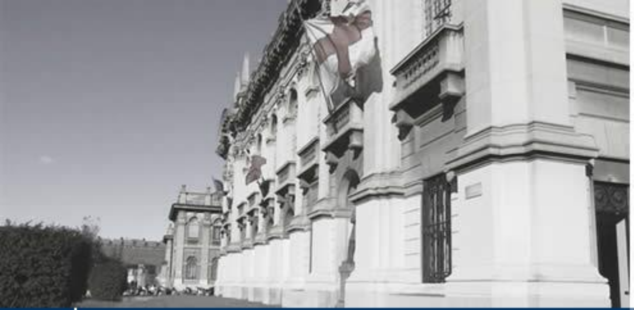


SCUOLA DI INGEGNERIA INDUSTRIALE E DELL'INFORMAZIONE

DIPARTIMENTO DI CHIMICA, MATERIALI E INGEGNERIA CHIMICA «GIULIO NATTA»

LAUREA MAGISTRALE IN INGEGNERIA CHIMICA

POLITECNICO DI MILANO

Conceptual Design of Chemical Plants by Multi-Objective Optimization of Economic and Environmental Criteria

Relatore: Prof. Davide MANCA

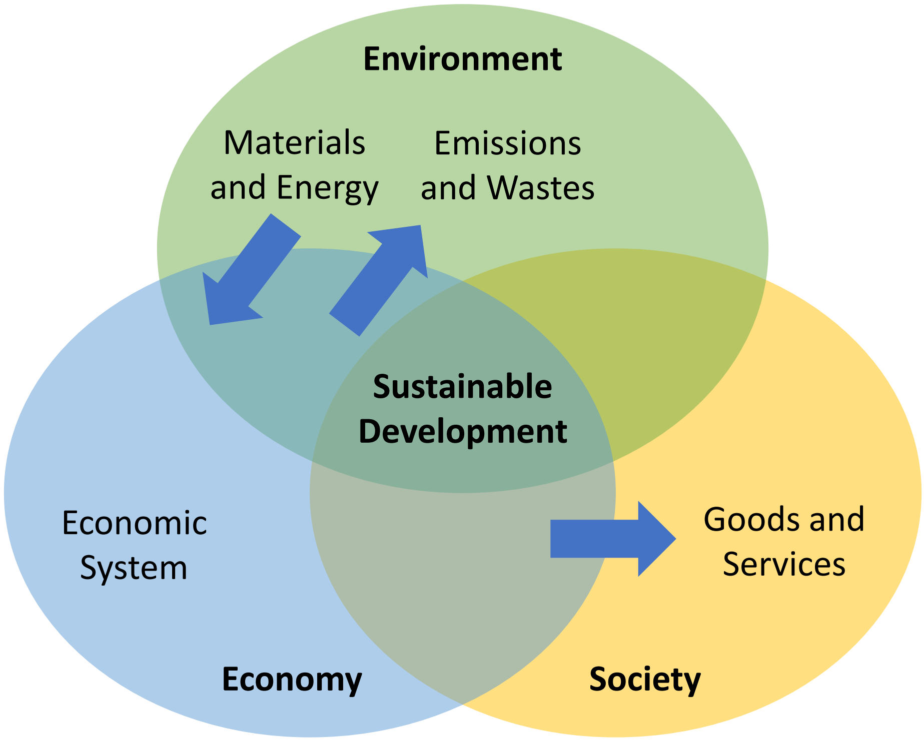
Tesi di
Piernico SEPIACCI matr. 837275

Anno Accademico 2015-2016

Definition of sustainability

A **sustainable** product or process:

- constraints **resource consumption** and **waste generation** to an acceptable level;
- makes a positive contribution to the satisfaction of human needs;
- provides **enduring economic value** to the business enterprise.



