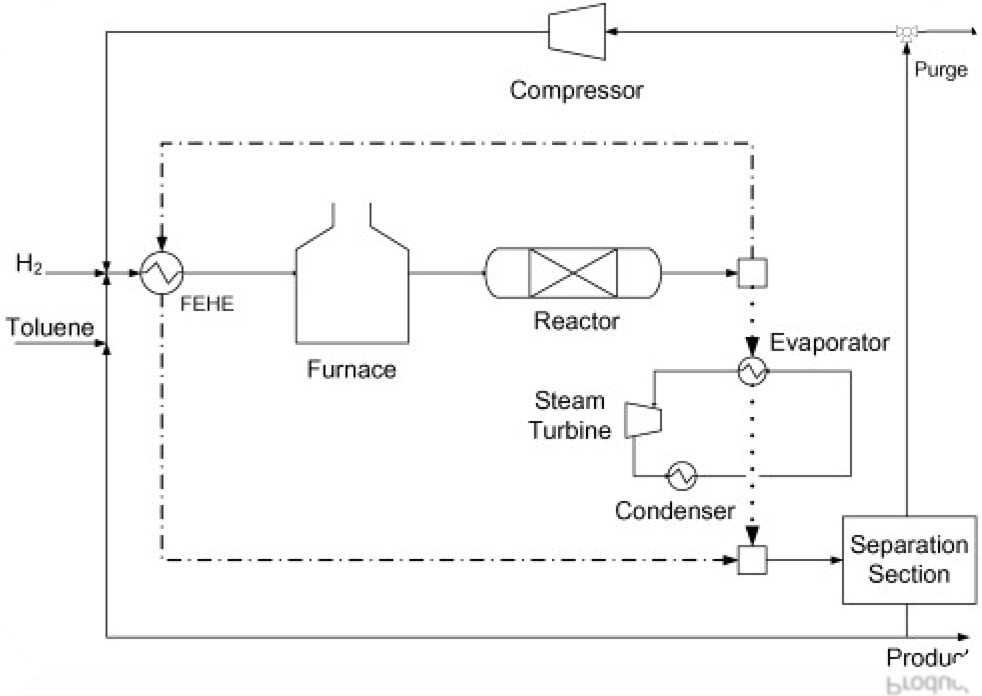

Dynamic Conceptual Design

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Lesson 3 of "Process Systems Engineering" – Master Degree in Chemical Engineering – Politecnico di Milano

Feasibility study of industrial processes

- The feasibility study of industrial processes calls for the economic assessment of both CAPEX and OPEX terms.
- This happens for both **green-field** and **brown-field** projects.

- **FEASIBILITY STUDY = CAPEX + OPEX**

The term **greenfield** was originally used in construction and development to reference land that has never been used, where there was no need to demolish or rebuild any existing structures. Today, the term greenfield project is used in many industries, where it means to start a project without the need to consider any prior work.
The term **brownfield** was originally used in construction and development to reference land that at some point was occupied by a permanent structure. In a brownfield project the structure would need to be demolished or renovated. Today, the term brownfield project is used in many industries to mean to start a project based on prior work or to rebuild a product from an existing one.

www.webopedia.com

CAPEX terms

Feasibility study of industrial processes

- **CAPEX** terms are evaluated during the design phase by:
  - updating previous quotations of similar pieces of equipment by means of suitable **cost indexes**.
  - evaluating the investment/installation cost of a process unit with the **Guthrie's formulae** (if no other proprietary methods/data are available).

Cost indexes

The **cost index** is a number that allows determining the value of a piece of equipment at a given time compared to that of the same unit at a reference time.

$$\text{Current Cost} = \text{Original Cost}\left(\frac{\text{Cost Index}_{\text{Current}}}{\text{Cost Index}_{\text{Original}}}\right)$$

Cost indexes are used to perform an **estimate** of the actual cost of a piece of equipment if one knows the cost of that same unit quoted in the past.

N.B.: it is not recommended to make use of cost indexes when the time interval between quotations is longer than 10 years.

N.B.: the cost index can also be used to **extrapolate** the present value of a piece of equipment or of a whole plant in the near future (*i.e.* for a maximum of 2-3 years; for instance when the equipment will be bought respect to available quotation at design time).

