032
O12	Methane	sRC,ir-dDS,op	34.3100	0.0000	-159.0000	0.1130	-159.1000
O13	Benzene	sRC,ir-dDB,op	9505.0000	0.0000	14870.0000	629.3000	14240.0000
O14	Biphenyl	sRC,ir-dDB,op	0.0000	0.0000	0.0000	0.0000	0.0000
O15	Toluene	sMI1,ip-dDB,op	2.7200	1.0220	-6.5380	0.1900	-6.7270
O16	Benzene	sRC,ir-dDT,op	0.0000	0.0000	0.0000	0.0000	0.0000
O17	Biphenyl	sRC,ir-dDT,op	200.7000	0.0000	-12.9900	267.2000	-280.2088
O18	Toluene	sRC,ir-dDT,op	0.3880	1.0220	-0.3920	0.6070	-0.9980
O19	Hydrogen	sMI1,ip-dRC,or	248.0000	1.0430	not defined	22.1900	-22.1900
O20	Toluene	sMI1,ip-dRC,or	11460.0000	1.0220	not defined	187.9000	-187.9000

Mass indicators value for the open paths in the alternative design

HDA process: Evaluate new alternative

Indicators for mass cycle paths

Cycle path	Component	Path	Flowrate (k	AF	RQ	EWC (10^3 $	TVA (10^3 $/
C1	Methane	Gas cycle	0.0000	0.0000	0.0000	0.0000	0.0000
C2	Hydrogen	Gas cycle	1338.0000	154.7000	1.0430	183.5000	-183.5000
C3	Benzene	Gas cycle	358.9000	0.0149	-0.0214	11.0300	-11.0300
C4	Biphenyl	Gas cycle	0.0000	0.0000	0.0000	0.0000	0.0000
C5	Toluene	Gas cycle	47.6200	0.0048	1.0220	1.1290	-1.1290
C6	Methane	Liquid cycle	0.0000	0.0000	0.0000	0.0000	0.0000
C7	Hydrogen	Liquid cycle	0.0000	0.0000	0.0000	0.0000	0.0000
C8	Benzene	Liquid cycle	95.9900	0.0097	-0.0214	52.1900	-52.1900
C9	Biphenyl	Liquid cycle	0.0000	0.0000	0.0000	0.0000	0.0000
C10	Toluene	Liquid cycle	3768.0000	74.2400	1.0220	1845.0000	-1845.0000
C11	Methane	Quench cycle	7.3390	0.0035	0.0000	0.0241	-0.0241
C12	Hydrogen	Quench cycle	0.4510	0.0003	0.0000	0.0083	-0.0083
C13	Benzene	Quench cycle	1950.0000	0.1960	0.0000	3.3100	-3.3100
C14	Biphenyl	Quench cycle	40.7400	0.2030	0.0000	0.1200	-0.1200
C15	Toluene	Quench cycle	765.6000	0.2010	0.0000	1.3690	-1.3690

Mass indicators value for cycle paths in the alternative design

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HDA Process: Comparison of alternative

- A simple economical study including all the associate cost with the HDA process was performed
- The values shows the improvement obtained by mass indicators analysis

The base design:

•Benefit = -1579 (k$/year)

The alternative design:

•Benefit = 2309 (k$/year)

HDA Process: Measures of sustainability

Sustainability Metrics

Total Net Primary Energy Usage Rate = Imports – Exports-$75.09e^{+4}$GJ/y

Total Net Primary Energy Usage Rate per kg Product -$78.58e^{+6}$kJ/kg

Total raw materials used per kg product 1.27 kg/kg

Hazardous raw material per kg product 1.22 kg/kg

Net water consumed per unit mass of product 184.62 kg/kg

Base Case

Total Net Primary Energy Usage Rate = Imports – Exports-$53.61e^{+4}$GJ/y

Total Net Primary Energy Usage Rate per kg Product -$55.24e^{+6}$kJ/kg

Total raw materials used per kg product 1.22 kg/kg

Hazardous raw material per kg product 1.19 kg/kg

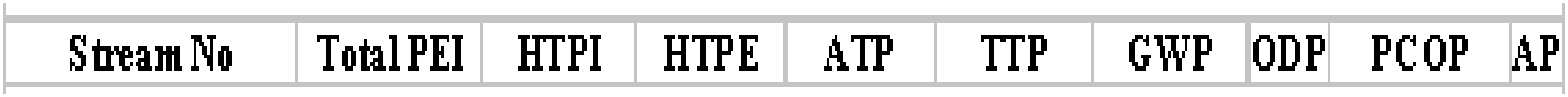
Net water consumed per unit mass of product 171.35 kg/kg

Generated Alternative

SPEED

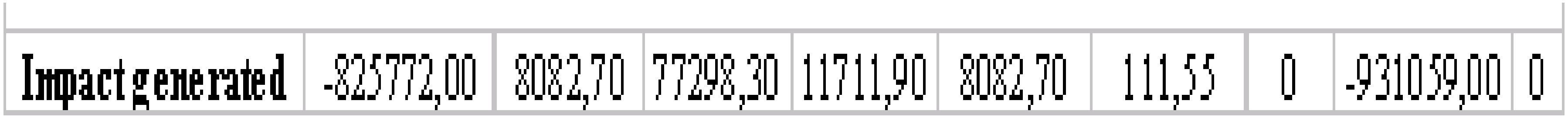
HDA Process: measures of sustainability

Environmental Impact



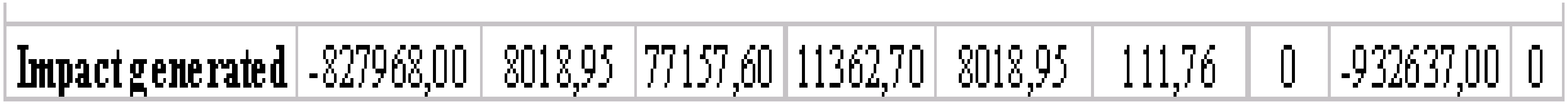
Stream No	Total PEI	HTPI	HTPE	ATP	TTP	GWP	ODP	PCOP	AP

Base Case



Impact generated	-825772,00	8082,70	77298,30	11711,90	8082,70	111,55	0	-931059,00	0

Generated Alternative

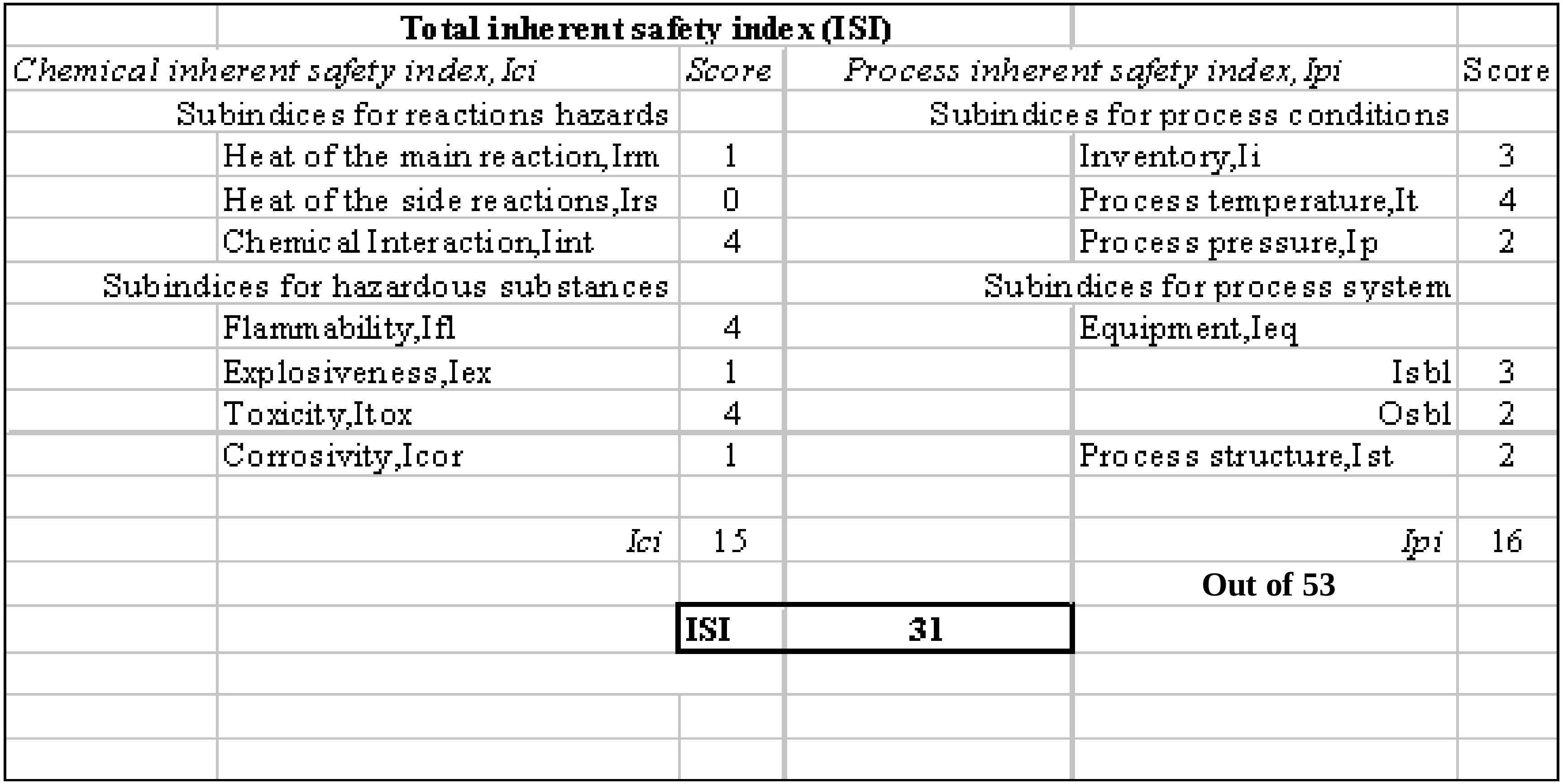


Impact generated	-827968,00	8018,95	77157,60	11362,70	8018,95	111,76	0	-932637,00	0

HDA Process: Measures of safety

Safety Factors

Base Case & Generated Alternative



	Total inherent safety index (ISI)				
Chemical inherent safety index, Ici		*Score*	*Process inherent safety index, Ipi*		Score
Subindices for reactions hazards			Subindices for process conditions		
	Heat of the main reaction, Irm	1		Inventory, Ii	3
	Heat of the side reactions, Irs	0		Process temperature, It	4
	Chemical Interaction, Iint	4		Process pressure, Ip	2
Subindices for hazardous substances			Subindices for process system		
	Flammability, Ifl	4		Equipment, Ieq	
	Explosiveness, Iex	1		Isbl	3
	Toxicity, Itox	4		Osbl	2
	Corrosivity, Icor	1		Process structure, Ist	2
	Ici	15		*Ipi*	16
				Out of 53	
		ISI	**31**		

Dow CEI = 801.6 mg/m^3; $HD_1 > 10000$ m, $HD_2 = 8016.4$ m

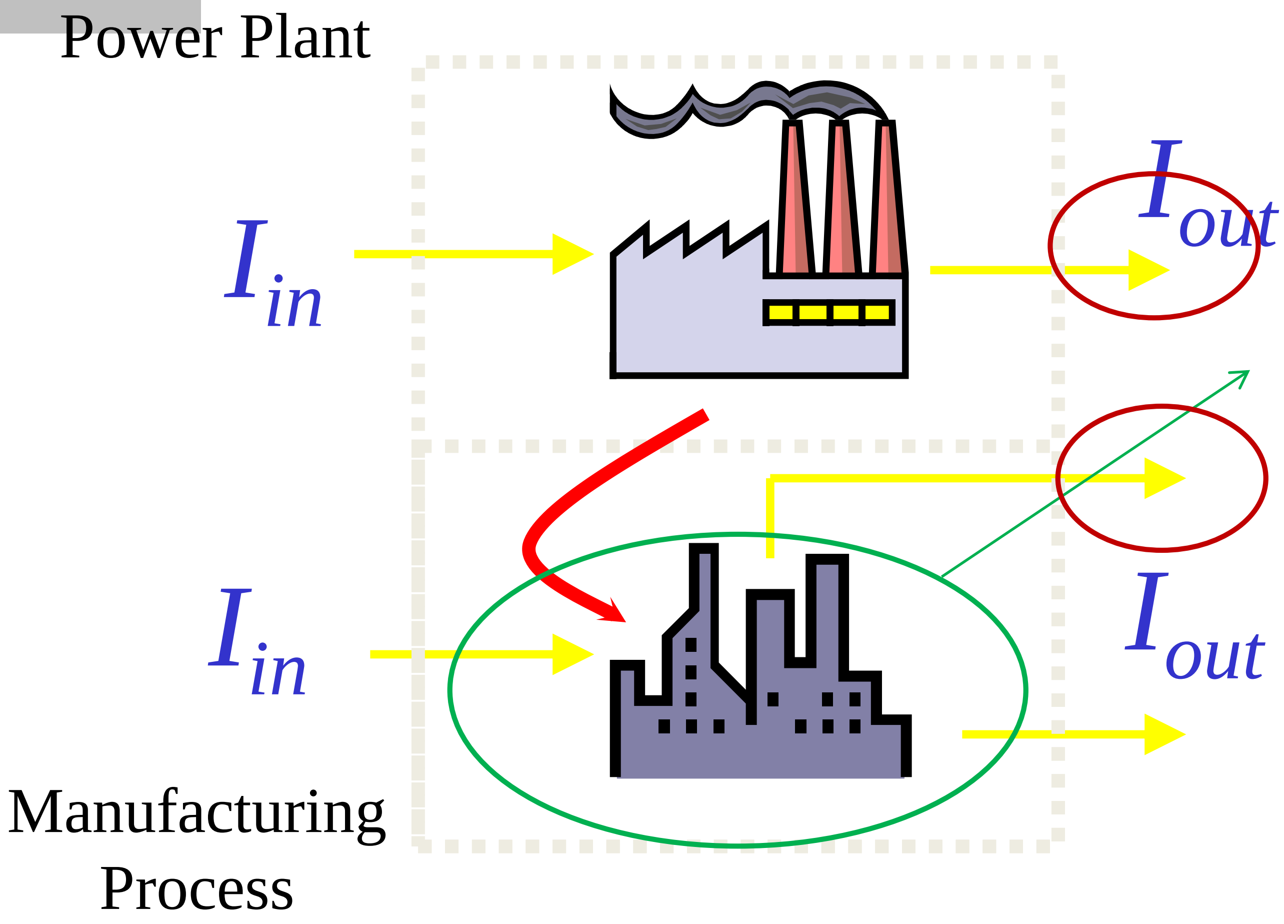
Summary: Indicator-based methodology

- A systematic model-based method to generate alternatives that improves the ability of the process to be flexible and adapt to future demands has been presented and its application illustrated through examples.
- The indicators point to process/operation alternatives that affects the sustainability metrics parameters in the desired direction, avoiding, thereby, tradeoffs in design (decisions).
- The models and methodology are generic and can easily be applied in other targeted design problems.
- Industrial process flowsheets are being labelled in terms of their potential for improvement.

Sustainable hybrid separation schemes

CO2 footprint - energy usage – waste – profit?