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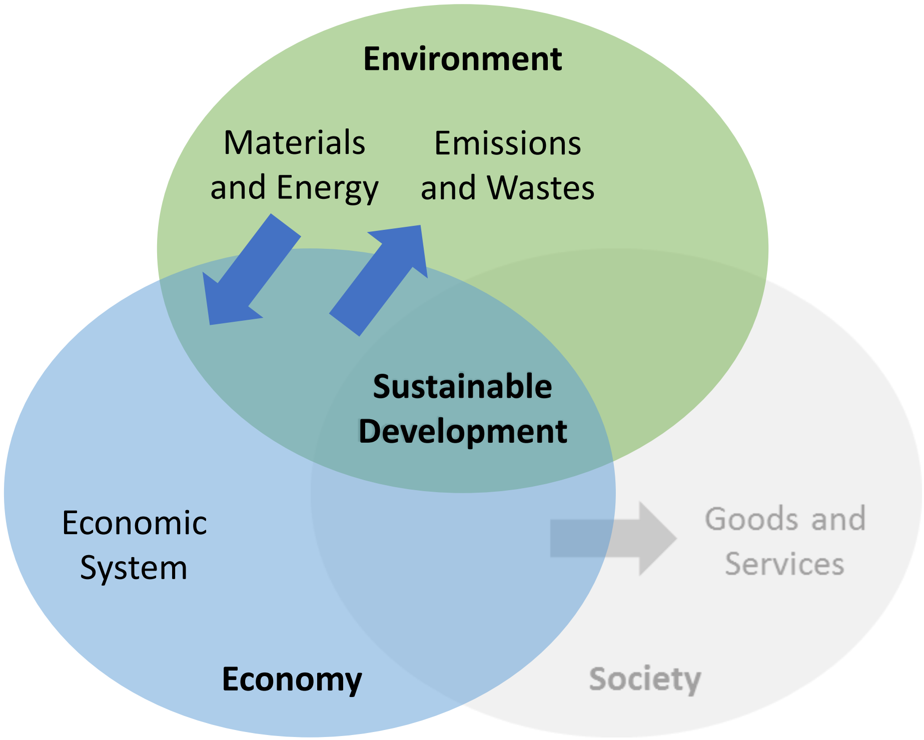
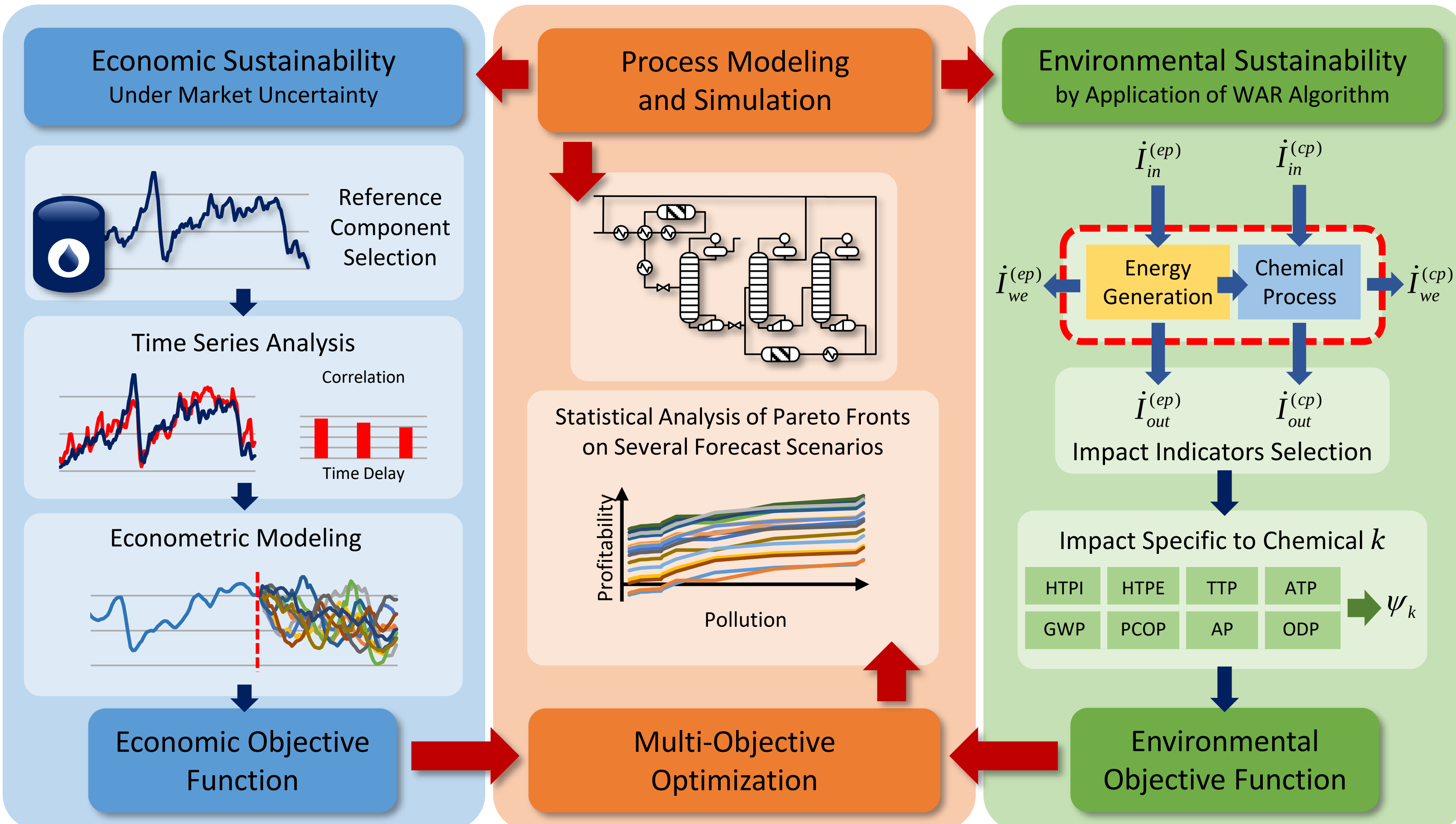
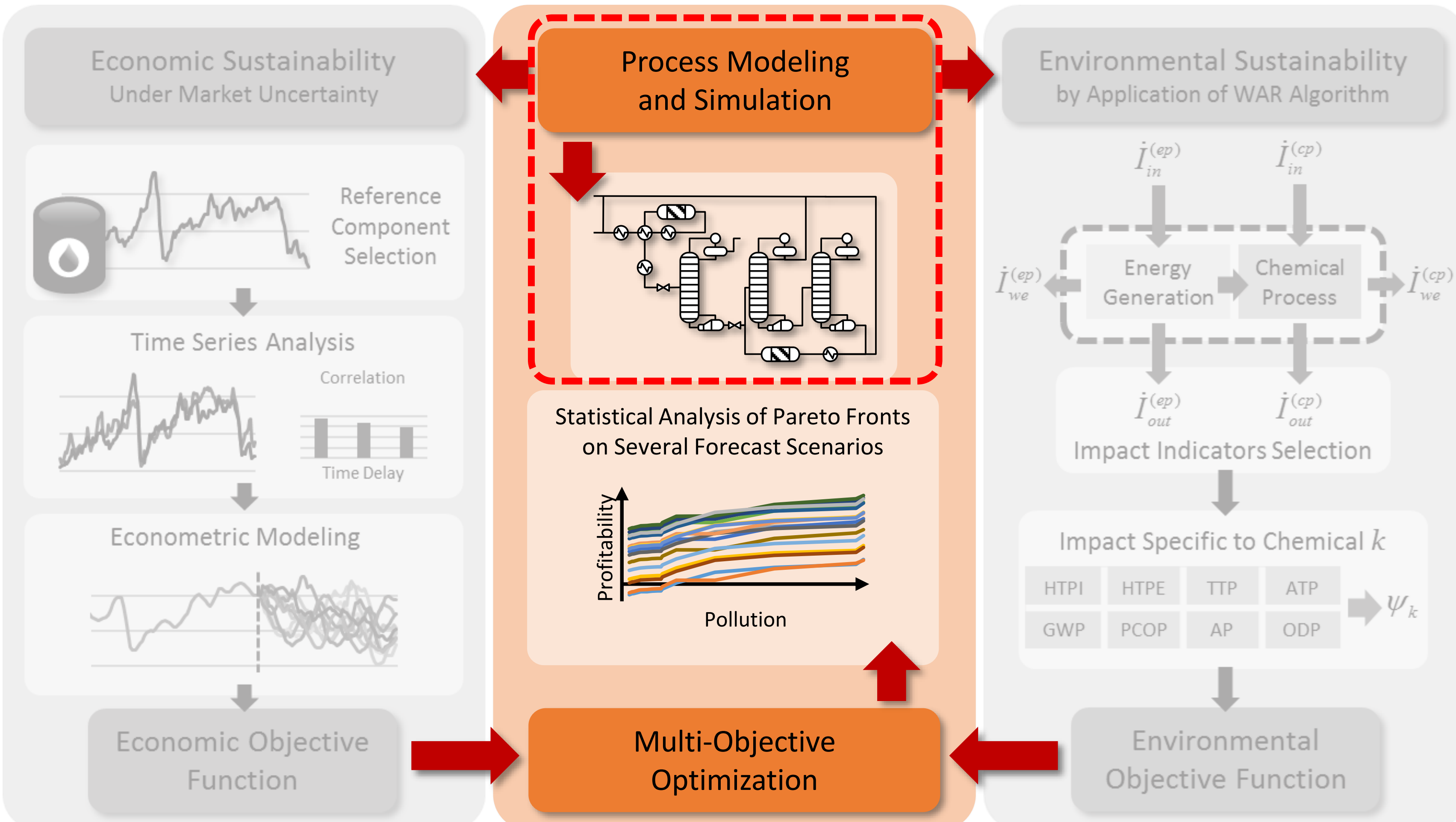