Cost indexes

The most used cost indexes in the process industry are:

Marshall & Swift (M&S): (base 100 in 1926)

- *All industries*
- *Process Industry*

Chemical Engineering (CEPCI): *Plant cost index* (base 100 in 1959)

Nelson-Farrar: *Refinery (inflation) index* (base 100 in 1946)

Vatavuk (VAPCCI): *Air pollution Control* (base 100 in 1994)

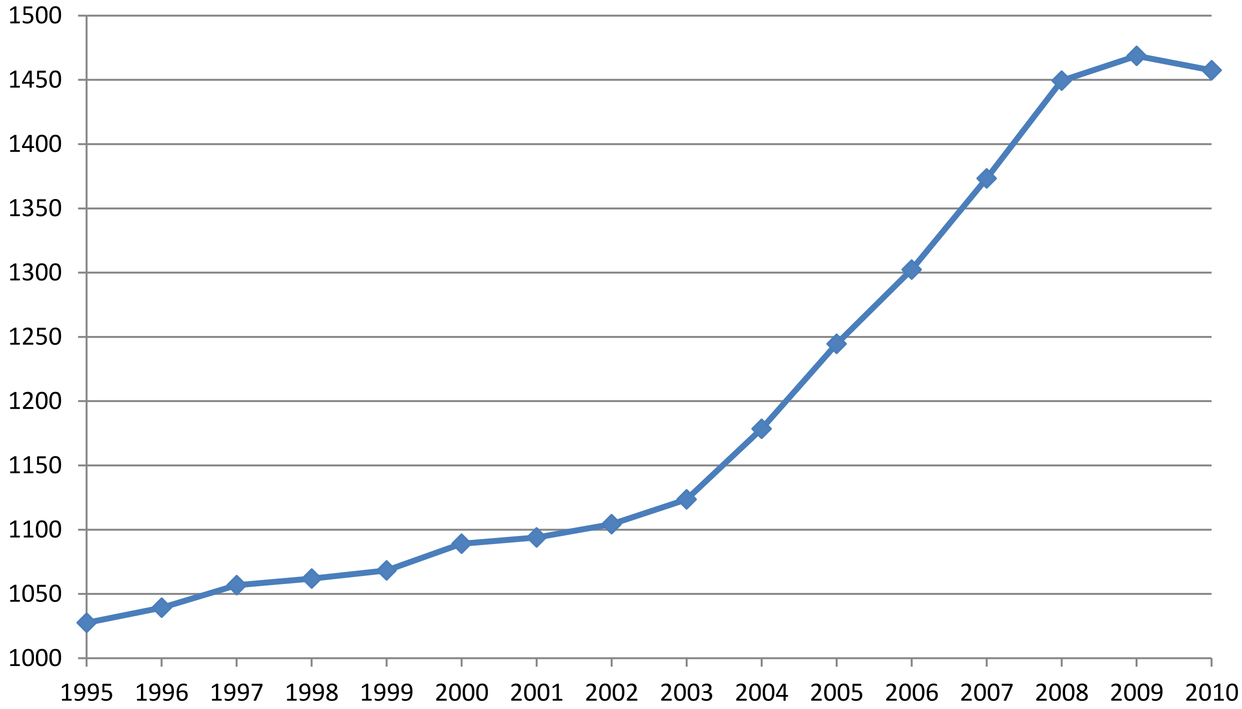
Cost indexes

	Marshall and Swift Equipment Cost Index		Nelson-Farrar Refinery (inflation) index	Chemical Engineering Plant Cost Index (CEPCI)
Year	All Industries	Process Industry		
1995	1027.5	1029.0	1392.1	381.1
1996	1039.2	1048.5	1418.9	381.7
1997	1056.8	1063.7	1449.2	386.5
1998	1061.9	1077.1	1477.6	389.5
1999	1068.3	1081.9	1497.2	390.6
2000	1089.0	1097.7	1542.7	394.1
2001	1093.9	1106.9	1579.7	394.3
2002	1104.2	1116.9	1642.2	395.6
2003	1123.6		1710.4	402.0
2004	1178.5		1833.6	444.2
2005	1244.5		1918.8	468.2
2006	1302.3		2008.1	499.6
2007	1373.3		2251.4	525.4
2008	1449.3		n.a.	575.4
2009	1468.6		2217.7	521.9
2010	1457.4		2337.6	550.8
2011			2435.6	585.7
2012				584.6