SPEED



Reduction in process utility demand

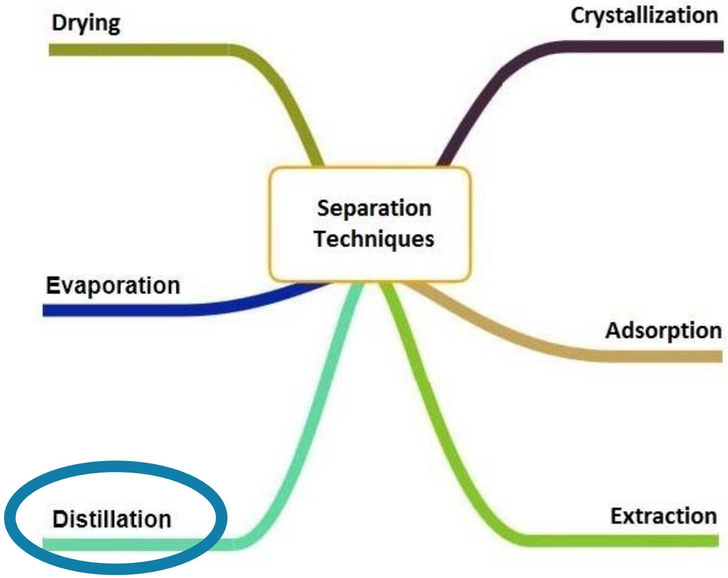
= less energy consumption, less waste and less CO2-footprint

= more profit

Direct & indirect CO2 emission

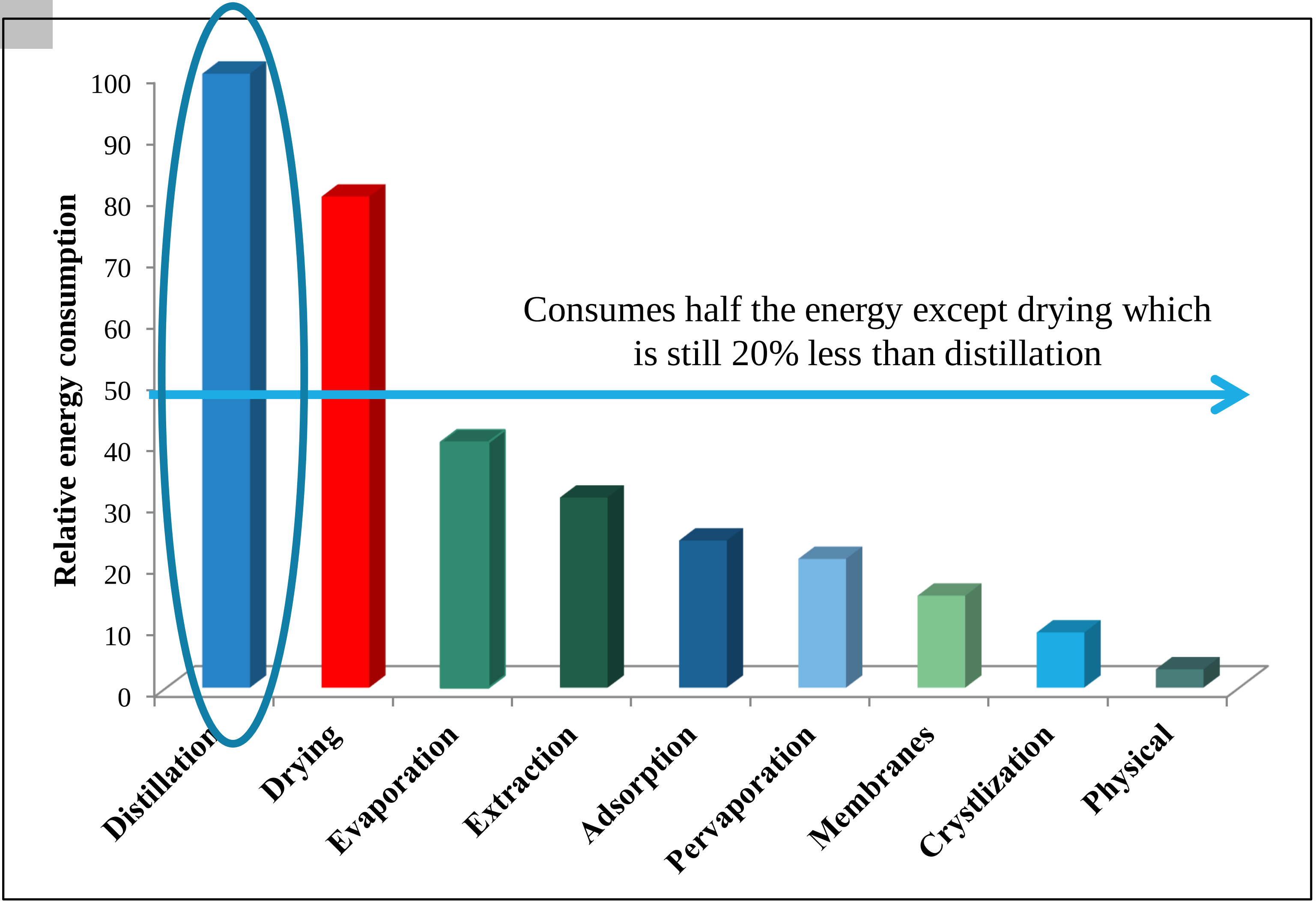
Energy intensive operations in chemical processes

- Separation Processes are indispensable in chemical industry
- Distillation is one of most used separation techniques among all
- 80 % of all the Vapor-Liquid separations are performed by distillation
- Distillation is among highly energy intensive techniques with lower thermal efficiency
- More than 40,000 distillation units alone in US (2005) using nearly 75 million KW of energy



$$Thermal\ efficiency = \frac{Net\ work\ done}{Heat\ supplied}$$

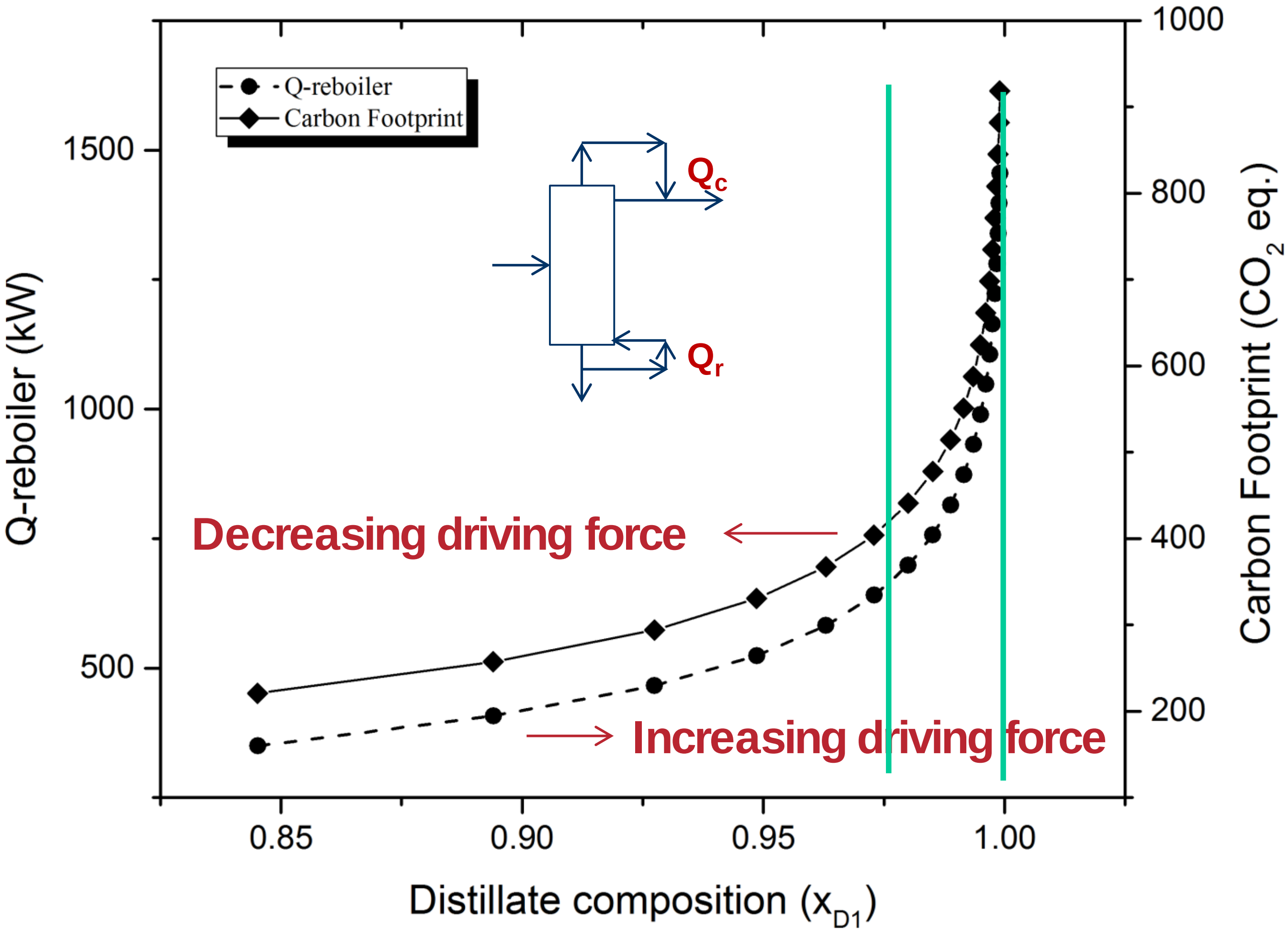
Energy intensive operations in chemical processes