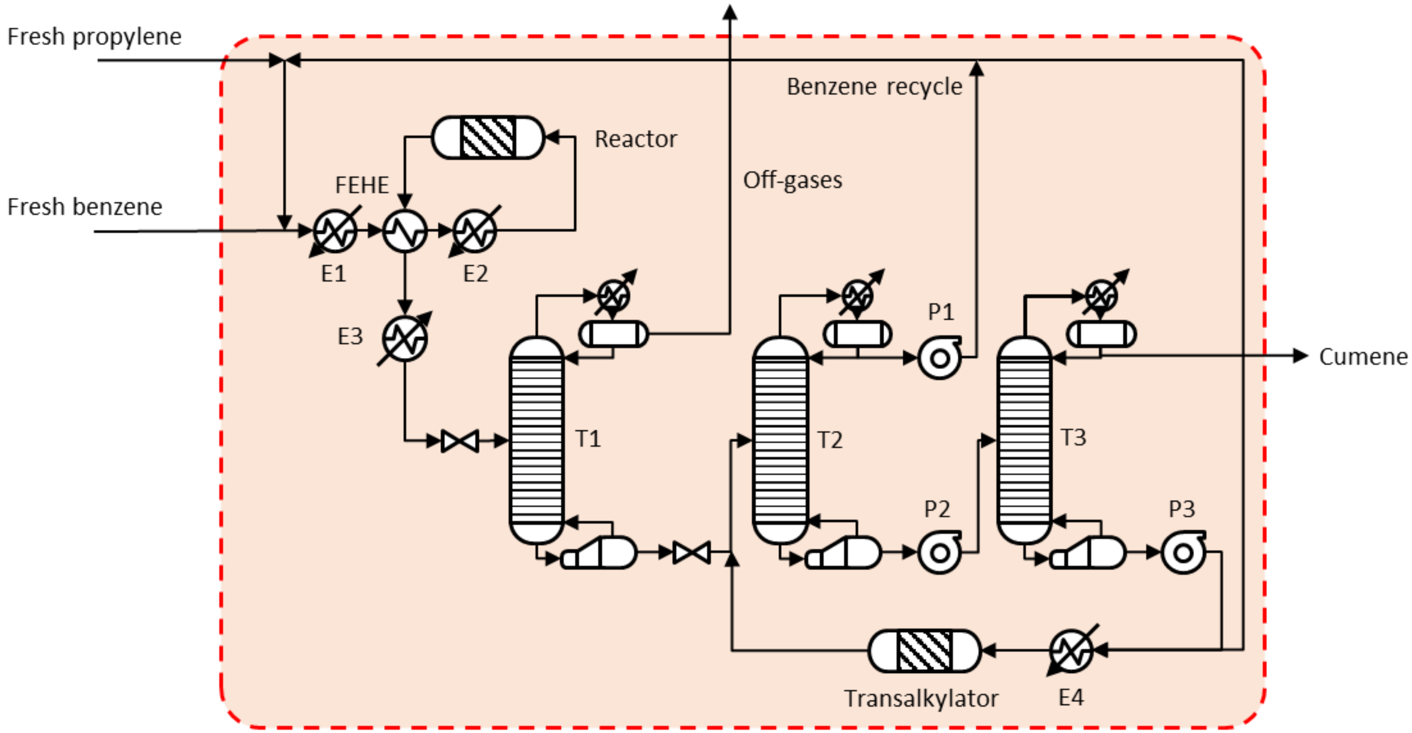
Structure of the work



Process modeling and simulation



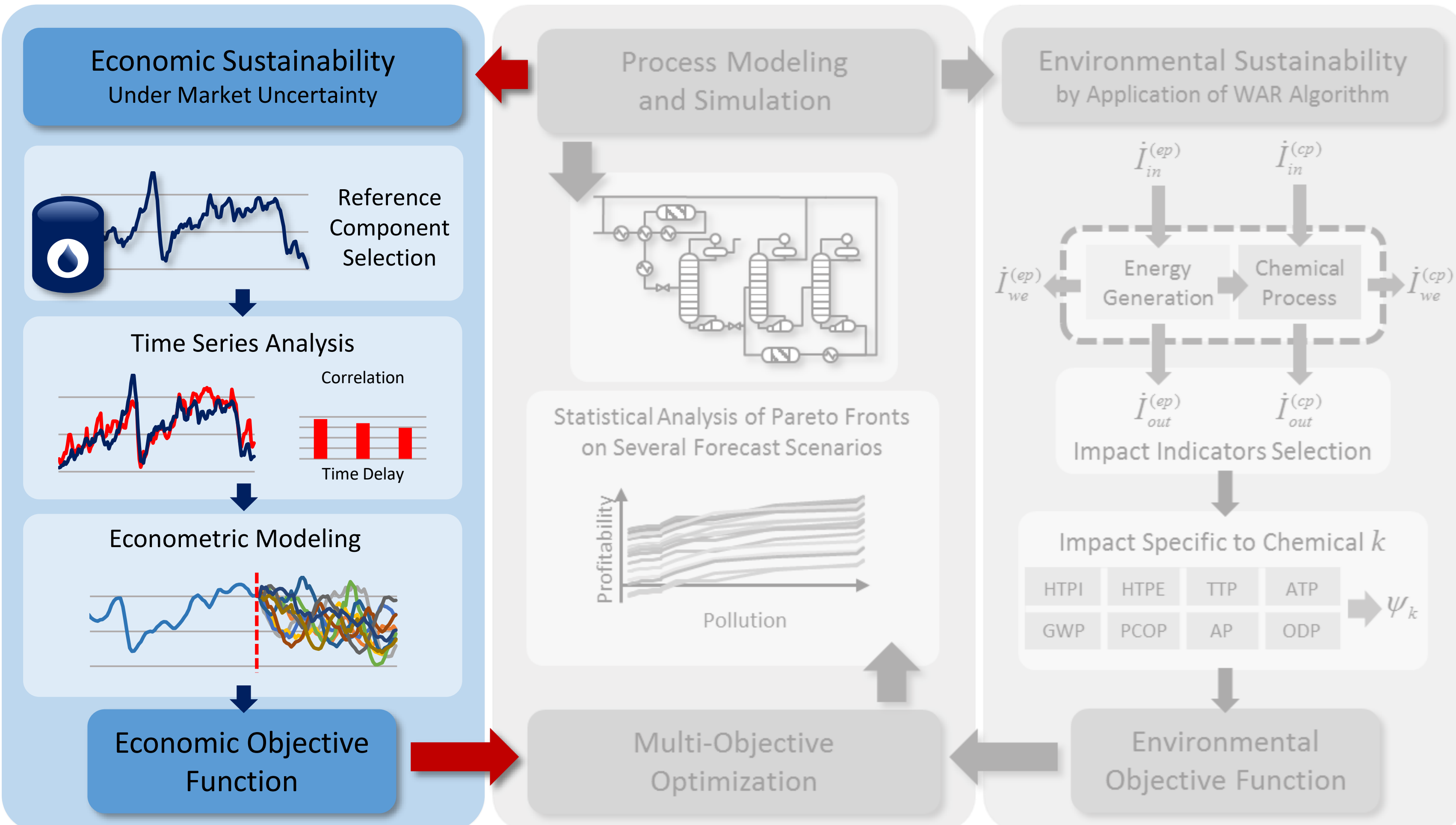
The cumene manufacturing process



Reactions		Kinetics
1) Cumene reaction	$C_3H_6 + C_6H_6 \rightarrow C_9H_{12}$	$r_1 = 2.8 \cdot 10^7 \exp\left[-104{,}181/(RT)\right] C_B C_P$
2) DIPB reaction	$C_3H_6 + C_9H_{12} \rightarrow C_{12}H_{18}$	$r_2 = 2.32 \cdot 10^9 \exp\left[-146{,}774/(RT)\right] C_C C_P$
3) Transalkylation	$C_{12}H_{18} + C_6H_6 \rightleftarrows 2C_9H_{12}$	$r_{3,f} = 2.529 \cdot 10^8 \exp\left[-100{,}000/(RT)\right] x_B x_D$ $r_{3,b} = 3.877 \cdot 10^9 \exp\left[-127{,}240/(RT)\right] x_C^2$

Pathak, A. S., Agarwal, S., Gera, V., & Kaistha, N. (2011). Design and control of a vapor-phase conventional process and reactive distillation process for cumene production. *Industrial & Engineering Chemistry Research*, 50(6), 3312-3326.