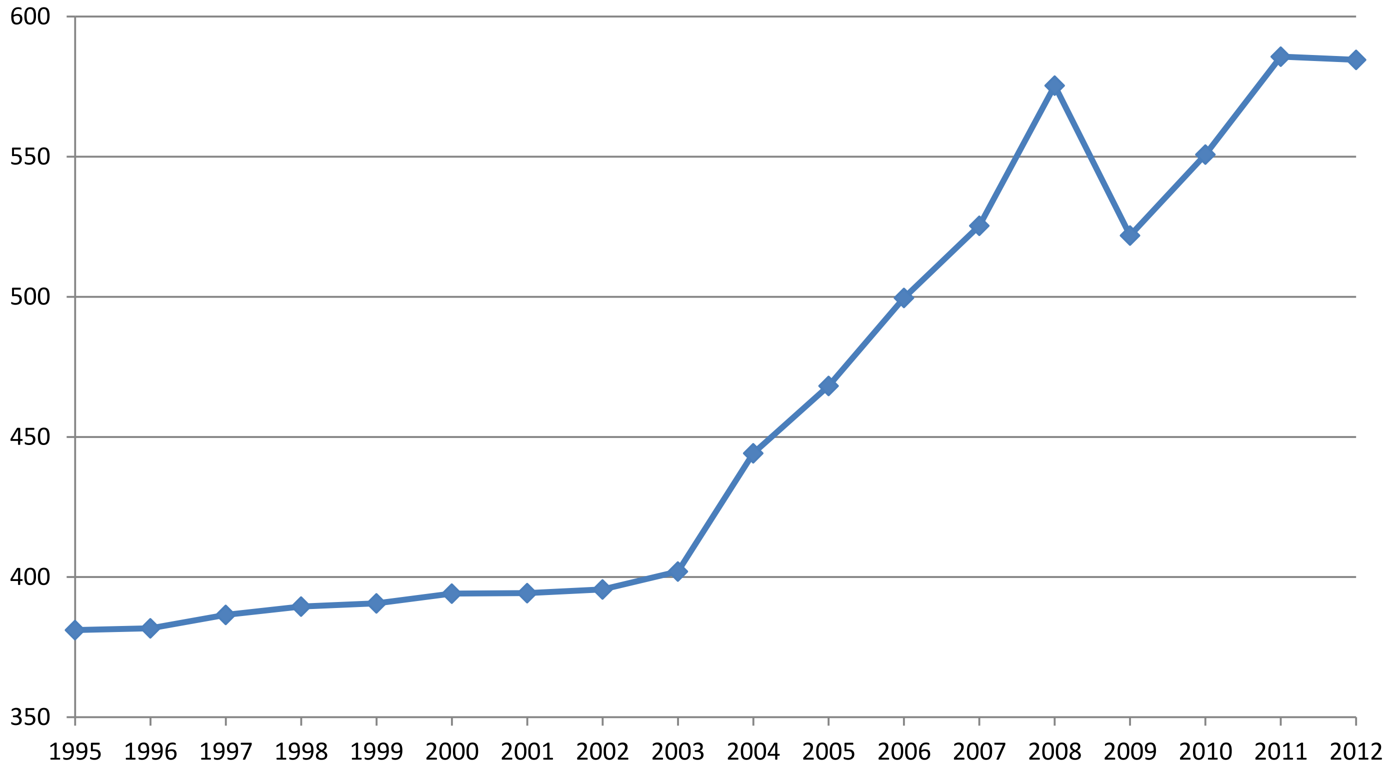
Plant Design and Economics for Chemical Engineers, M. S. Peters, K. D. Timmerhaus, R. E. West, Mc Graw Hill, 2003