Consumes half the energy except drying which is still 20% less than distillation

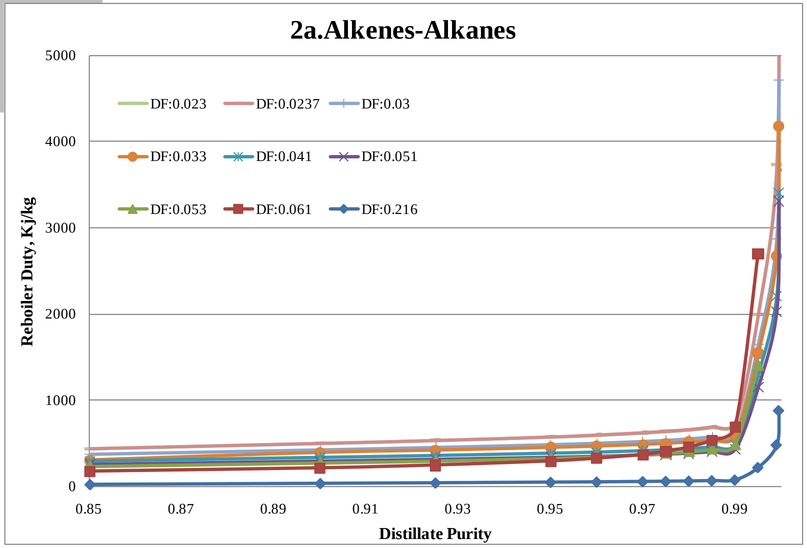
Analysis of design: distillation column

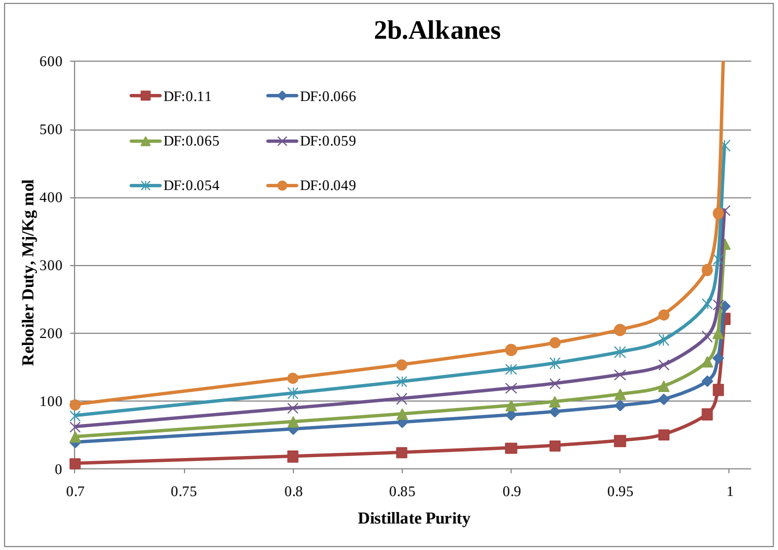
Design specification versus energy cost

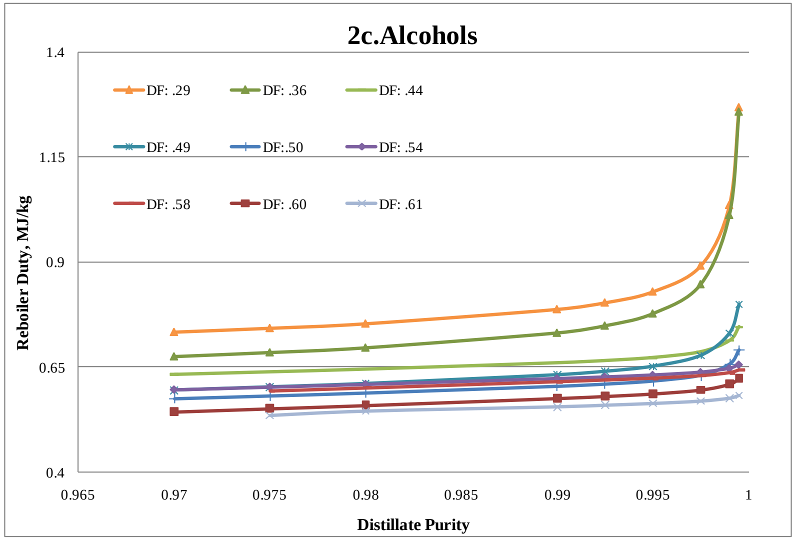


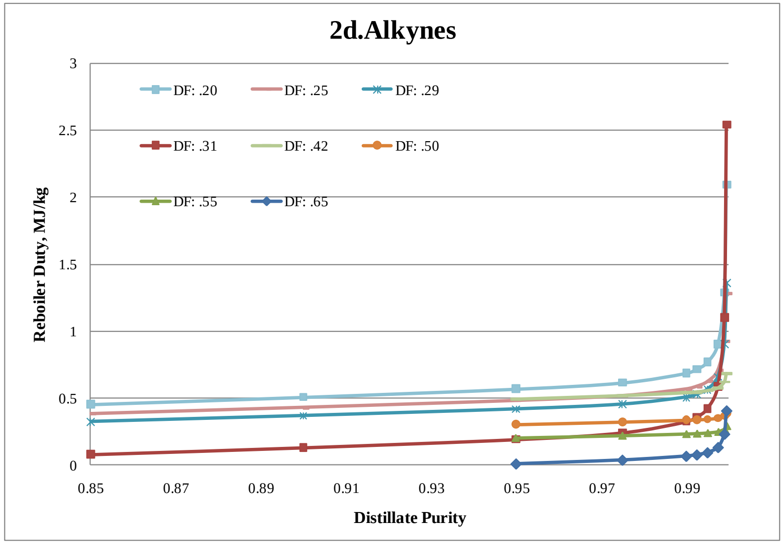
SPEED

Analysis of numerous distillation columns



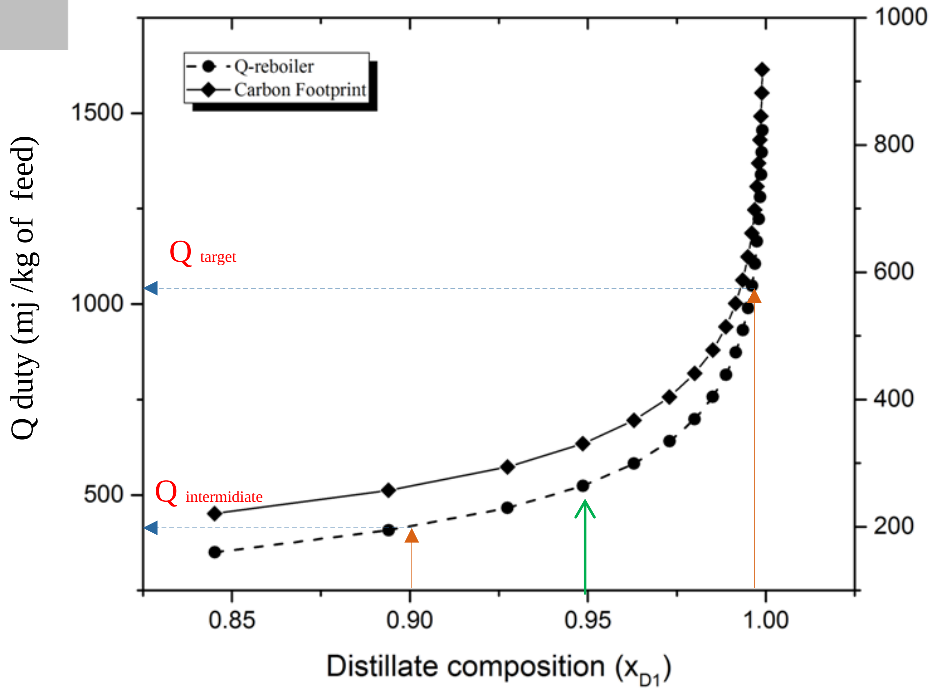


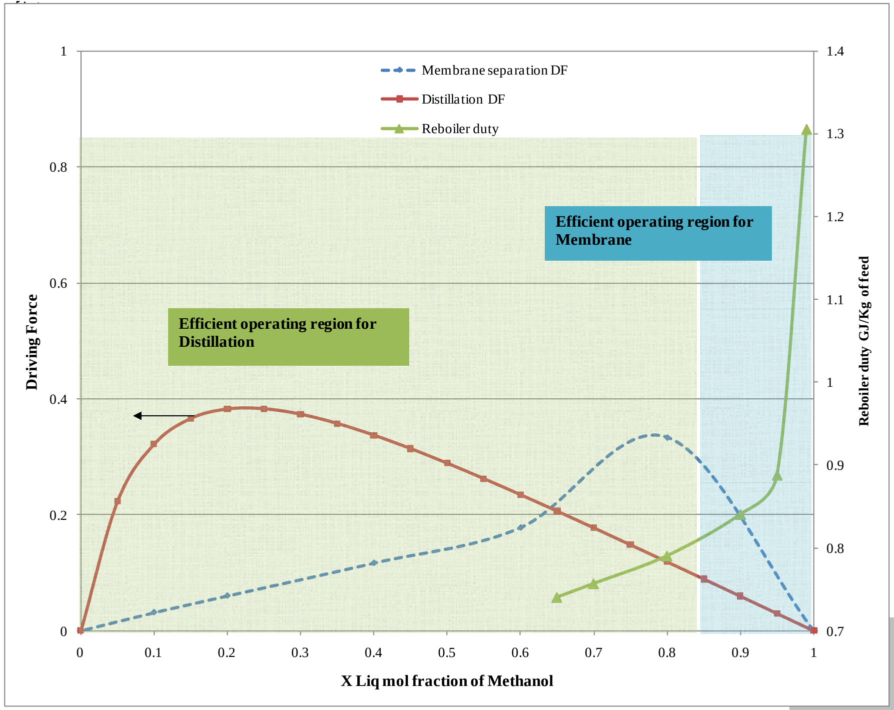




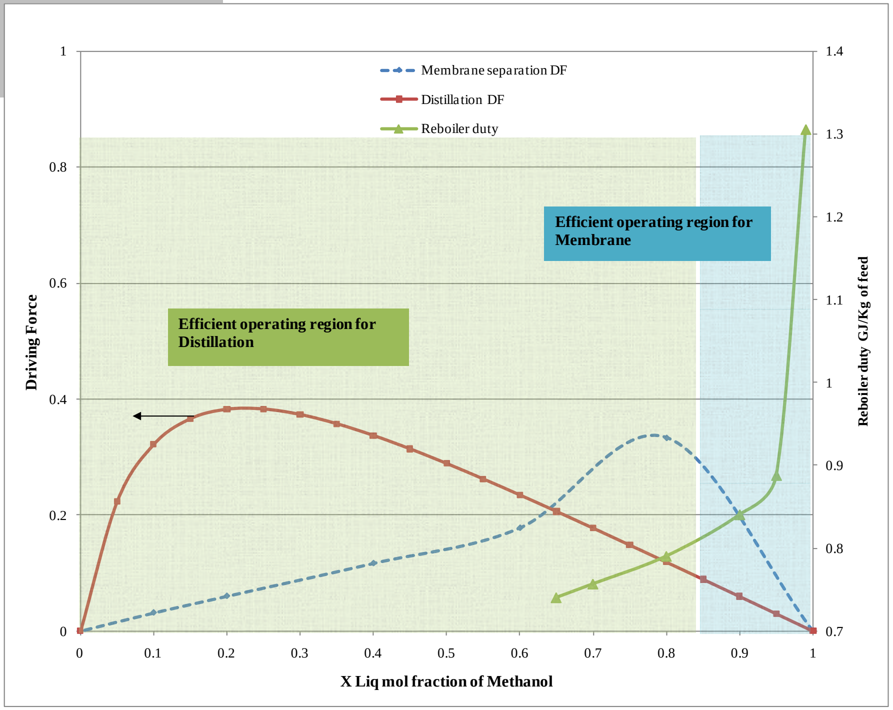
SPEED

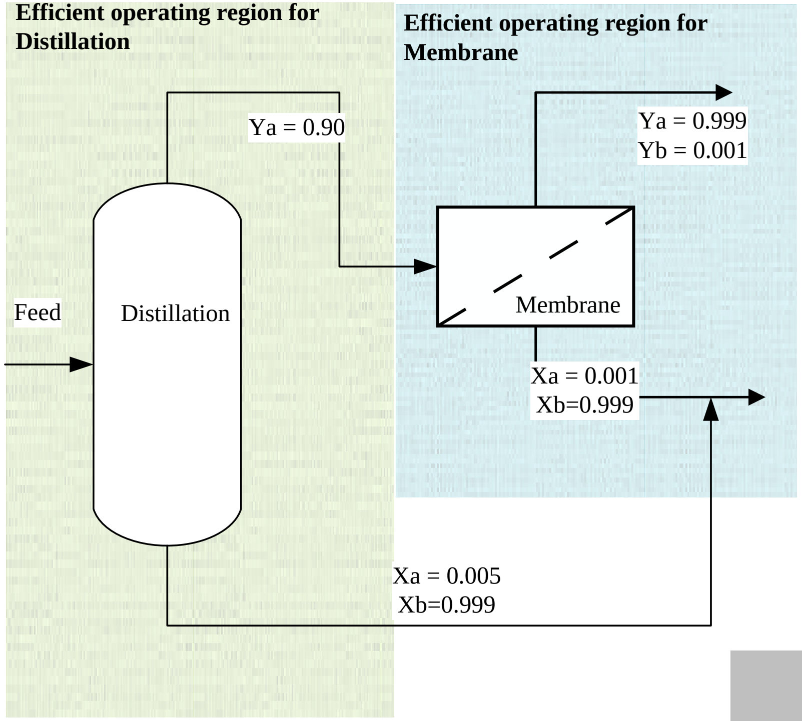
Basis for hybrid separation scheme





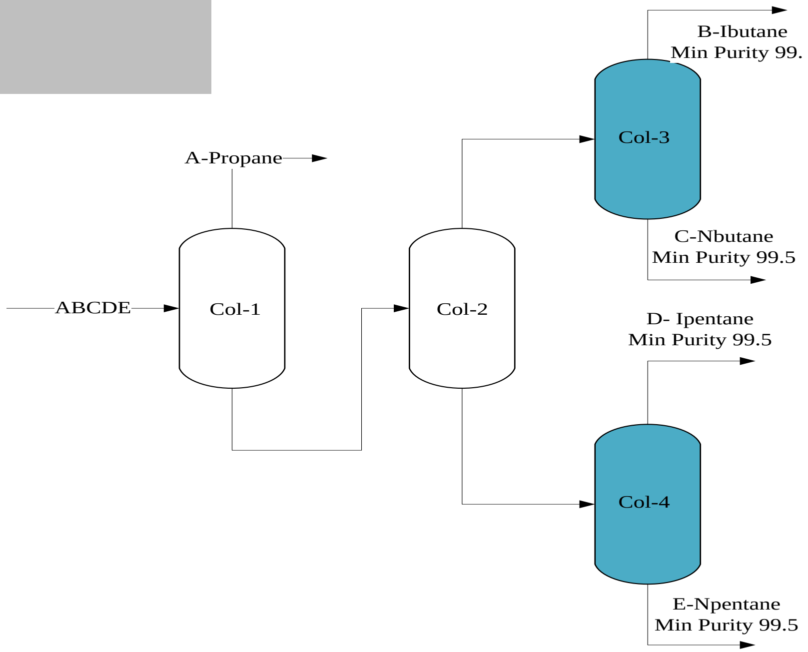
Hybrid distillation + membrane scheme

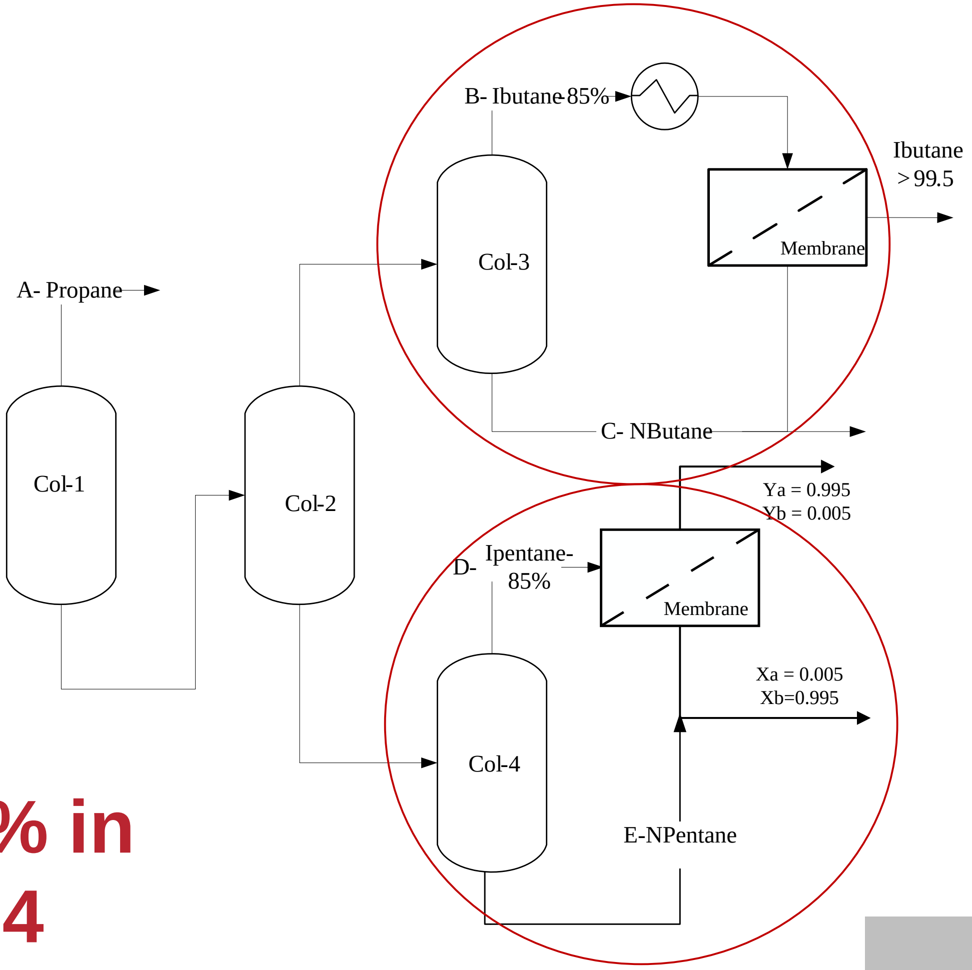




Use membranes to remove from distillate the compound in the smaller amount ~ to increasing the purity of the compound in the larger amount!

New energy efficient sustainable design - 1



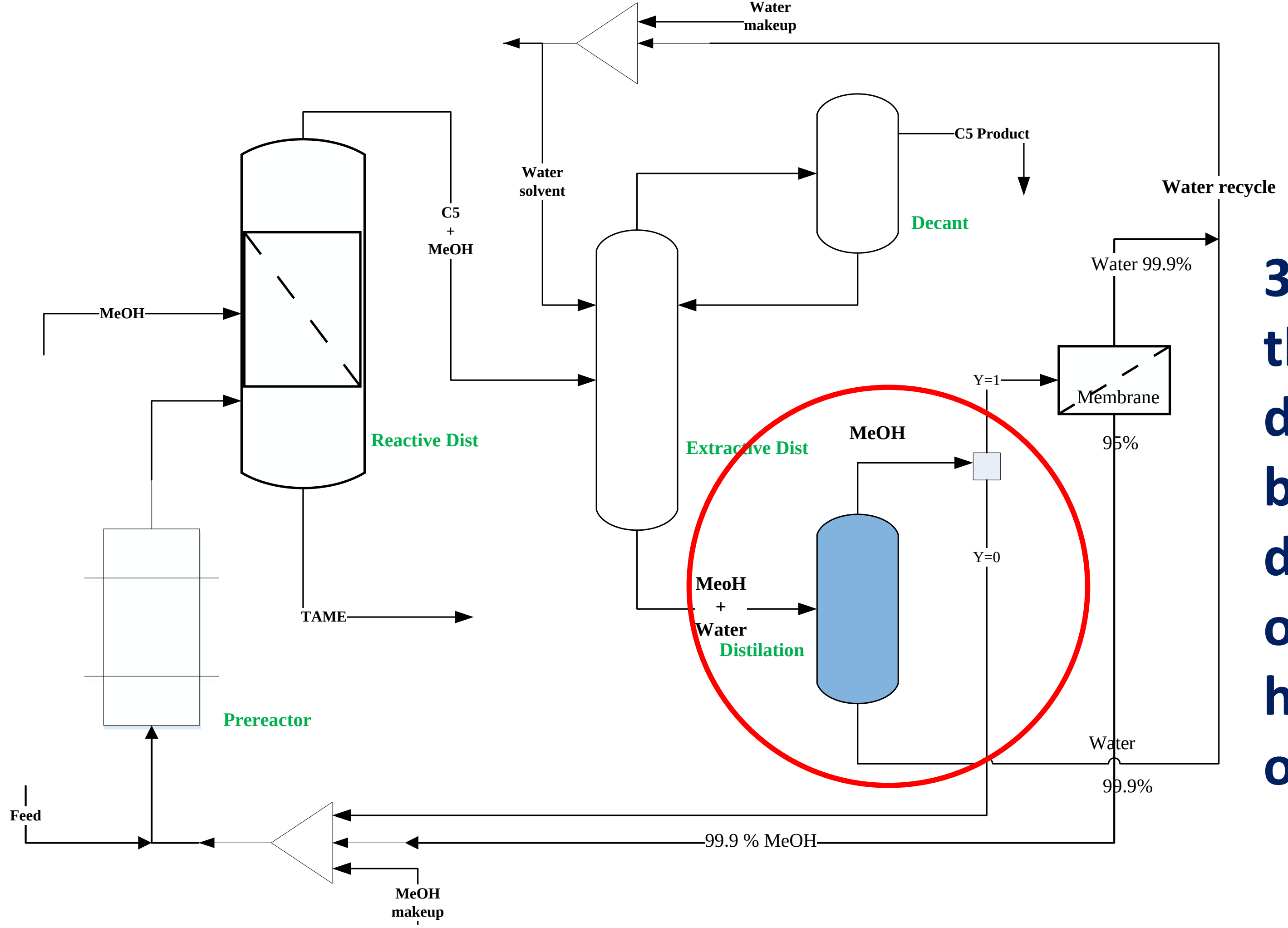


Energy reduction: 44.4% in Col-3 and 37.6% in Col-4

New energy efficient sustainable design - 2

SPEED

Separation Task



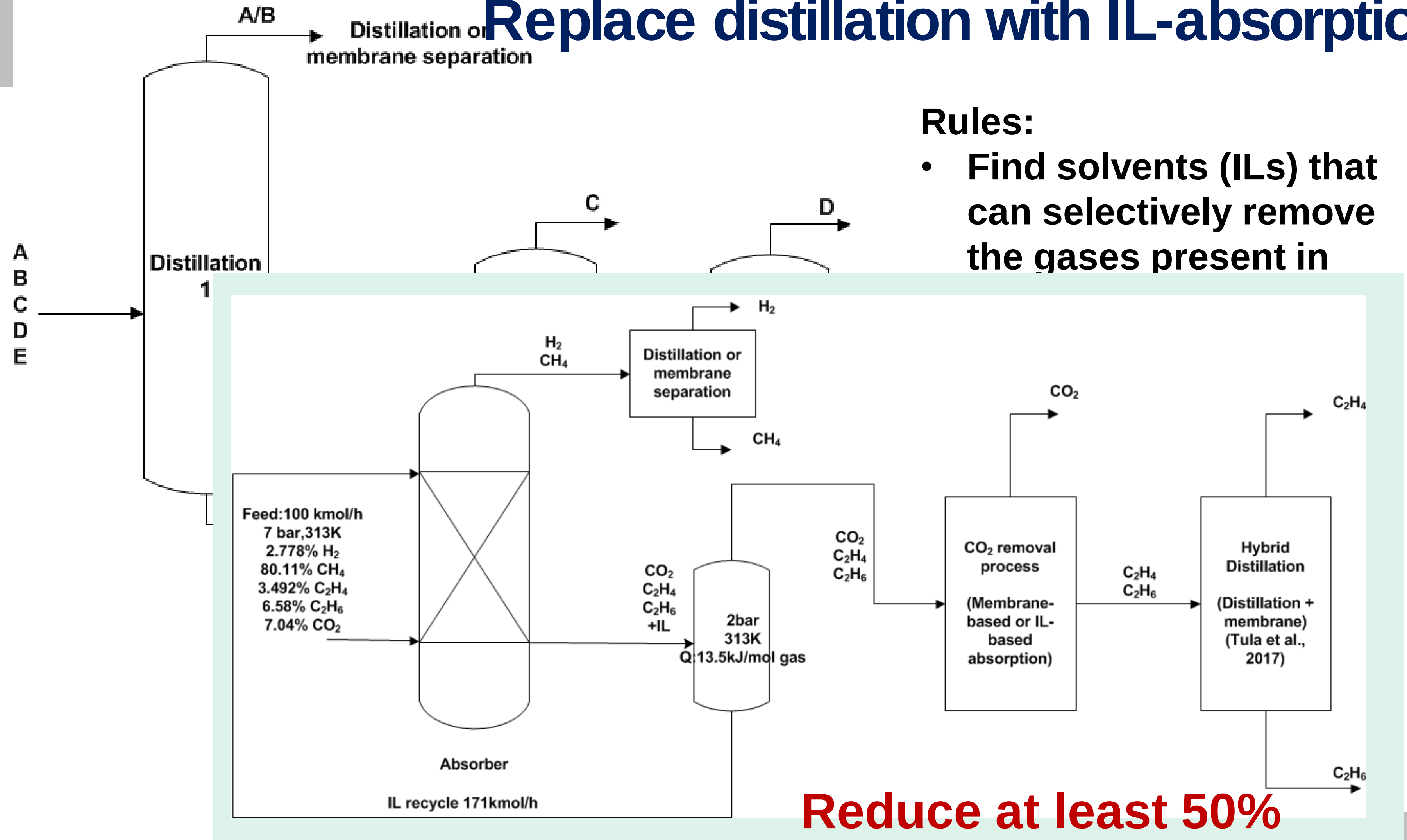
39% energy on the base case design is saved by replacing the distillation operation with hybrid operation