Economic sustainability



Conceptual design

The feasibility assessment of chemical plants traditionally follows the economic guidelines suggested in the ***Conceptual Design of Chemical Processes*** by **Douglas** (1988).

Hierarchy of decisions

1. Batch vs. Continuous;

2. Input-Output Structure of the flowsheet;

$$EP2 = (Product\ Price) - (Raw\ Materials\ Cost)$$

3. Recycle structure of the flowsheet;

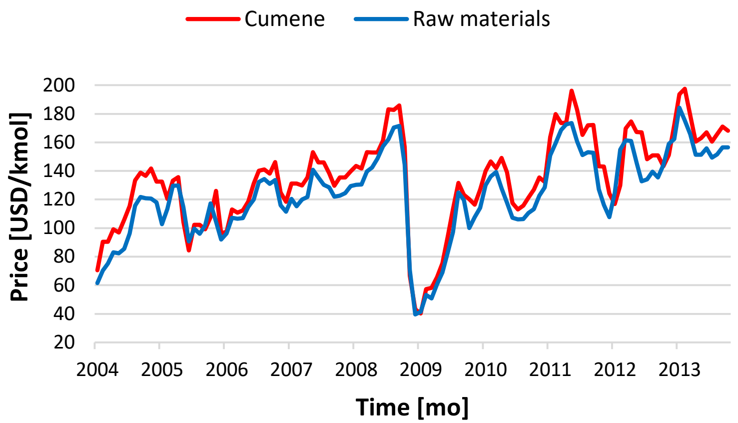
$$EP3 = EP2 - Reactor\ Cost\ (CAPEX + OPEX)$$

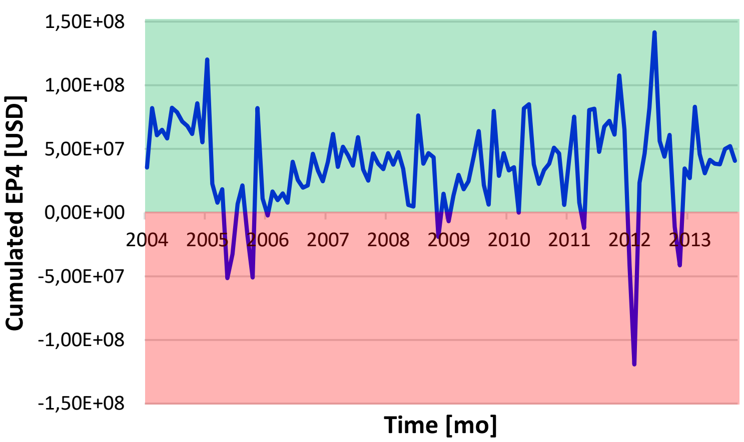
4. General structure of the separation system;

$$EP4 = EP3 - Separation\ Cost\ (CAPEX + OPEX)$$

$$Cumulated\ EP4 = \sum_{t=1}^{nMonths} EP4_t = nMonths \cdot EP4$$

5. Heat exchanger networks.





Methodology

1. Selection of a suitable **reference component**, which must be:

   - chosen according to the **market field** of the chemical plant;
   - a **key component** for either the process or the sector where the plant operates.

   For the **O&G sector** and **petrochemical industry**, a good candidate for the reference component is **crude oil**.

2. Definition of the **sampling time** and **time horizon** of the economic assessment;

3. Identification of an **econometric model** for the **reference component**;

4. Identification of an econometric model for the **raw materials** and **(by)products**;

5. Identification of an econometric model for the **utilities**;

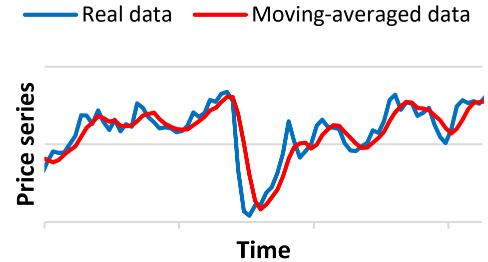
6. Use of the identified econometric models to determine the economic impact of the designed plant in terms of **Dynamic Economic Potentials** (**DEPs**).

Time series analysis

Use of moving-averaged values

Moving average allows eliminating most of the high-frequency fluctuations and catching the price trend.

$$m = \frac{1}{n}\sum_{i=0}^{n-1} Y_{t-1}$$

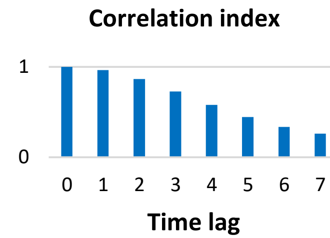


(Auto)correlation analysis

(Auto)correlograms report the (auto)correlation index of the time series X and Y based on the time lag between them.

$$\operatorname{corr}\left(Y_t, Y_{t-j}\right) = \frac{\operatorname{cov}\left(Y_t, Y_{t-j}\right)}{\sqrt{\operatorname{var}\left(Y_t\right)\operatorname{var}\left(Y_{t-j}\right)}}$$

$$\operatorname{corr}\left(X, Y\right) = \frac{\operatorname{cov}\left(X, Y\right)}{\sqrt{\operatorname{var}\left(X\right)\operatorname{var}\left(Y\right)}}$$



Identification of the candidate econometric model

Autoregressive model

$$X_t = a_0 + a_1 X_{t-1} + a_2 X_{t-2} + \ldots + a_q X_{t-q}$$

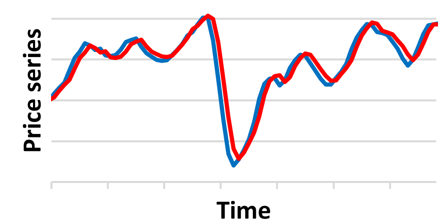
Autoregressive Distributed Lag model

$$Y_t = a_0 + a_1 X_{t-1} + a_2 X_{t-2} + \ldots + a_q X_{t-q} + b_1 Y_{t-1} + b_2 Y_{t-2} + \ldots + b_p Y_{t-p}$$

Evaluation of the adaptive parameters

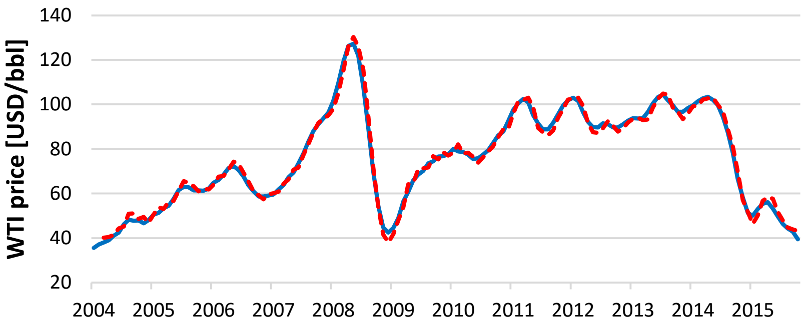
It requires a linear regression procedure that minimizes the sum of square errors between real and model prices.