Oil&Gas Journal, 2014 – www.ogj.com

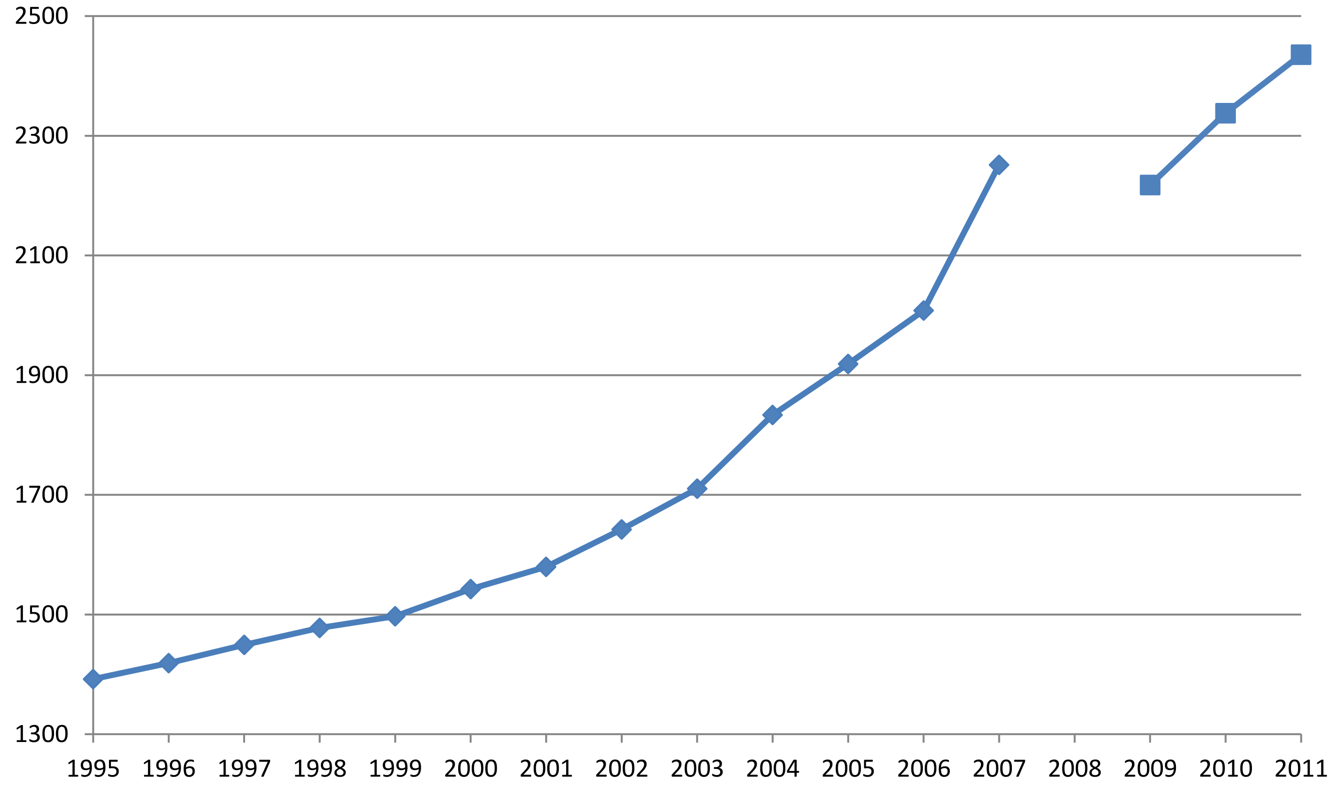
Marshall and Swift – Equipment Cost Index



Chemical Engineering – Plant Cost Index (CEPCI)



Nelson-Farrar – Refinery (inflation) index



Guthrie's formulae

- Guthrie's formulae allow evaluating the cost of either investment or installation of several process units by non-linearly regressed economic data referred to specific **categories** of equipment and on some **characteristic dimensions** of the process units. They take into account also the **material** and the **operating conditions** of the equipment to be quoted. The general formulation is:

$$CE_{inv/inst} = a \frac{M\,\&\,S}{280} L_1^b L_2^c d_1 d_2$$

- For instance:

$$C_{comp_{Inst}} = 517.5 \cdot \left(\frac{M\,\&\,S}{280} \right) \cdot W^{0.82} \left(2.11 + F_C \right)$$

$$C_{rec_{Inst}} = 101.3 \cdot \left(\frac{M\,\&\,S}{280} \right) \cdot A^{0.65} \left(2.29 + F_C \right)$$