New energy efficient sustainable design – 3b

Replace distillation with IL-absorption

Rules:

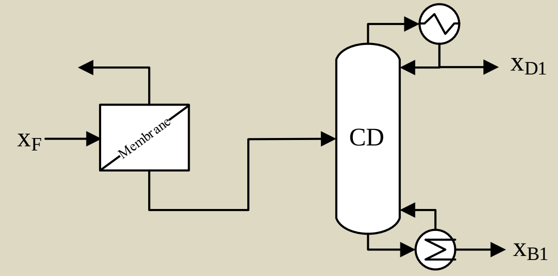
- **Find solvents (ILs) that can selectively remove the gases present in**



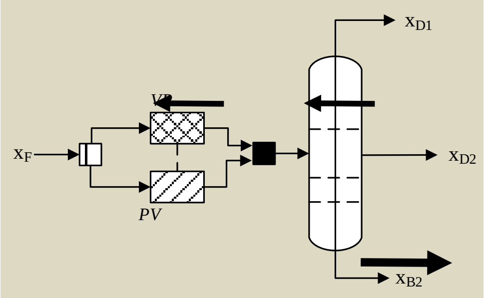
Reduce at least 50% energy consumption

Design of hybrid –intensified modules

Apply these hybrid modules whenever they match the design targets



1



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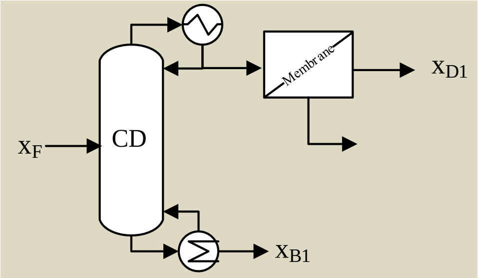

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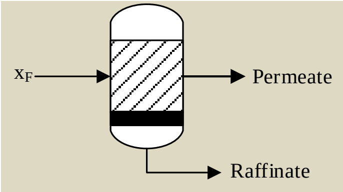

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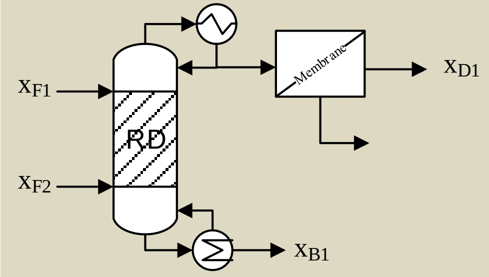

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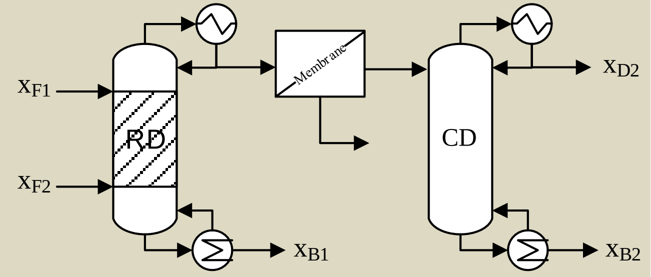
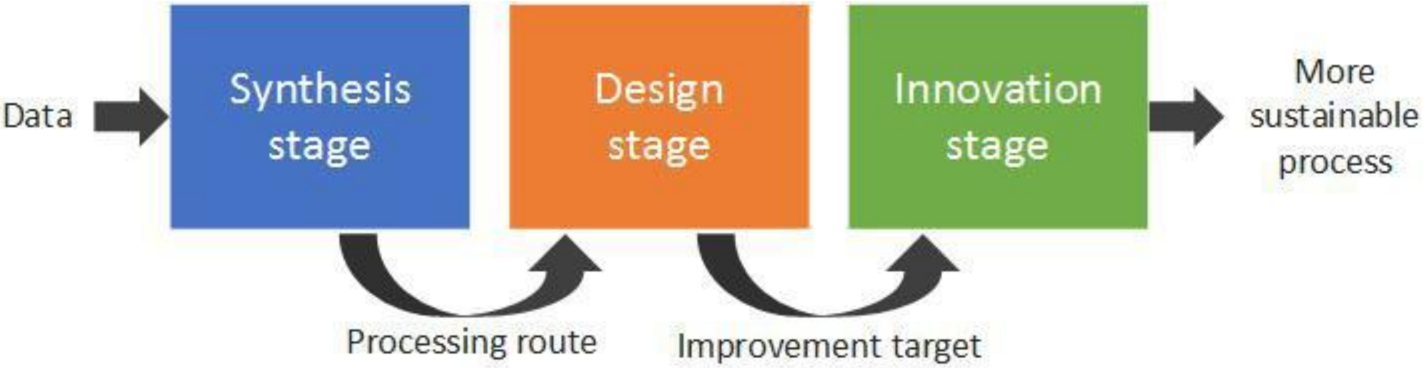


4

Close to 50% or more energy reduction compared to original process achievable

Sustainable Product-Process Development

SPEED



Data

Synthesis stage

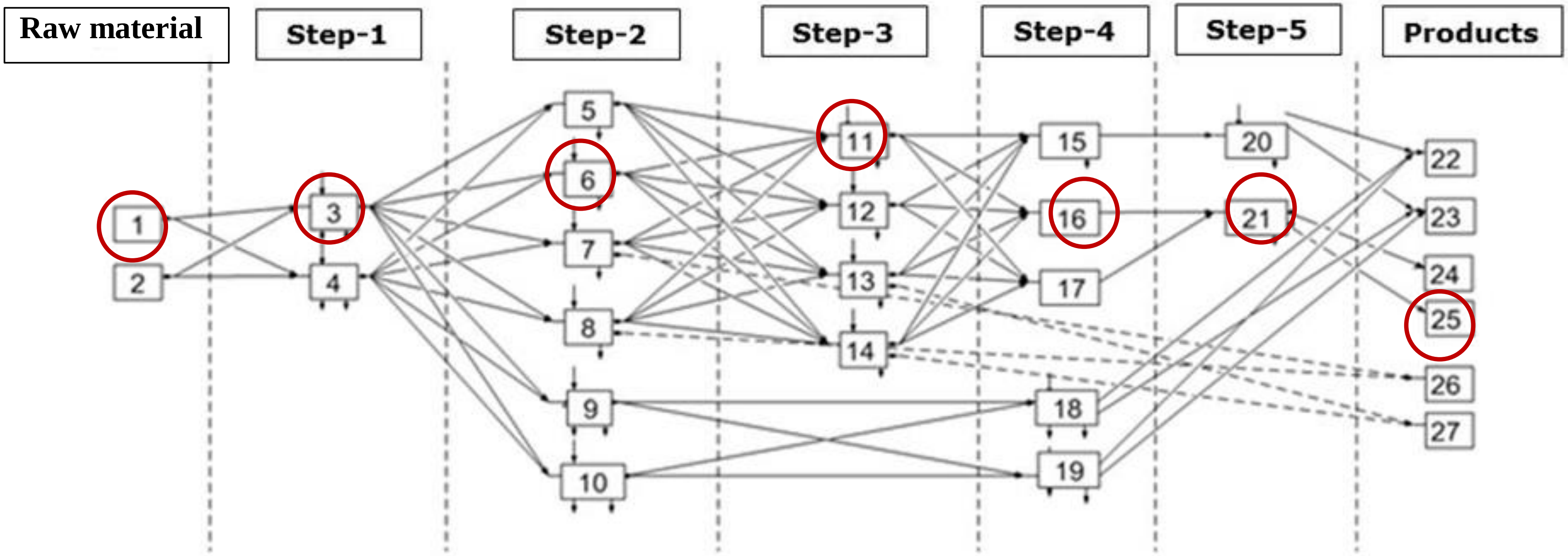
Design stage

Innovation stage

More sustainable process

Processing route

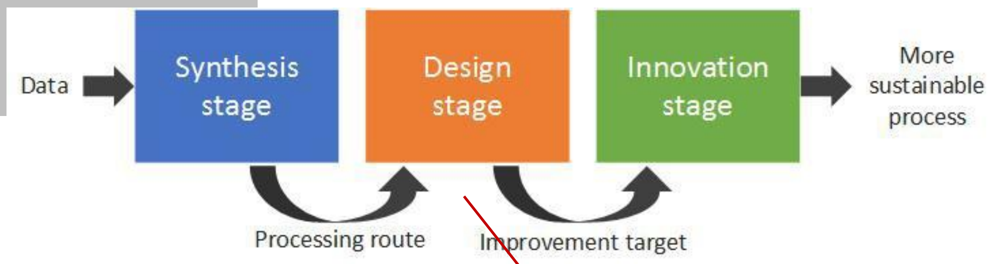
Improvement target



Synthesis stage: find the optimal processing route

Sustainable Product-Process Development

SPEED


Data

Synthesis stage

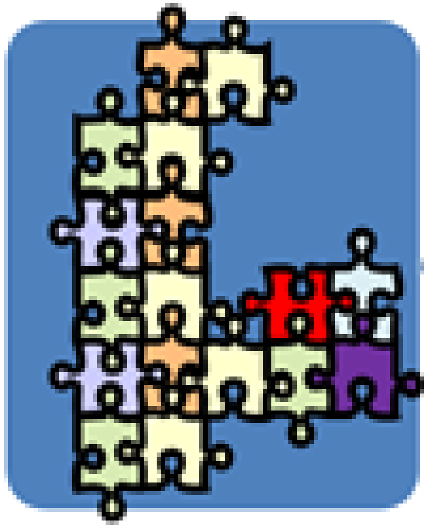
Design stage

Innovation stage

More sustainable process

Processing route

Improvement target



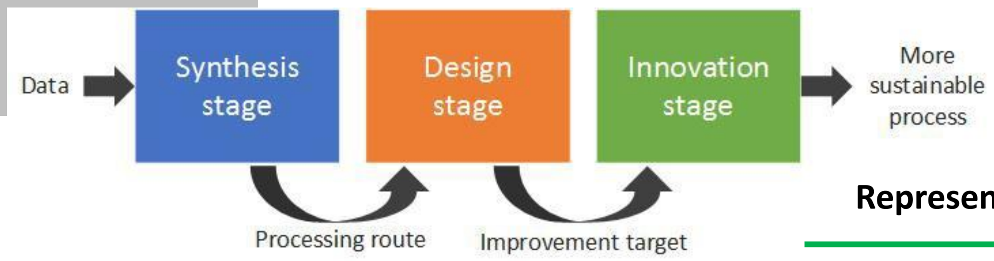
Design targets:

more profit; less energy consumption; less waste; lower environmental impact;

…..

Sustainable process synthesis-design-intensification

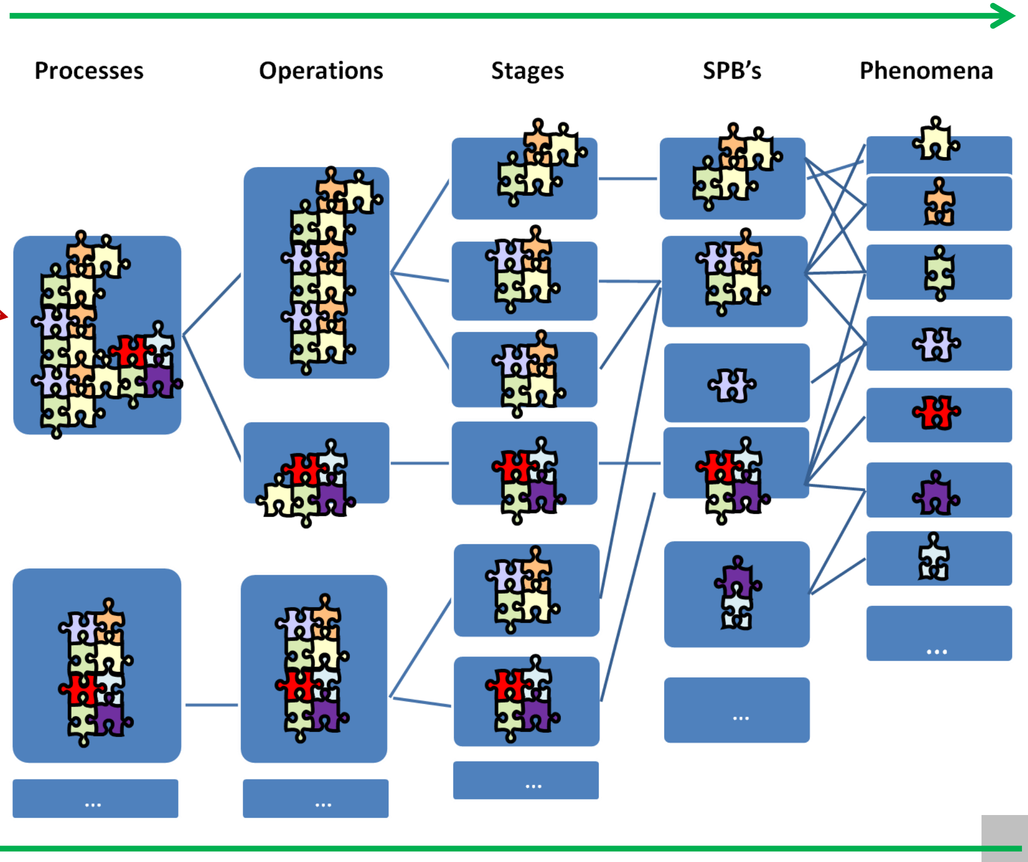
SPEED



CACE, PI-special issue, 2017; CACE, 81, 2015)

Intensification method:
Starting with a base case design (synthesis stage), set targets for improvement (design stage), generate new intensified options that match design targets and make the process more sustainable (innovation stage)

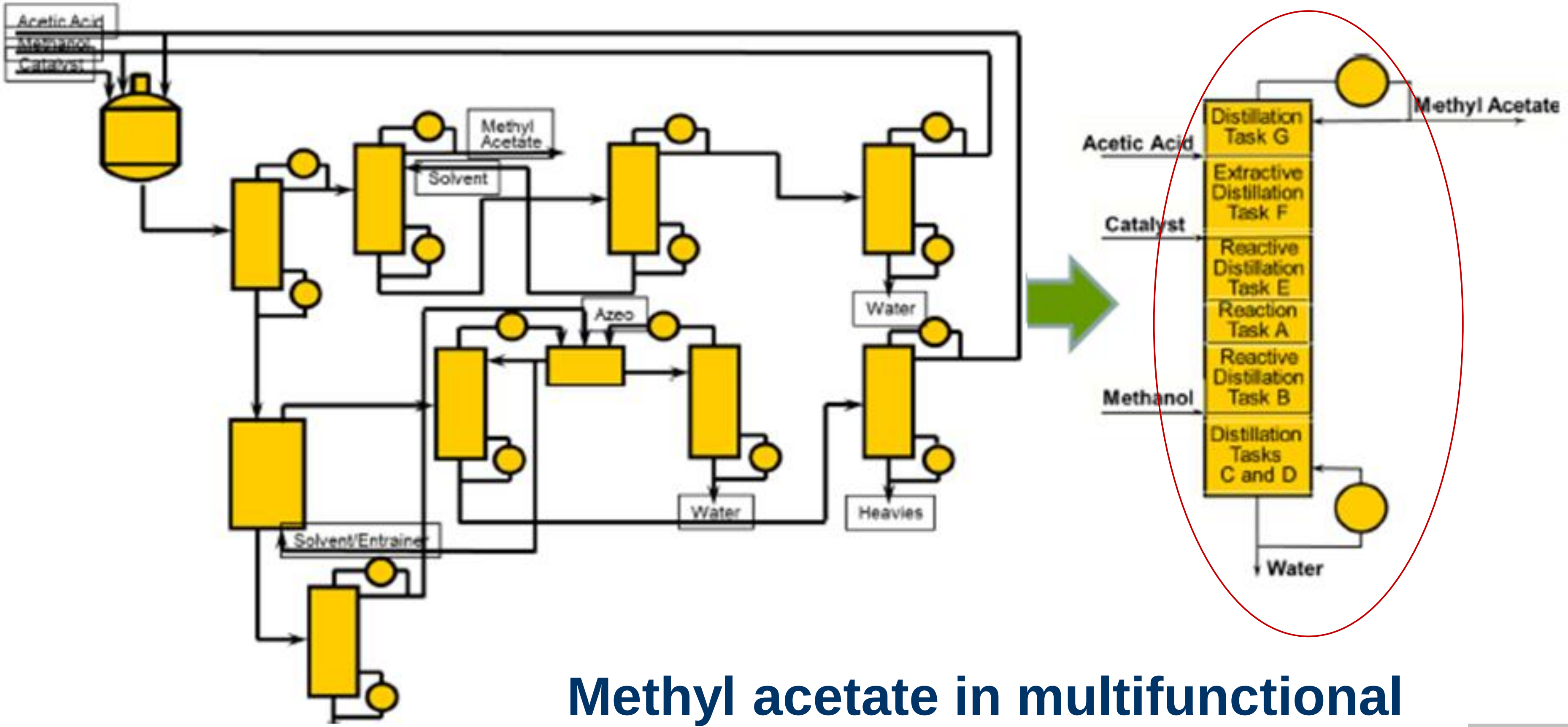
Represent base case process wrt to operations to phenomena