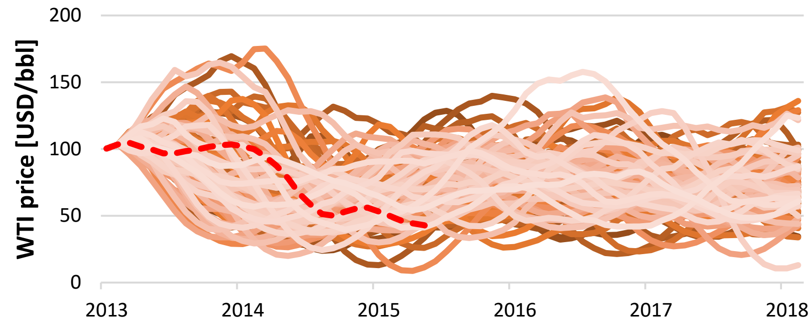
$$\min_{a,b} \sum_{t=1}^{nMonths} \left(\bar{Y}_t - Y_t\right)^2$$



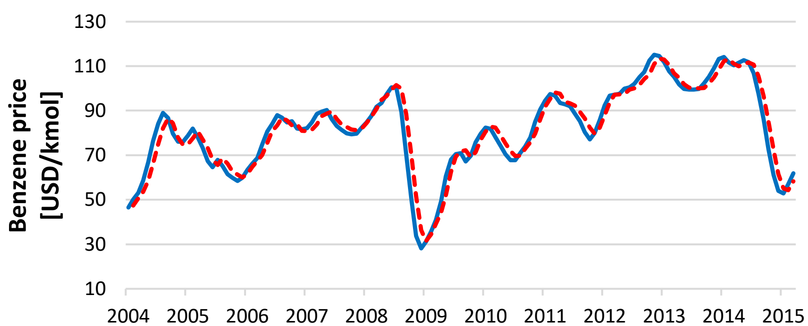
Econometric models

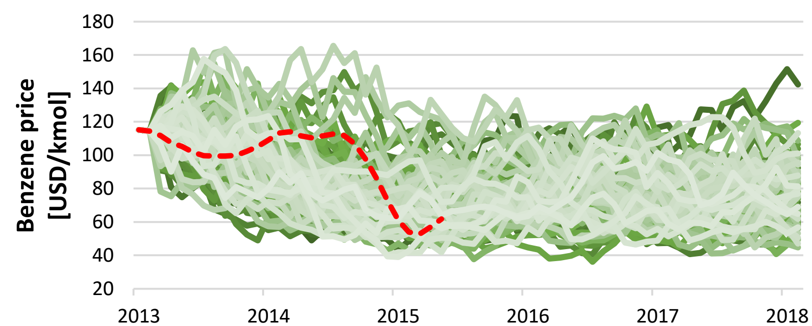
$$P_{Crude\ Oil,t} = \left(a_0 + a_1 P_{Crude\ Oil,t-1} + a_2 P_{Crude\ Oil,t-2}\right)\left(1 + RAND \cdot \sigma_{Crude\ Oil} + \bar{X}_{Crude\ Oil}\right)$$





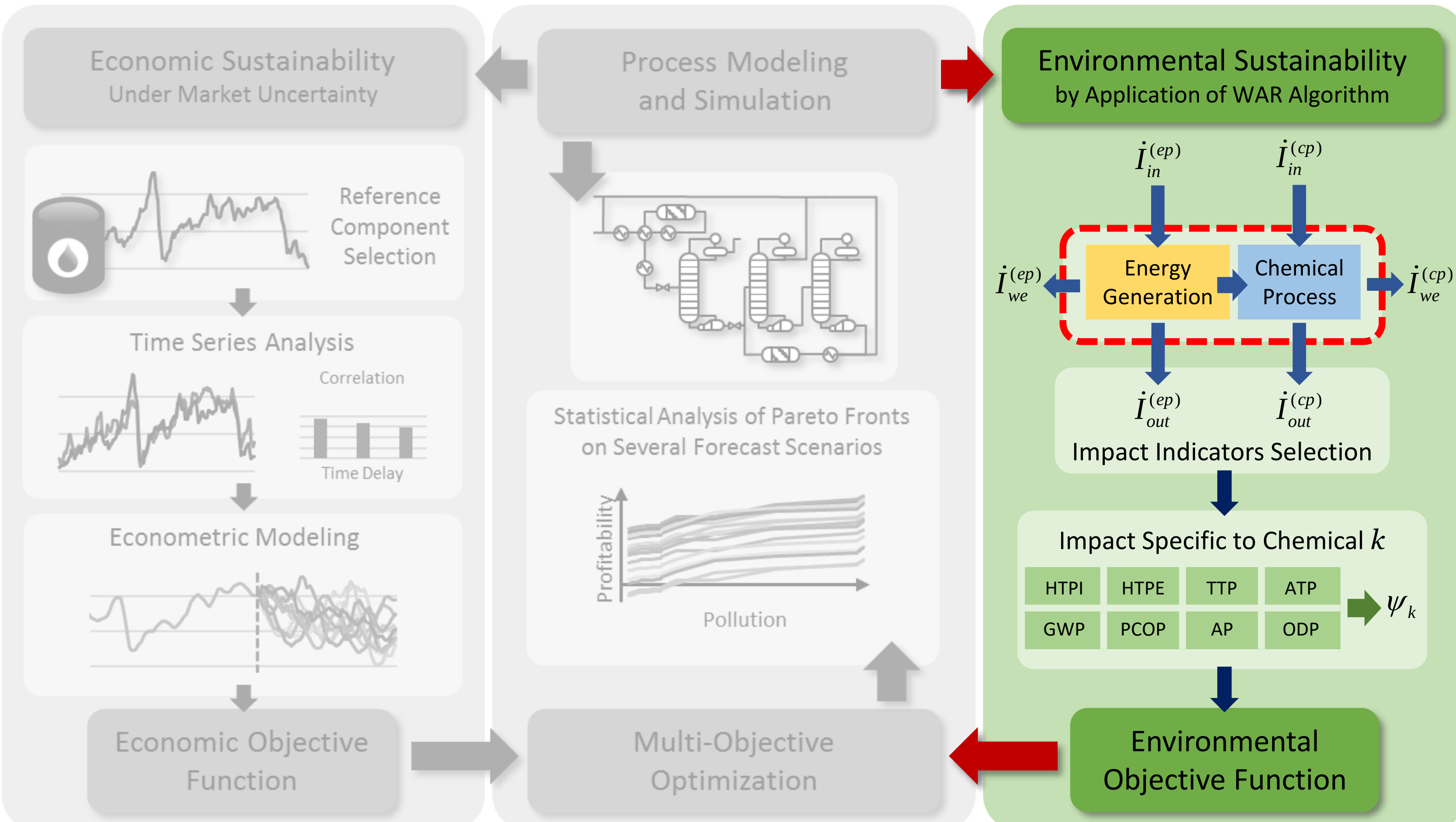
$$P_{Benzene,t} = \left(a_0 + a_1 P_{Crude\ Oil,t} + b_1 P_{Benzene,t-1}\right)\left(1 + RAND \cdot \sigma_{Benzene} + \bar{X}_{Benzene}\right)$$