Recombine the phenomena to generate new intensified options

Stage – 3: Find innovative solutions

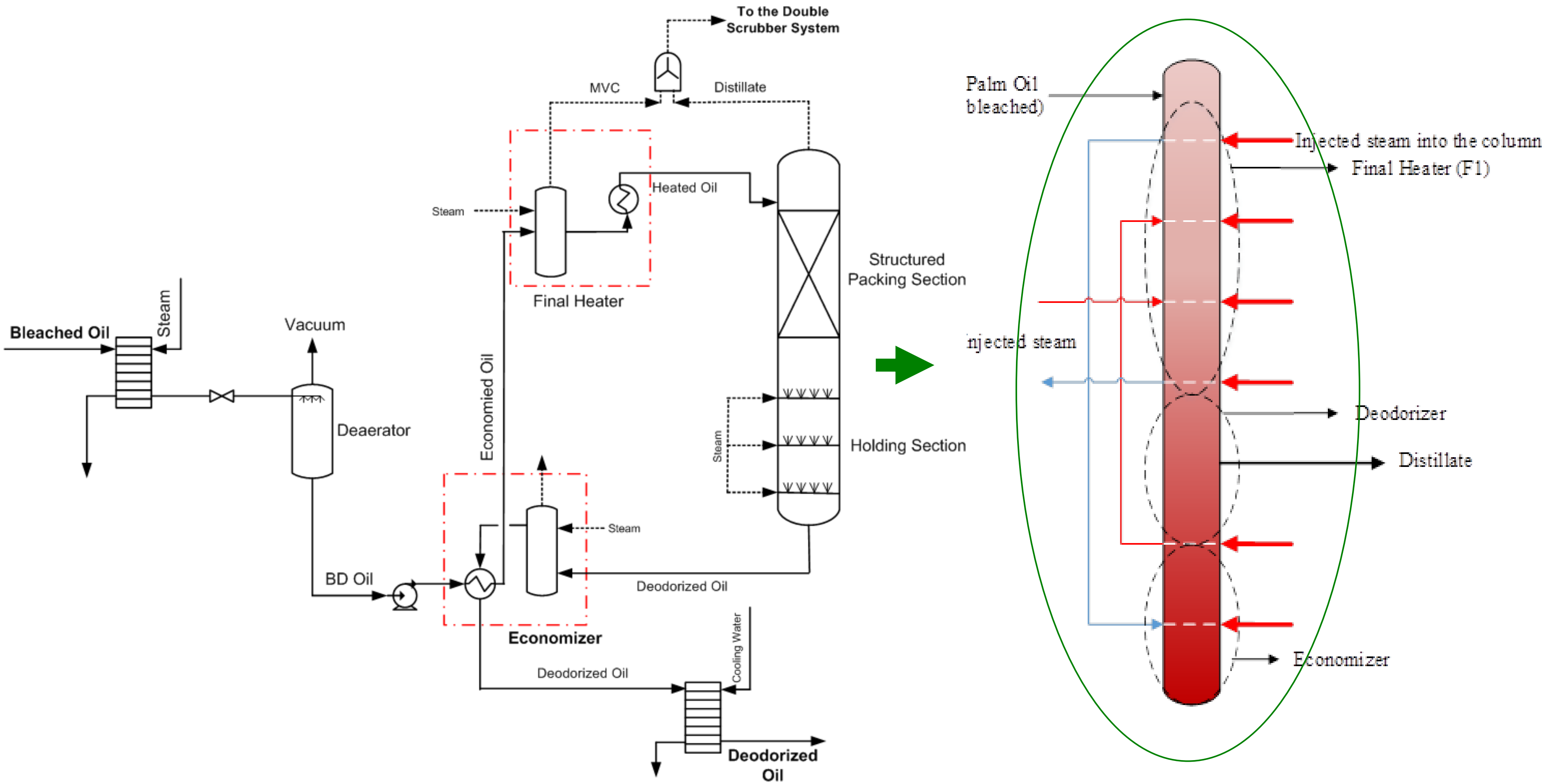
Target: Intensify (reduce number of operations) as well as operational cost



Methyl acetate in multifunctional reactor (Eastman Chemicals)

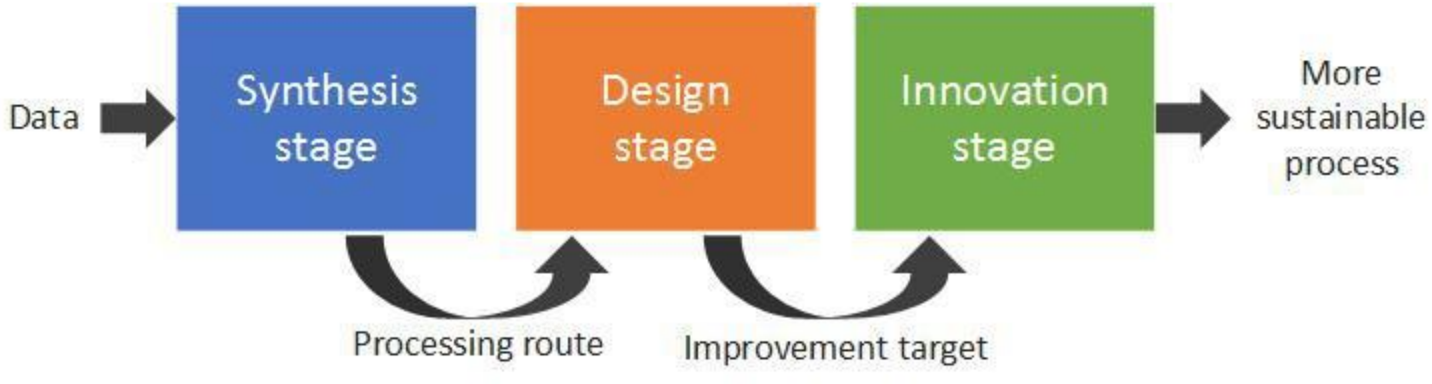
SPEED

Industrial example of process intensification



Deordorization Plant – Alfa Laval, Copenhagen

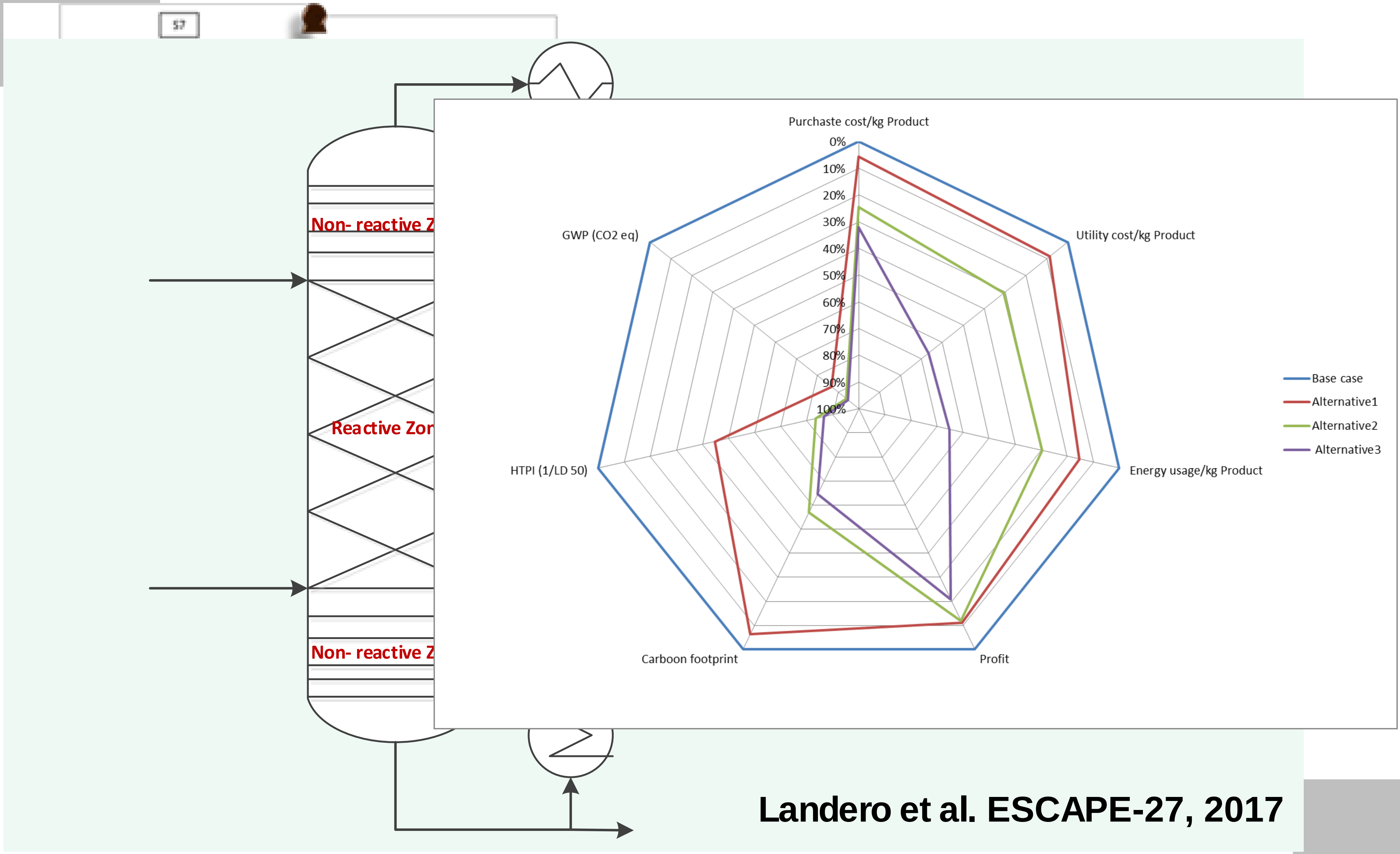
Energy efficient innovative designs for stage 3



Note: for existing process, stage-1 is not necessary and we start with stage-2 to define the targets for sustainable & innovative design

SPEED

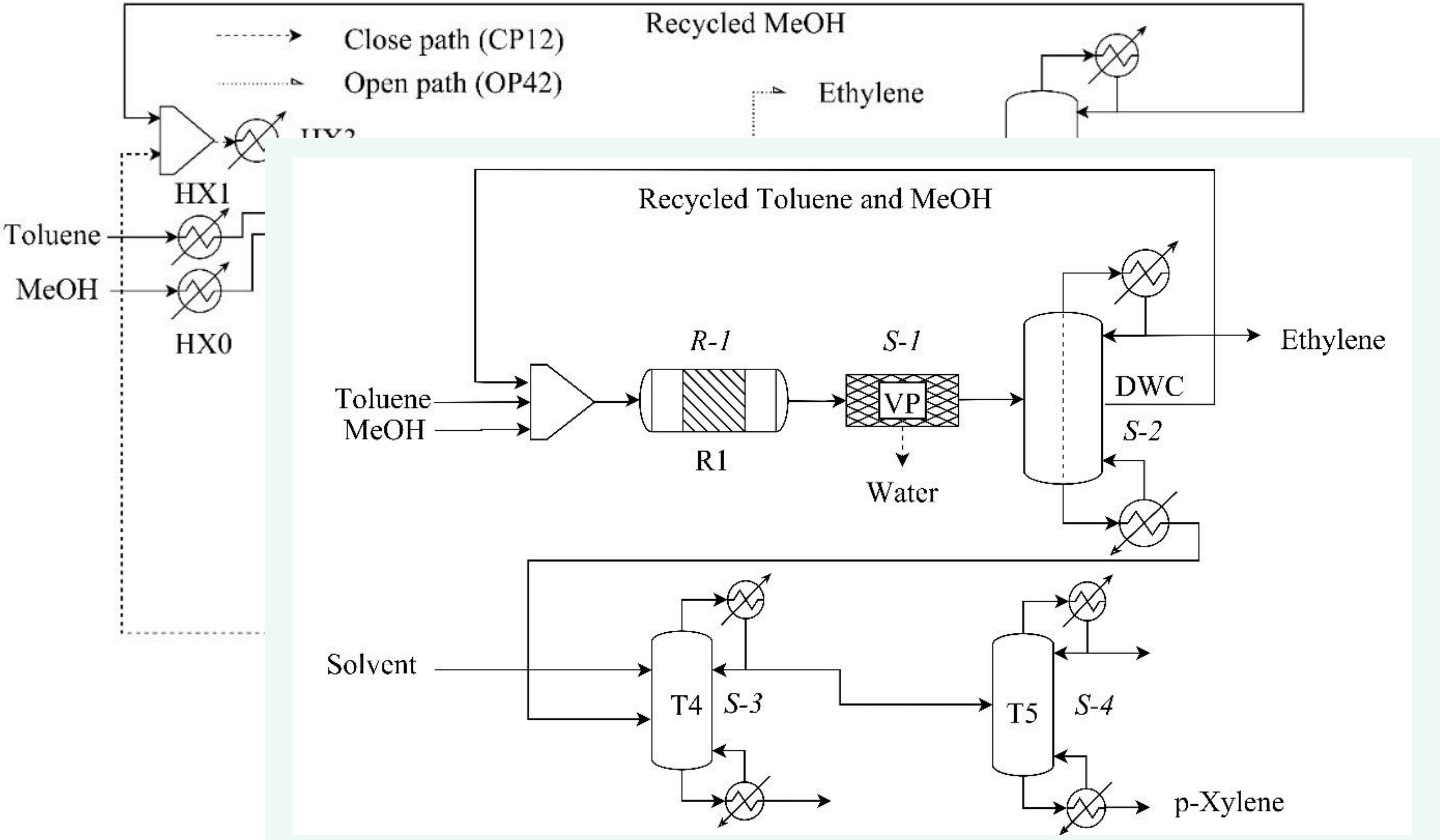
More examples (synthesis of dioxolane products)



Landero et al. ESCAPE-27, 2017

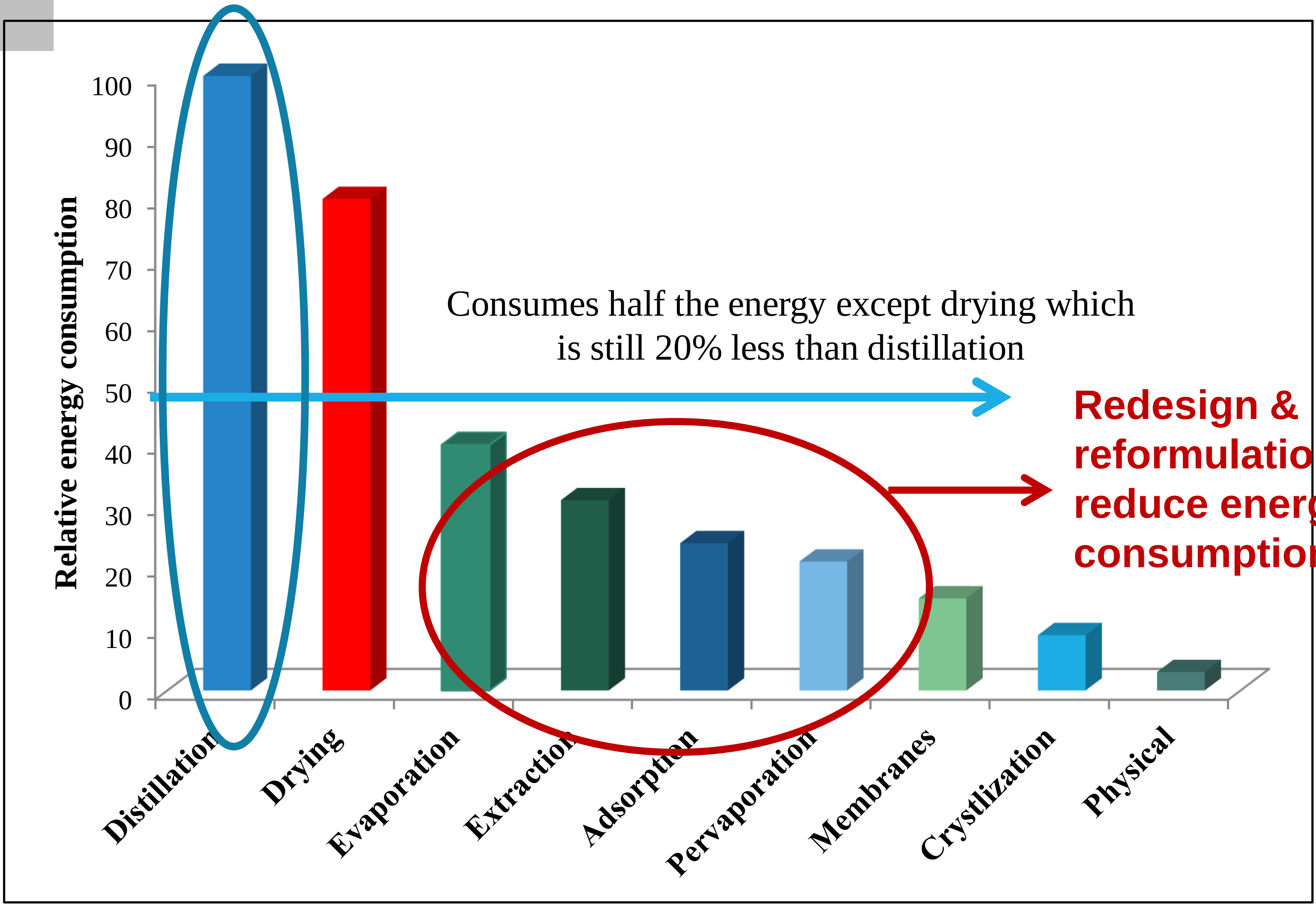
SPEED

More examples (toluene to p-xylene)