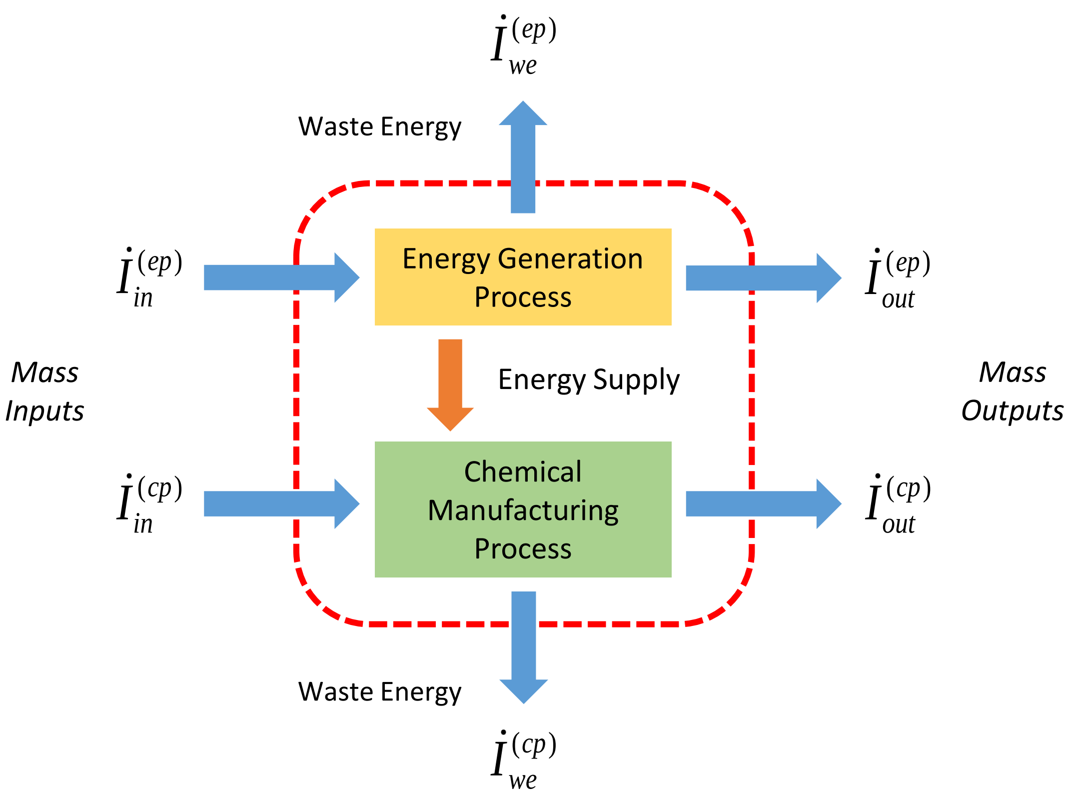
Commodity	a_0	a_1	b_1	$\bar{R}^2$	σ	$\bar{X}$
Crude oil	3.3207	1.8286	-	98.13%	0.0313	−0.0028
Benzene	2.6984	0.0754	0,9012	94.07%	0.0843	−0.0098

Environmental sustainability



The Waste Reduction algorithm

The **Waste Reduction** (**WAR**) **algorithm** is a tool to determine the **potential environmental impact** (**PEI**) of a chemical process.



Total rate of PEI output

$$\dot{I}_{out}^{(tot)} = \dot{I}_{out}^{(cp)} + \dot{I}_{out}^{(ep)}$$

PEI output from the chemical process

$$\dot{I}_{out}^{(cp)} = \sum_{j}^{cp} \dot{M}_j^{(out)} \sum_k x_{kj} \psi_k$$

Where:

- $M_j^{(out)}$ is the output mass flow rate of stream j;
- x_{kj} is the mass fraction of chemical k in stream j.

PEI output from the energy generation

$$\dot{I}_{out}^{(ep)} = \sum_{j}^{ep\text{-}g} \dot{M}_j^{(out)} \sum_k x_{kj} \psi_k$$

Overall PEI for chemical *k*

ψ_k ?

The Waste Reduction algorithm

Overall PEI for chemical *k*

$$\psi_k = \sum_l \alpha_l \psi_{kl}^s$$

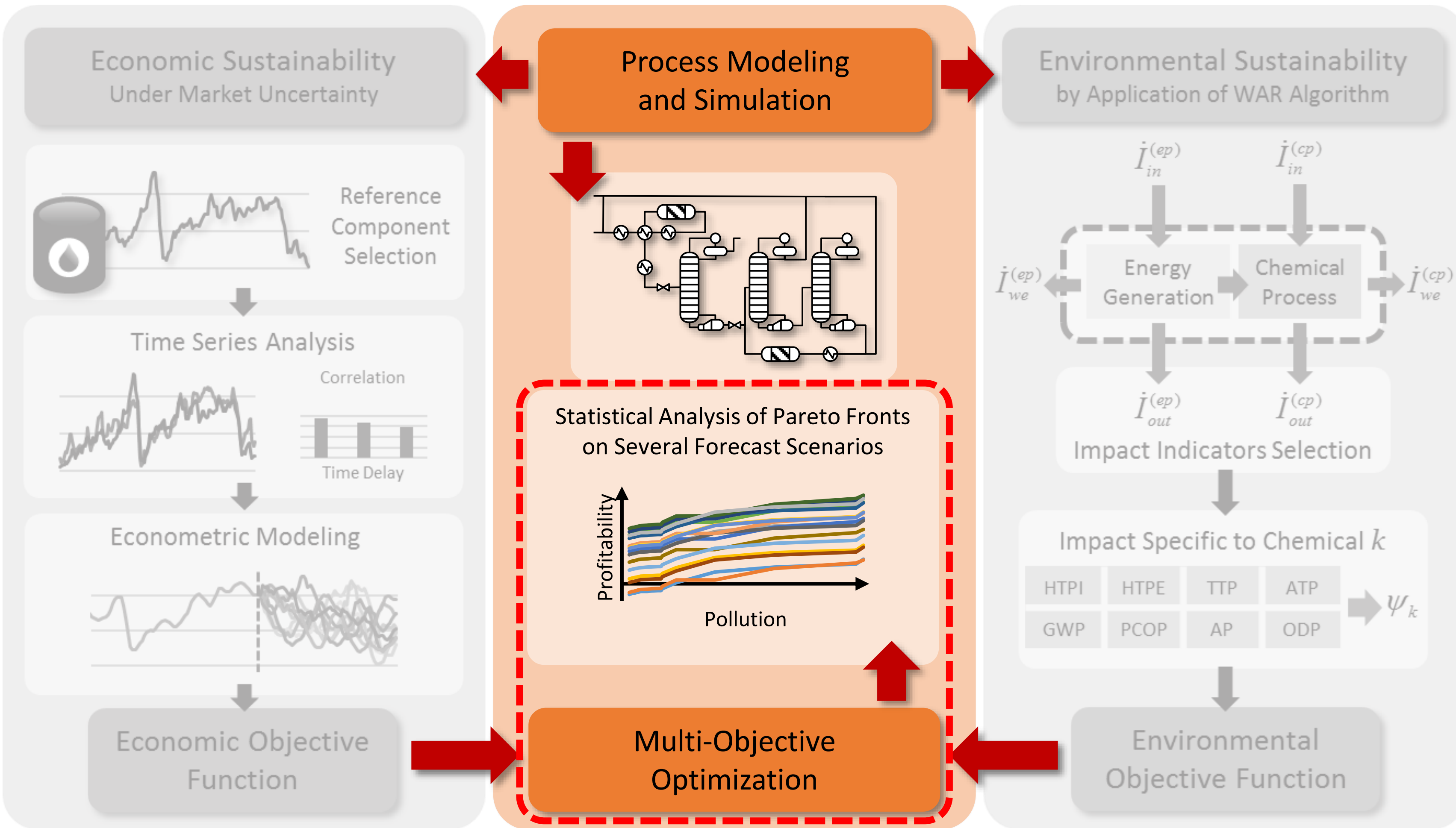
Where:

- ψ_{kl}^s is the specific PEI of chemical k for the impact category l;
- α_l is the weighing factor of the impact category l.

General impact category	Impact category	Measure of impact category
Human toxicity	Ingestion	LD_{50}
	Inhalation/dermal	OSHA PEL
Ecological toxicity	Aquatic toxicity	Fathead minnow LC_{50}
	Terrestrial toxicity	LD_{50}
Global atmospheric impacts	Global warming potential	GWP
	Ozone depletion potential	ODP
Regional atmospheric impacts	Acidification potential	AP
	Photochemical oxidation potential	PCOP

Chemical	Mass flow [kg/h]	ψ_k [PEI/kg]	$\dot{I}_{out,k}^{(tot)}$ [PEI/h]
Benzene	22.537	0.837	18.863
Propylene	53.473	3.838	205.251
Propane	232.293	0.155	36.010
Cumene	12.682	1.196	15.164
DIPB	0.001	7.898	0.010
NO_2	3.624	2.483	8.999
CO	1.594	0.305	0.486
CO_2	2275.783	0.001	2.387
SO_2	0.012	0.719	0.008
Methane	0.045	0.472	0.021

Multi-objective optimization



Multi-objective optimization

General formulation:

$$\underset{\mathbf{x}}{Optimize} \quad \boldsymbol{F}(\mathbf{x}) = \left[F_1(\mathbf{x}), F_2(\mathbf{x}), \ldots, F_n(\mathbf{x})\right]$$

$$s.t. \quad h_j(\mathbf{x}) = 0 \qquad j = 1, 2, \ldots, n_e$$

$$g_j(\mathbf{x}) \leq 0 \qquad j = 1, 2, \ldots, n_i$$

$$\mathbf{x}_l < \mathbf{x} < \mathbf{x}_u$$

Objective functions:

$$Cumulated\ DEP4_k = \sum_{t=1}^{nMonths} DEP4_{t,k} \quad k = 1, \ldots, nScenarios$$

To be maximized

$$Cumulated\ PEI = \dot{I}_{out}^{(tot)} \cdot nHpM \cdot nMonths$$

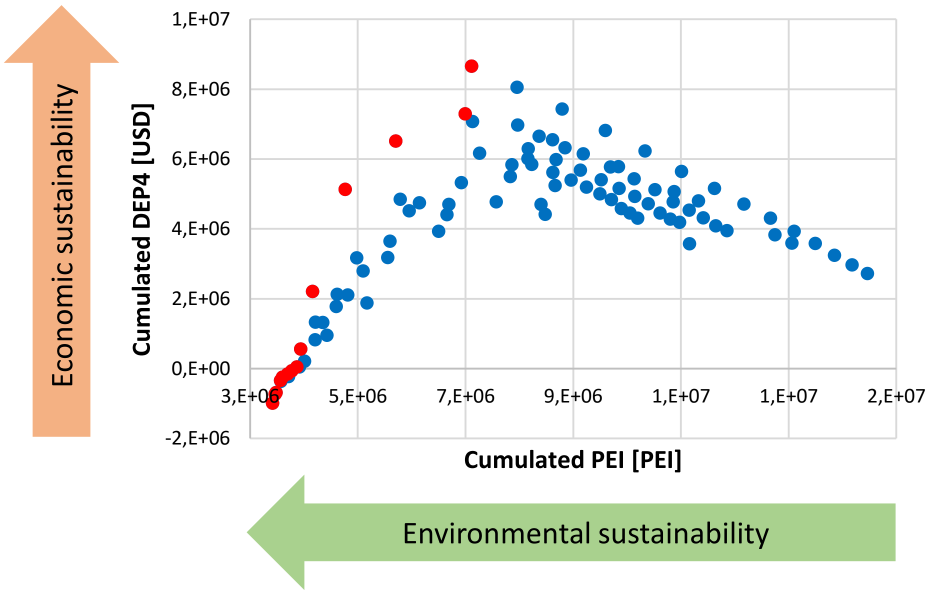
To be minimized

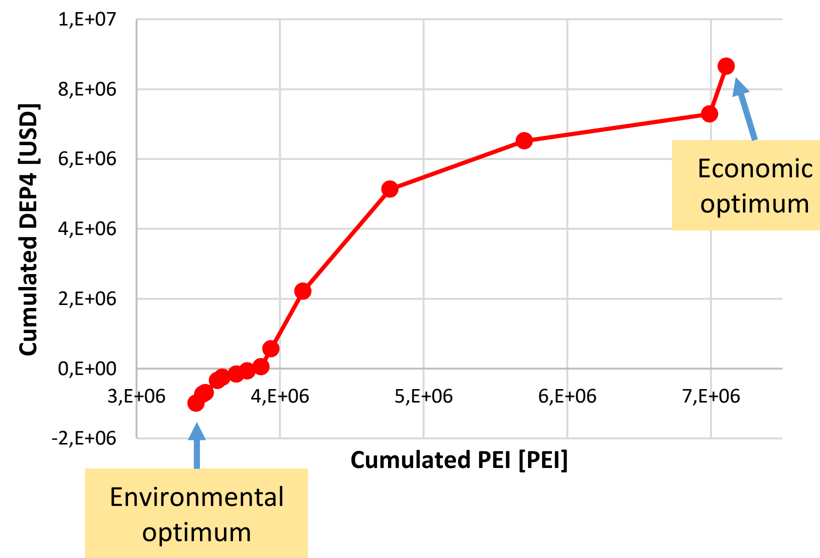
Optimization algorithm: grid-search method.

Design variable	Lower bound	Upper bound	Step size	Steps number
Reactor length [m]	4	10	1	7
Inlet temperature [°C]	300	390	5	19

Pareto optimal solutions

These plots show the non-Pareto and **Pareto optimal solutions** for an **arbitrarily chosen economic scenario**. Each solution corresponds to a discrete point of the grid-search domain, *i.e.* a plant configuration.