Anantasarn et al, CACE 2017 (PI Special Issue)

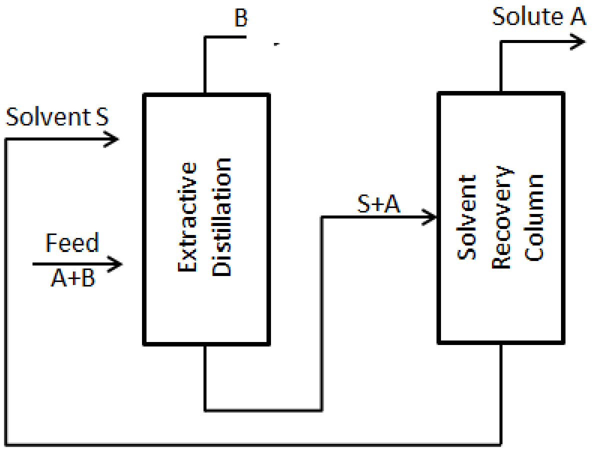
Energy intensive operations in chemical processes



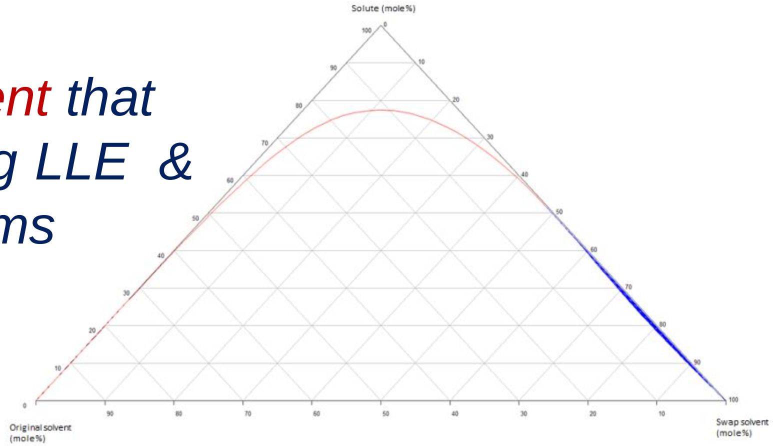
Consumes half the energy except drying which is still 20% less than distillation

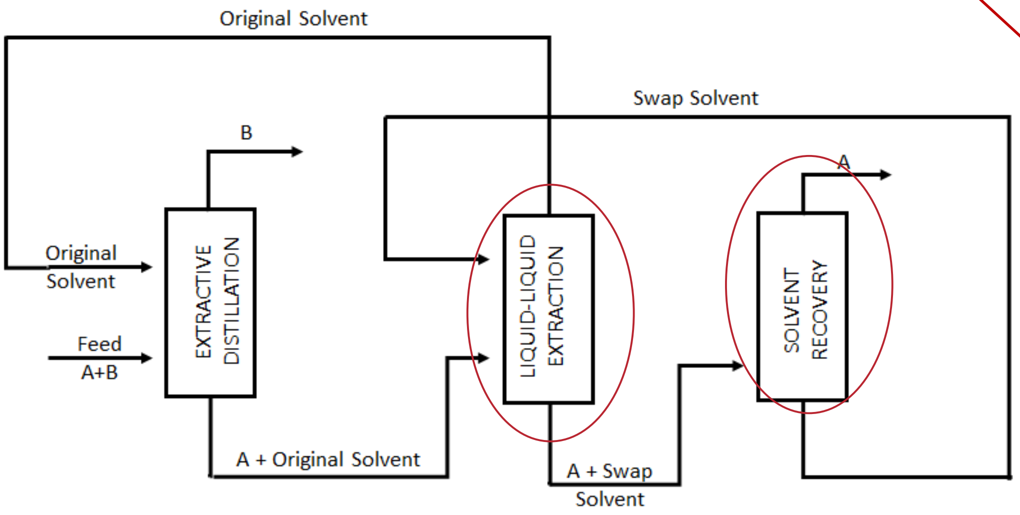
Redesign & reformulation can reduce energy consumption

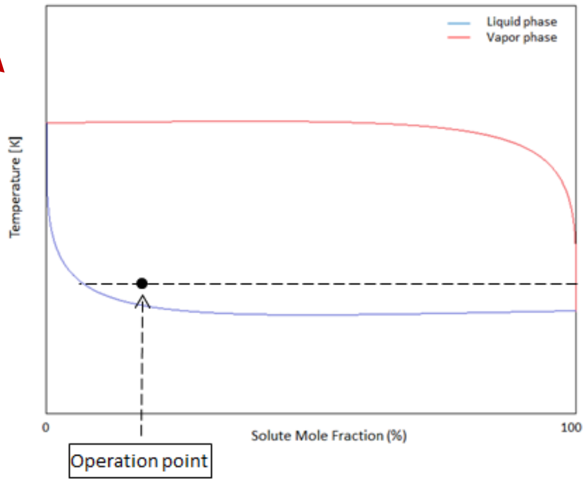
Idea-1: Swap solvent based design



Find *swap solvent* *that gives the following LLE & VLE diagrams*

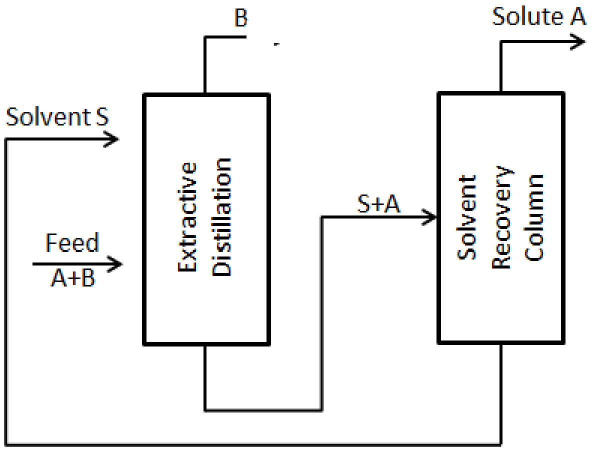






SPEED

Idea-1: Swap solvent based design



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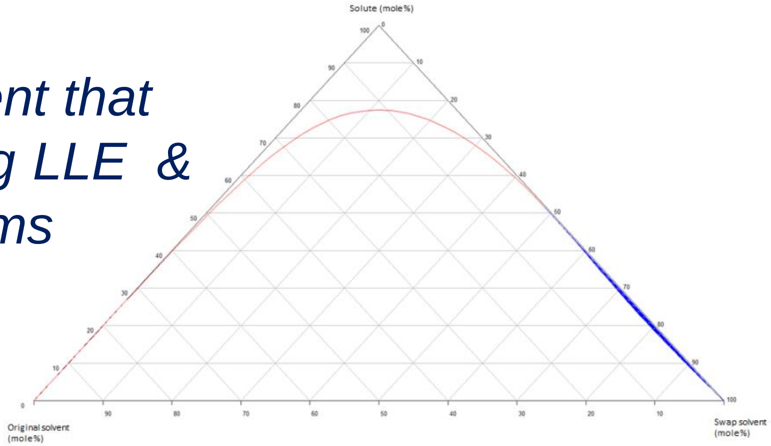
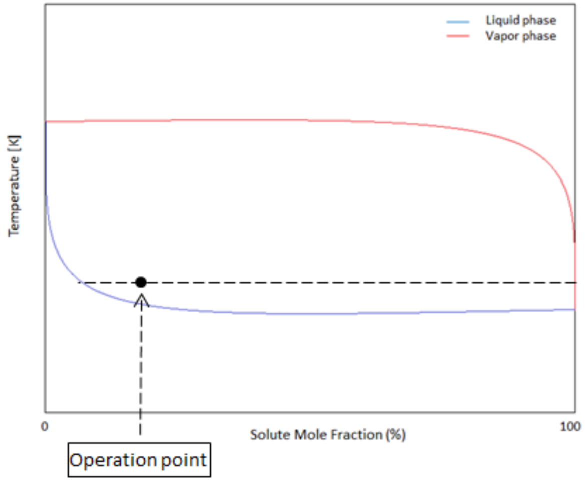
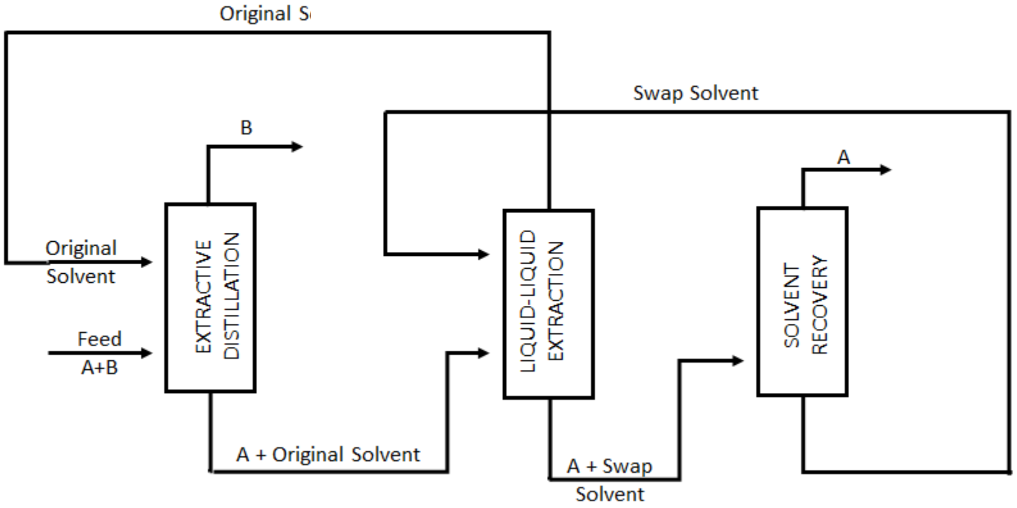


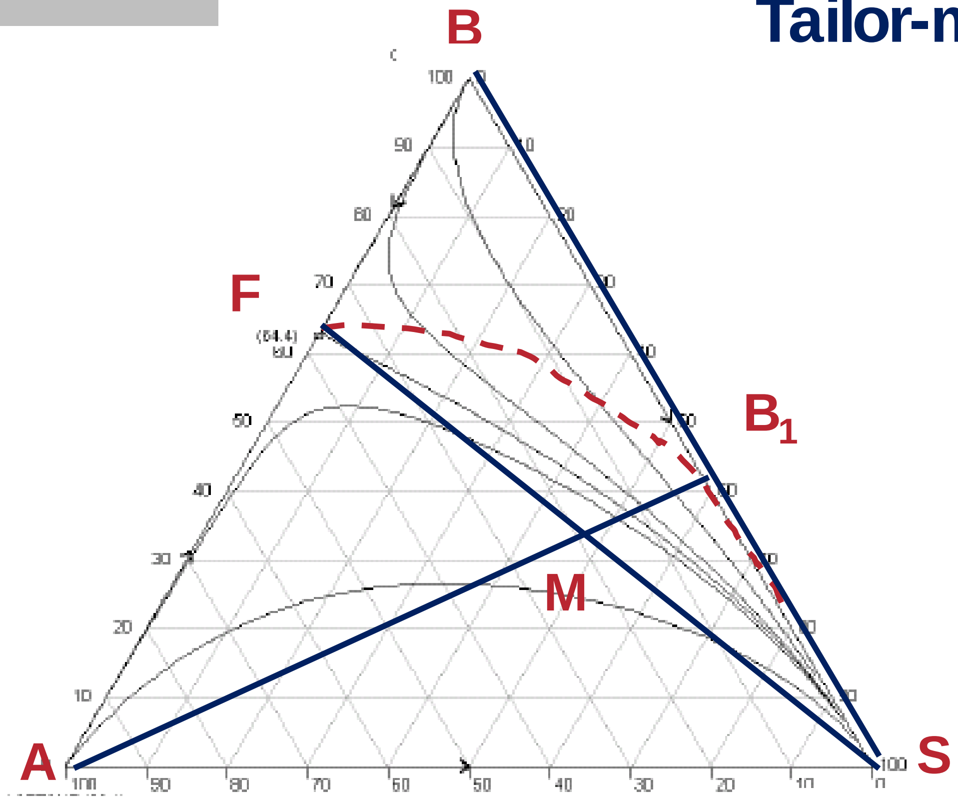


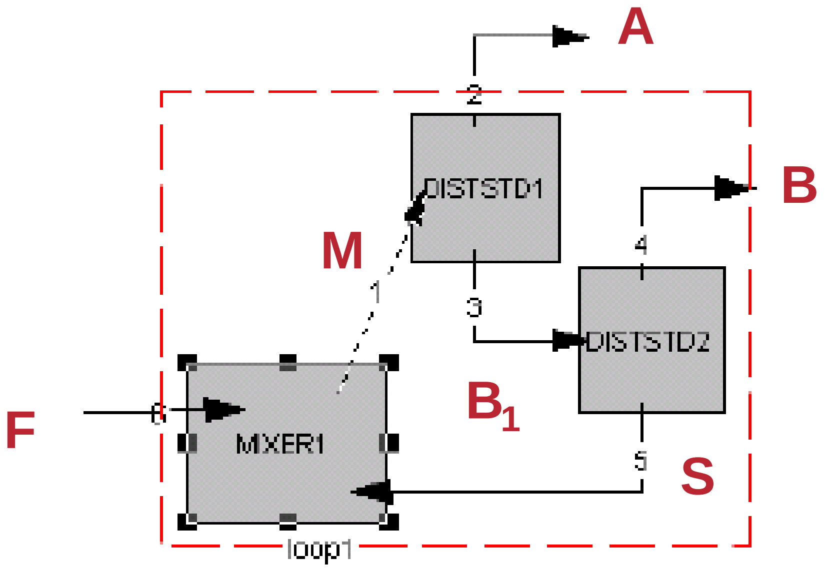


Application: Acetone-methanol-water (original solvent)

Idea-2: Main concept

Tailor-made design of solvents-process





If a solvent could be found that **i)** matches a desired distillation boundary; **ii)** is selective to B; **iii)** is environmentally acceptable; does not form azeotropes with A or B; **iv)** is miscible in the liquid phase,

Then an apriori optimal design is applicable for these azeotropes

Idea 2: Method development steps

Driving force concept ⟷ **Solvent-mixture behavior**

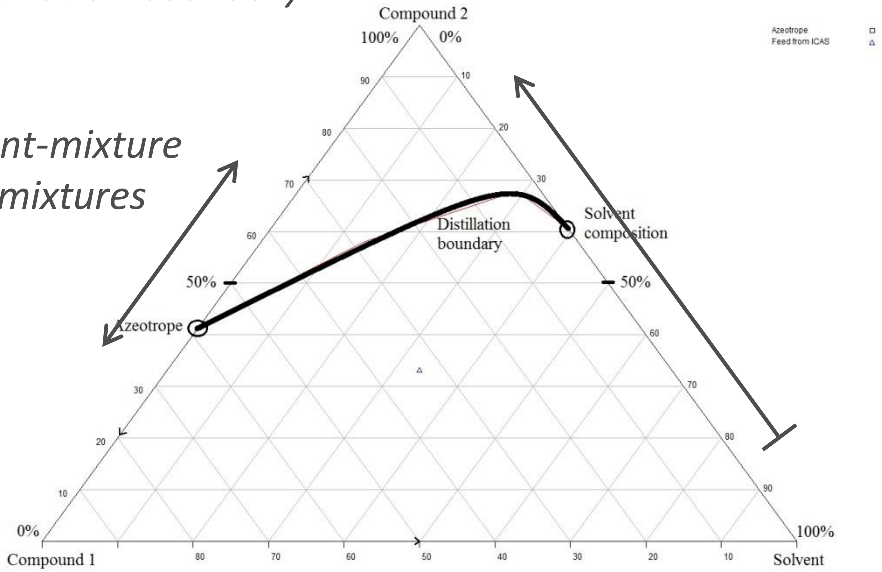
More sustainable energy efficient process

No unique solvent-mixture behavior for all mixtures

Classification

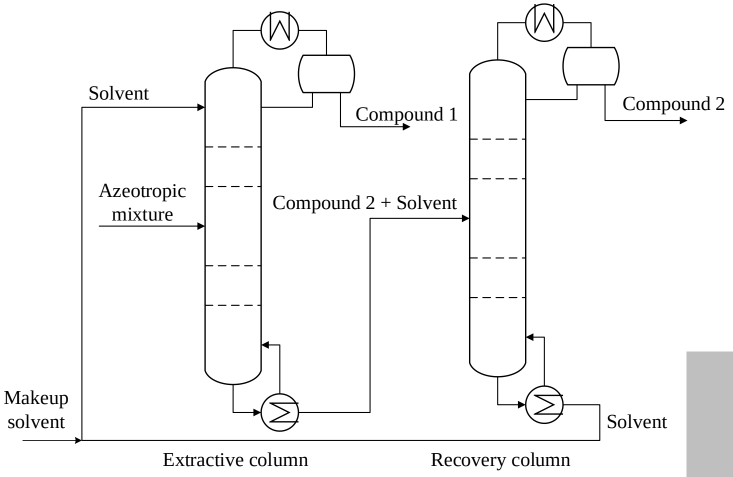
Ternary plot and the position of the distillation boundary

Distillation boundary



***A priori* process design**

Properties of the system



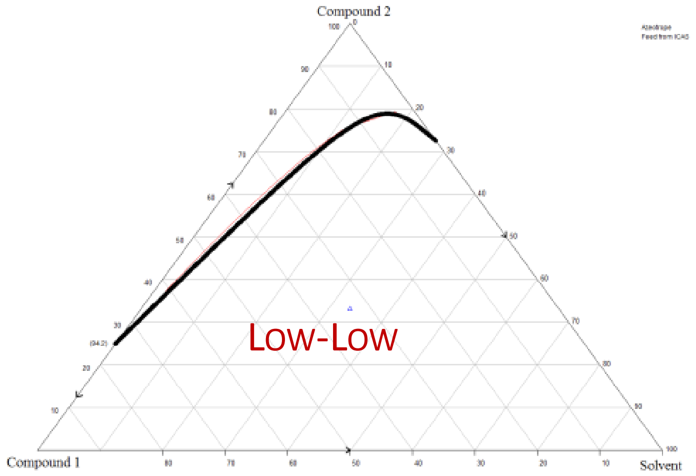
Correlations

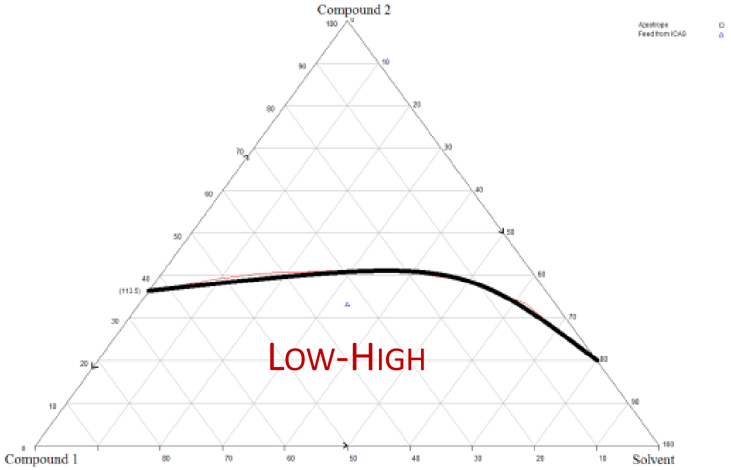
- *Process design parameters*
- *Solvent behavior parameters*

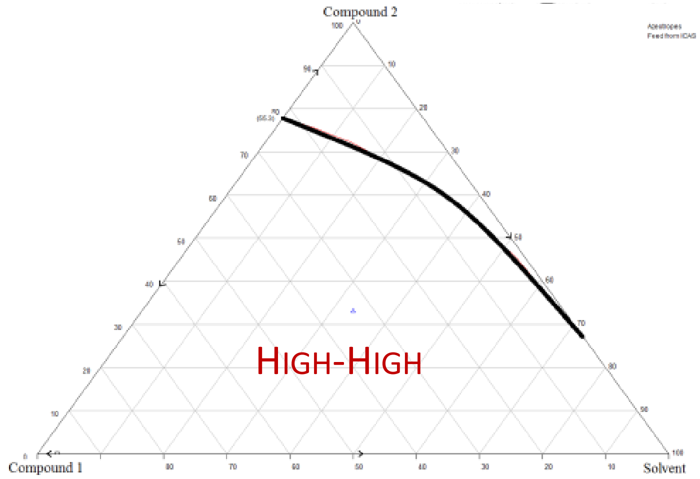
Idea 2: Method development steps

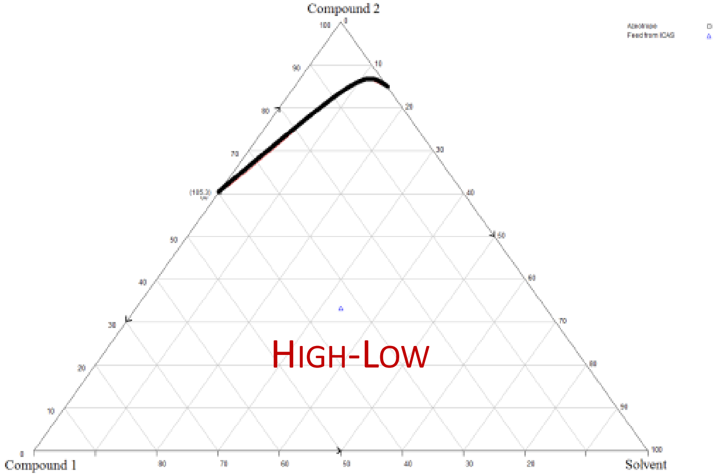
System classification

- Based on the **ternary plot** and the **position of the distillation boundary**









Idea 2: Method development steps

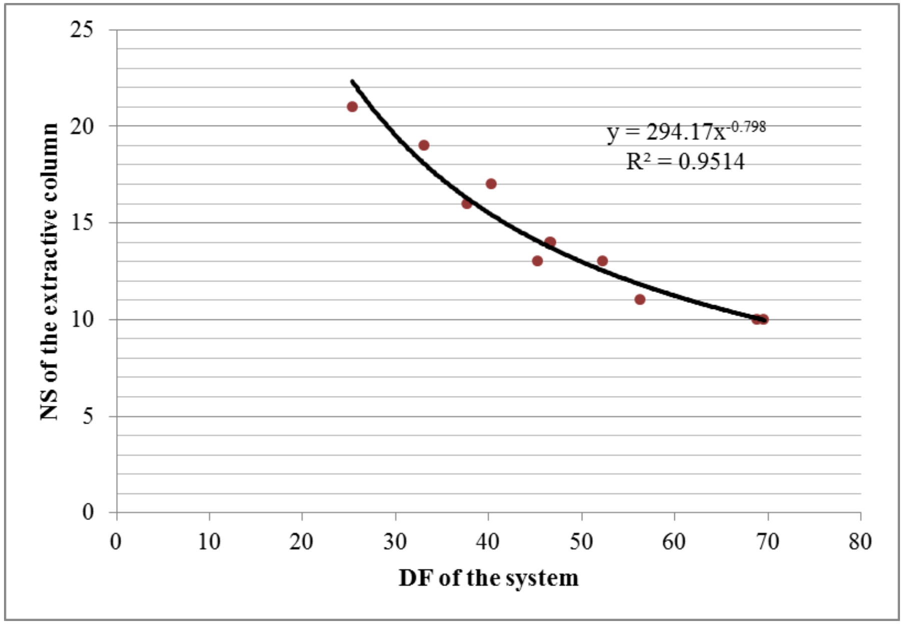
Apriori design & correlations

Process design parameters (NS, N_F and reboiler duty) with respect to solvent behavior parameters (SFR and DF) for each class

- **SFR_{PD} vs DF**
- **SFR_{TP} vs %S**
- **NS vs DF**
- **RD vs DF**

For extractive and recovery columns;
RD = reboiler duty
DF = driving force
NS = number of stages

- **SFR_{SIM} vs SFR_{PD} or SFR_{TP}**



- ➢ **Good correlations for Low-Low and Low-High classes**
- ➢ **Not enough data available for High-Low and High-High classes**

Idea 2: Problem definition & solution

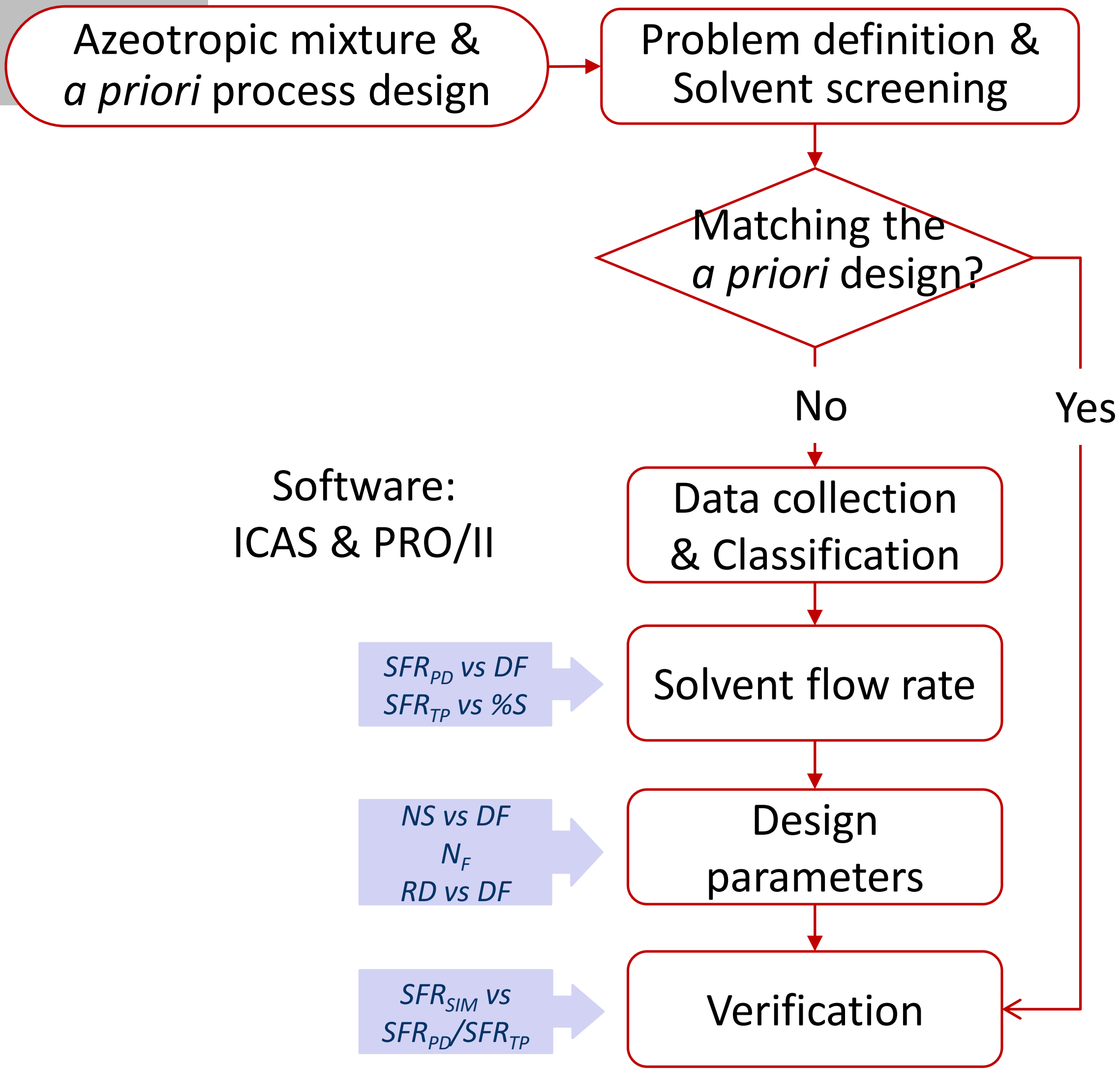
Starting point: homogeneous azeotropic mixture, desired driving force and desired distillation boundary

The method formulates and solves two sub-problems:

SUB-PROBLEM	GIVEN	FIND
1	• Homogeneous azeotropic mixture & known solvent • A priori process design matched	The best (optimal) solvent that satisfy the process design
2	• Homogeneous azeotropic mixture & known solvent • Solvent that does not match the *a priori* design	The optimal extractive distillation design from the correlations

SPEED

Tailor-made method: azeotrope separation



Software:
ICAS & PRO/II

Define the desired products and select the most optimal solvent matching the a priori design

Collect the necessary data for the azeotropic mixture and the solvent and check the classification of the system

Calculate the solvent flow rate, SFR_{PD} or SFR_{TP}, depending on the class

Calculate the design parameters, NS, N_F and RD, from the driving force

Rigorous simulation and verification of optimal design

Method (idea-2) application: Example

Problem definition & Solvent screening → Data collection & Classification → Solvent flow rate → Design parameters → Verification

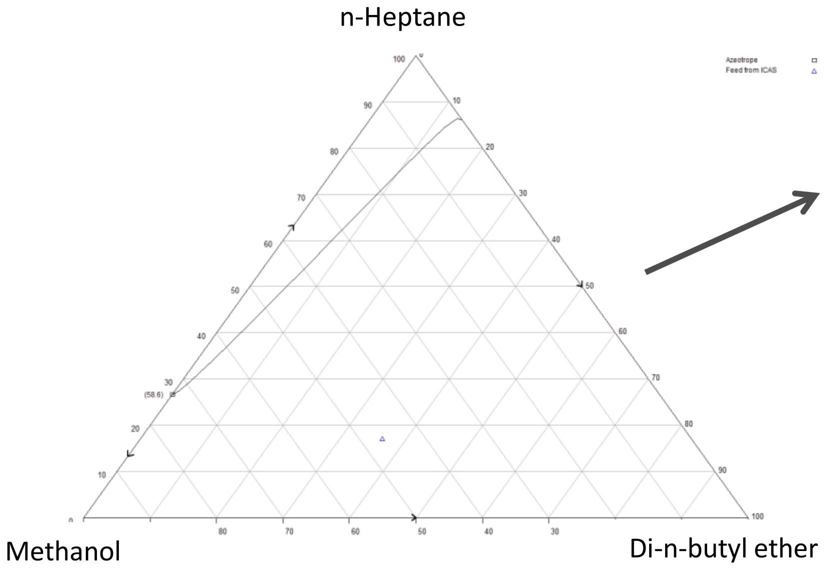
<u>Objective</u>: Define the products and select the most optimal solvent matching the *a priori* process design

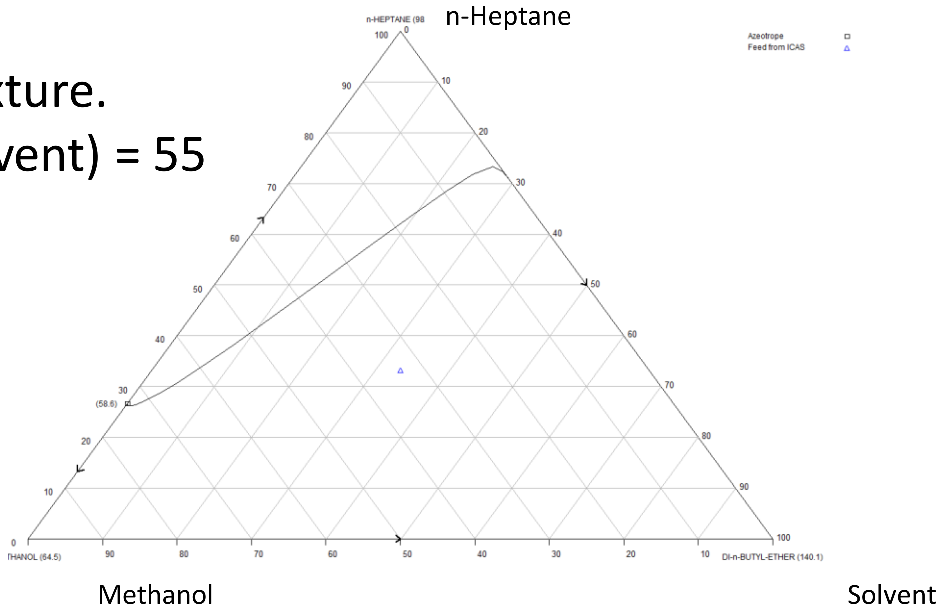
<u>INPUT</u>:

- Methanol/n-Heptane azeotropic mixture.
- DF (System) = 58, DF (Comp. 2 & Solvent) = 55

<u>SOLVENT SELECTION</u>:

Di-n-butyl ether, from CAPEC database.





The proposed distillation boundary does not match the desired distillation boundary

SPEED

Method (idea-2) application: Example

Problem definition & Solvent screening → Data collection & Classification → **Solvent flow rate** → Design parameters → Verification

Objective: Collect the necessary data, classify the system and calculate the solvent flow rate.