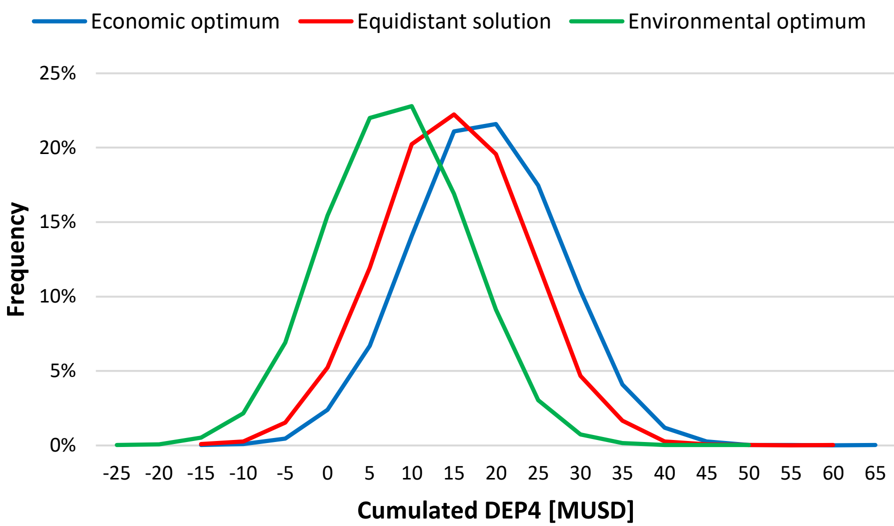


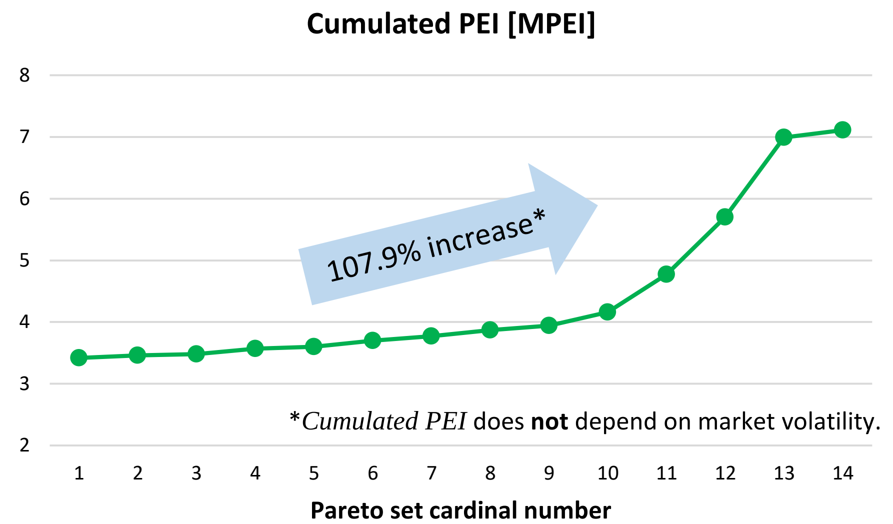


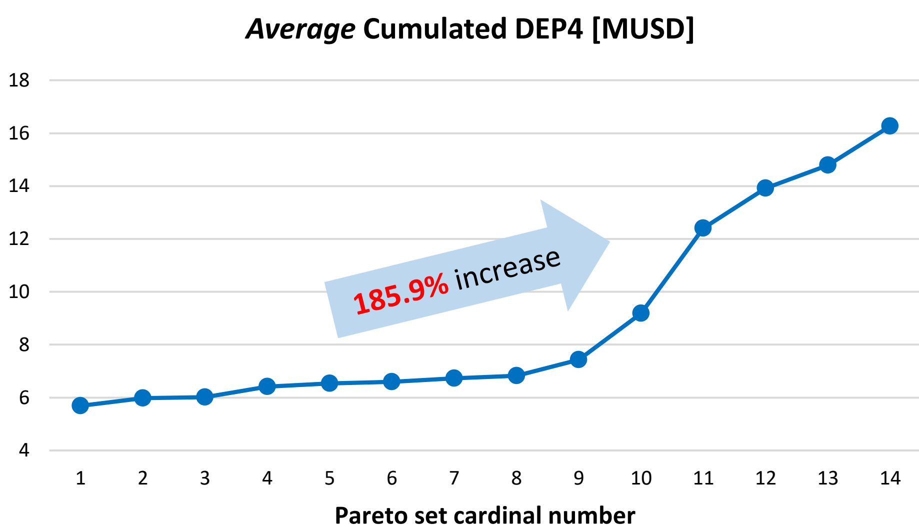
Configuration	Inlet temperature [°C]	Reactor length [m]	*Cumulated* $DEP4_k$ [MUSD]	*Cumulated PEI* [MPEI]
Economic optimum	365	7	8.66	7.11
Environmental optimum	390	10	−0.99	3.42
Equidistant solution	385	5	5.13	4.77

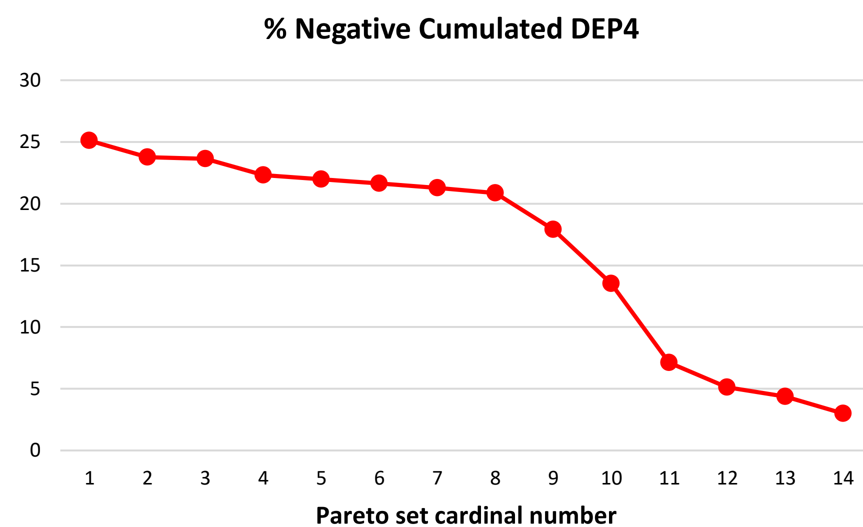
As **reactor length** and **inlet temperature increase**, propylene conversion increases, thus the total rate of PEI output decreases. At the same time, capital and energy costs increase, and selectivity decreases.

Pareto optimal solutions over 3000 scenarios









Conclusions and future developments

Conclusions

- The economic sustainability of the cumene plant is heavily conditioned by the **fluctuations of commodity and utility prices**.
- The **WAR algorithm** can be used in conjunction with **PCD** to achieve both environmental and economic sustainability.
- Whenever a modification is proposed to improve the environmental friendliness of a process, it is useful to question its **economic viability under market uncertainty**.

Future developments

- It will be worth considering new processes based on **a higher number of design variables** to make the optimization procedure more compliant with real plants.
- A further development could be **expanding the boundaries of the study** to include the upstream and downstream activities related to the main process.
- As far as the social attribute of sustainability is concerned, it will be worth developing practical ways to measure **social sustainability** for both **single-site** (*e.g.*, process synthesis) and **multi-site applications** (*i.e.* SCM/EWO).

Thank you for your attention