PURE COMPONENTS PROPERTIES:

Component	Boiling point (K)	MW (g/mol)
Methanol	337.5	32.04
n-Heptane	371.4	100.21
Di-n-butyl ether	413.1	130.23

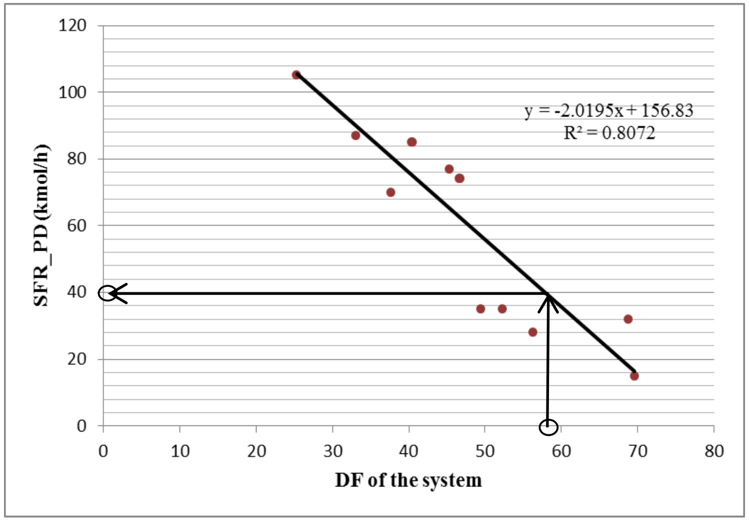
SYSTEM DATA:

- Azeo. Comp.: 27%mol Methanol, 73%mol n-Heptane
- % Solvent in comp.2-solvent line: 14%mol
- DF diagram of the system: DF=58, D_x=16
- DF diagram of comp. 2 and solvent: DF=55, D_x=22

Low-Low class

CALCULATION OF SOLVENT FLOW RATE:

SFR_{PD} = 39.7 kmol/h →

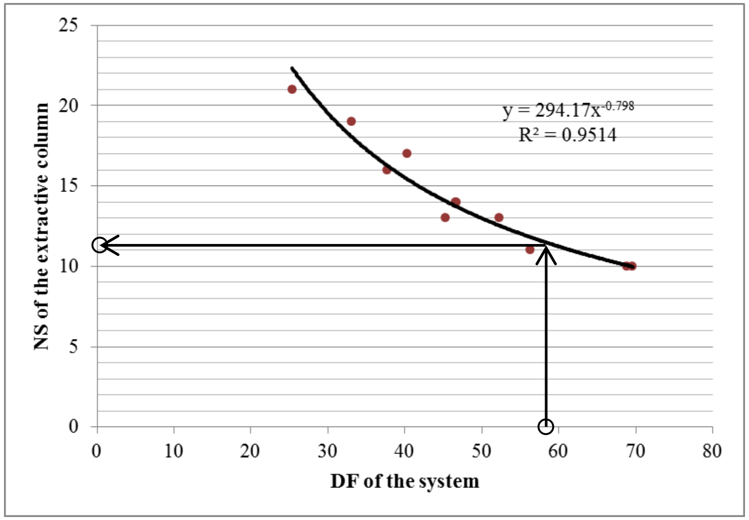


Method (idea-2) application: Example

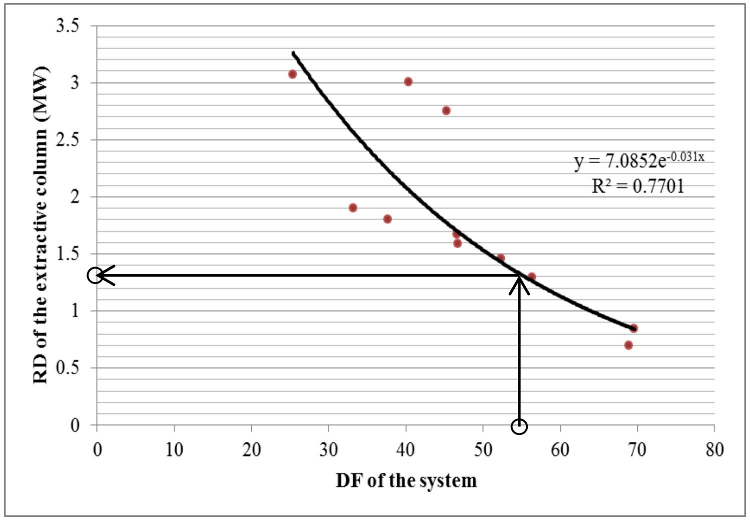
Problem definition & Solvent screening → Data collection & Classification → Solvent flow rate → **Design parameters** → Verification

Objective: Calculate the design parameters, NS, N_F and RD, from the driving force.

NUMBER OF STAGES:



REBOILER DUTY:

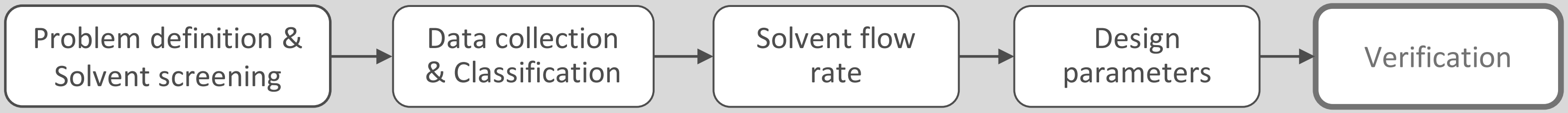


FEEDING STAGE LOCATION:

$$N_F = NS(1 - D_x)$$

	Extractive column	Recovery column
NS	12±2	13±2
N_F	10th±2	10th±2
RD (MW)	1.17	2.06

Method (idea-2) application: Example

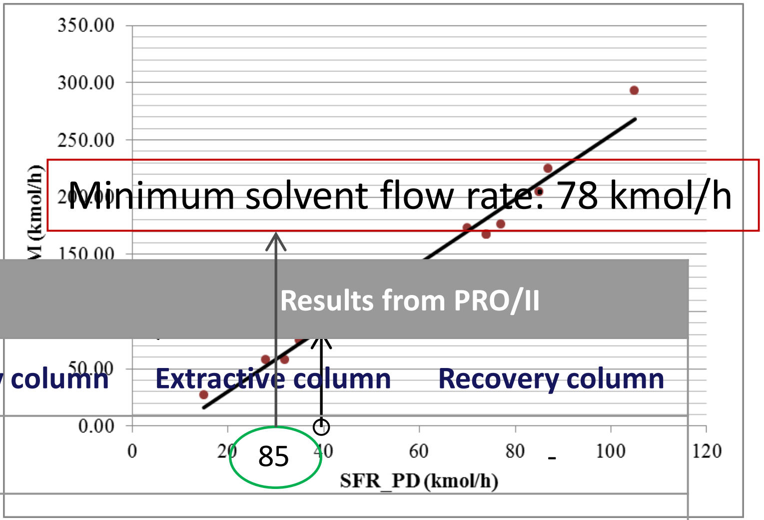


Problem definition & Solvent screening → Data collection & Classification → Solvent flow rate → Design parameters → Verification

Objective: Rigorous simulation and verification of optimal design.

SOLVENT FLOW RATE NECESSARY TO PERFORM THE RIGOROUS SIMULATION: SFR_{SIM}

SFR_{SIM} = 85.25 kmol/h →



Minimum solvent flow rate: 78 kmol/h

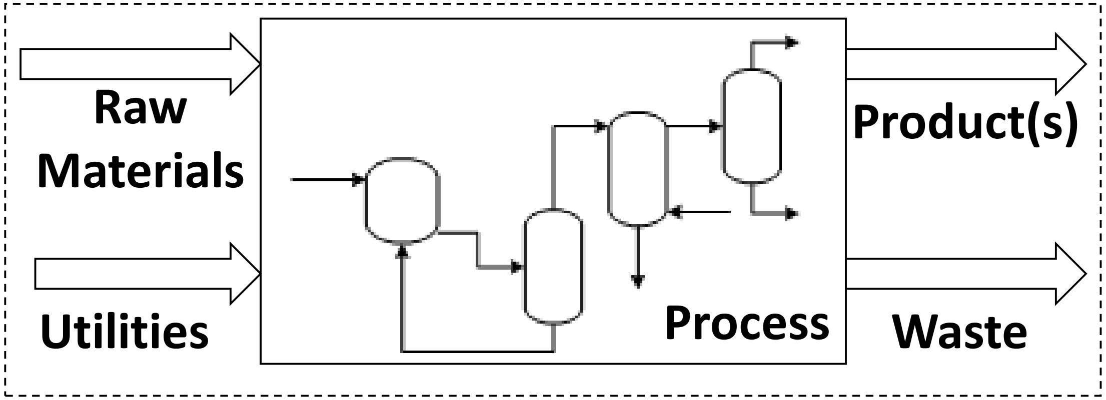
RIGOROUS SIMULATION:

	Method estimation		Results from PRO/II	
Design parameters	**Extractive column**	**Recovery column**	**Extractive column**	**Recovery column**
SFR (kmol/h)	85.25	-	85	-
NS	12±2	13±2	14	13
N_F	10^{th}±2	10^{th}±2	12^{nd}	7^{th}
Recovery of products (%mol)	99.5	99.5	99.5	99.5
Reboiler duty (MW)	1.17	2.06	1.48	1.72

Chemical and bio-based industry faces enormous challenges to achieve and/or respond to:

Establish sustainable production

Adopt to changing markets



Survive global competition

Demands for innovative products

Processes need to be:

Sustainable (Economically feasible; Reduced waste; Utility efficient; Environmentally acceptable); Safe; Operable; …….

Summary: Sustainable Process Design

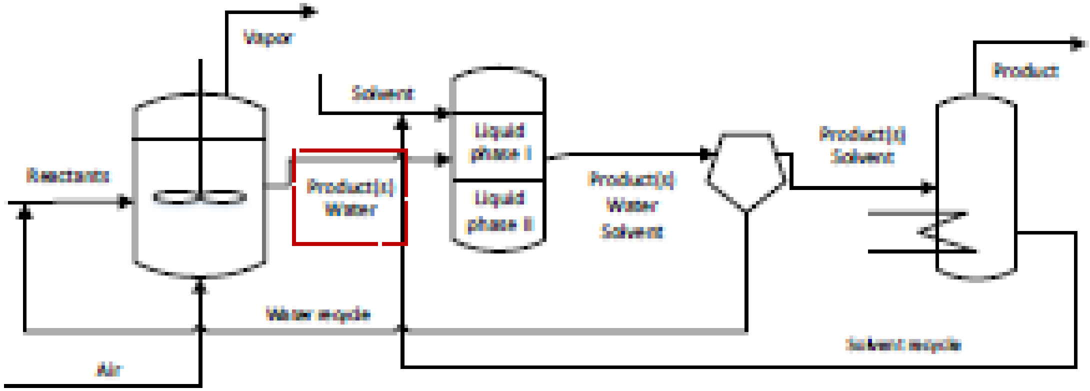
Chemical Process Design: Problem Definition

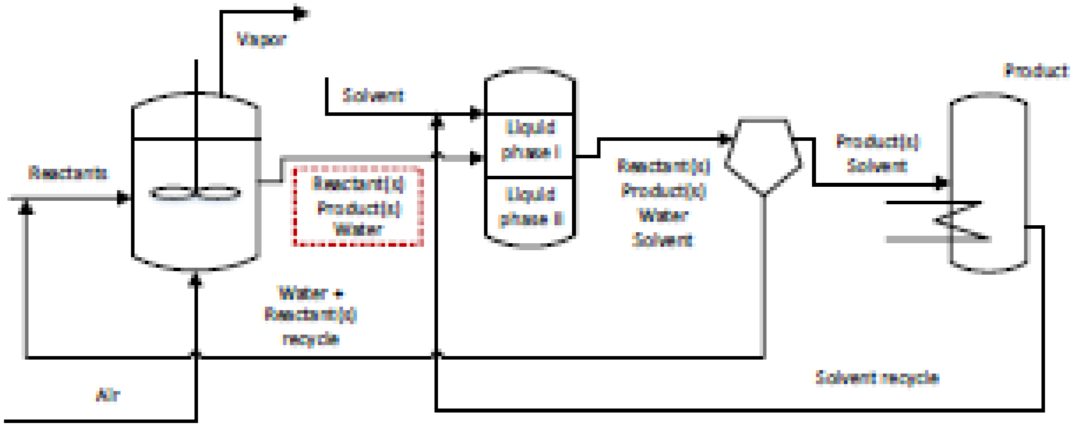
Given: Reference design of a process

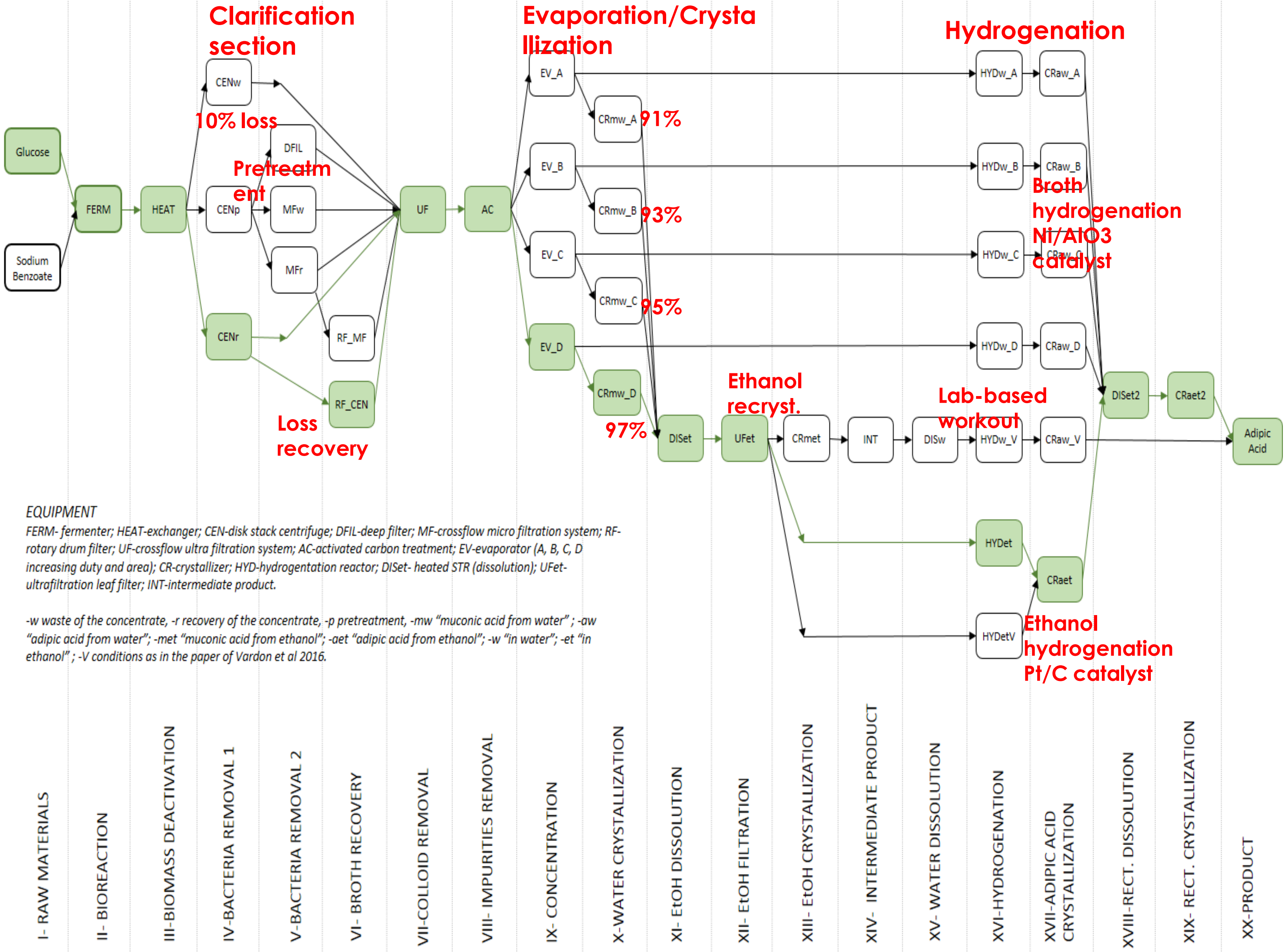
Objective: Generate design alternatives that can only improve one or more sustainability metrics and safety factors while remaining aprroximately neutral for all other metrics and factors

Determine: Mass & energy indicators for the process under investigation; identify the sensitive indicators; set target values for the sensitive indicator; find alternatives that match the targets

Application examples







Clarification section

10% loss

Pretreatment

Loss recovery

Evaporation/Crystallization

91%

93%

95%

97%

Ethanol recryst.

Hydrogenation

Broth hydrogenation Ni/AlO3 catalyst

Lab-based workout

Ethanol hydrogenation Pt/C catalyst

EQUIPMENT

FERM- fermenter; HEAT-exchanger; CEN-disk stack centrifuge; DFIL-deep filter; MF-crossflow micro filtration system; RF-rotary drum filter; UF-crossflow ultra filtration system; AC-activated carbon treatment; EV-evaporator (A, B, C, D increasing duty and area); CR-crystallizer; HYD-hydrogentation reactor; DISet- heated STR (dissolution); UFet-ultrafiltration leaf filter; INT-intermediate product.

-w waste of the concentrate, -r recovery of the concentrate, -p pretreatment, -mw "muconic acid from water" ; -aw "adipic acid from water"; -met "muconic acid from ethanol"; -aet "adipic acid from ethanol"; -w "in water"; -et "in ethanol" ; -V conditions as in the paper of Vardon et al 2016.