Guthrie's formulae

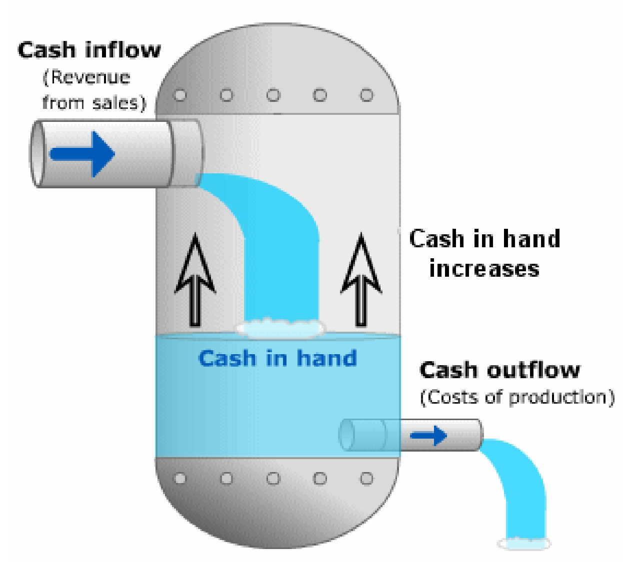
- Given the Guthrie's formula: $CE_{inv/inst} = a \frac{M\&S}{280} L_1^b L_2^c d_1 d_2$

- We have:
  - CE is the Equipment cost (either <u>inv</u>estment or <u>inst</u>allation).
    Actually, a constant varies according to the economic assessment
  - a is a suitable constant whose value allowed determining the real cost of the equipment when the formula was proposed in 1969 by Guthrie.
  - $M\&S$ is the Marshall and Swift index at present time
  - 280 was the Marshall and Swift index in 1969
  - L_1 and L_2 are two characteristic dimensions of the equipment (L_2 can also be missing)
  - d_1 is an expression that usually takes into account the working pressure
  - d_2 is an expression that takes into account the building material

OPEX terms

Feasibility study of industrial processes

- The economic evaluation of plant design/retrofitting/revamping is based on the **discounted back** concept where the **net present value** plays a major role.
- **Net Present Value**, NPV, can be described as the “difference amount” between the sums of discounted cash inflows and cash outflows. It compares the present value of money today to the present value of money in the future, taking inflation and returns into account.
- The NPV of a sequence of cash flows takes as input the cash flows and a discount rate or discount curve and outputs a price.
- Each cash inflow/outflow is discounted back to its present value, PV.



Feasibility study of industrial processes

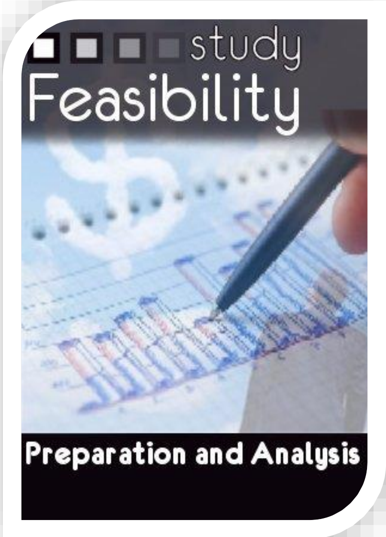
- Therefore NPV is the sum of all terms:

$$NPV = \sum_{t=1}^{NT} \frac{R_t}{(1+i)^t}$$

- Where:
  - t is the time of the cash flow
  - i is the discount rate (for industrial applications is the rate of return) that could be earned on an investment in the financial markets with similar risk
  - R_t is the net cash flow (the amount of cash, inflow minus outflow) at time t
  - NT is the total number of periods

Feasibility study of industrial processes

- To perform an efficient and straightforward feasibility study, **OPEX** terms are evaluated during the design phase by **assuming constant** the costs/prices of raw materials, products, utilities, and the like throughout the whole expected life of the plant (usually tens of years).
- Apparently, there are not any alternatives to quantify the OPEX terms but assuming their value constant and equal to the present value.
- This is a **significant problem** for the economic assessment of the feasibility study.



Feasibility study of industrial processes

- The steady state approach to the economic assessment of process design does not take into account the intrinsic variability of prices/costs due to:
  - Volatility of prices/costs
  - Market fluctuations
  - Demand modification
  - Financial fluctuations
  - Offer/demand oscillation
  - Climate change; Shortages; Overproduction; Seasonal/annual periodic variations; …
  - Natural disasters and anthropic events (*e.g.*, floods, earthquakes, wars, political and financial crises, …)

Feasibility study of industrial processes

QUESTION

Is there a methodology to take into account the dynamic features of OPEX terms?

Dynamic Conceptual Design

Methodology

1. Selection of a suitable **reference component**;
2. Definition of the **sampling time** and **time horizon** of the economic assessment;
3. Identification of an **econometric/economic/hybrid 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 econometric models to determine the economic impact of the designed plant in terms of **Dynamic Economic Potentials** (**DEPs**).

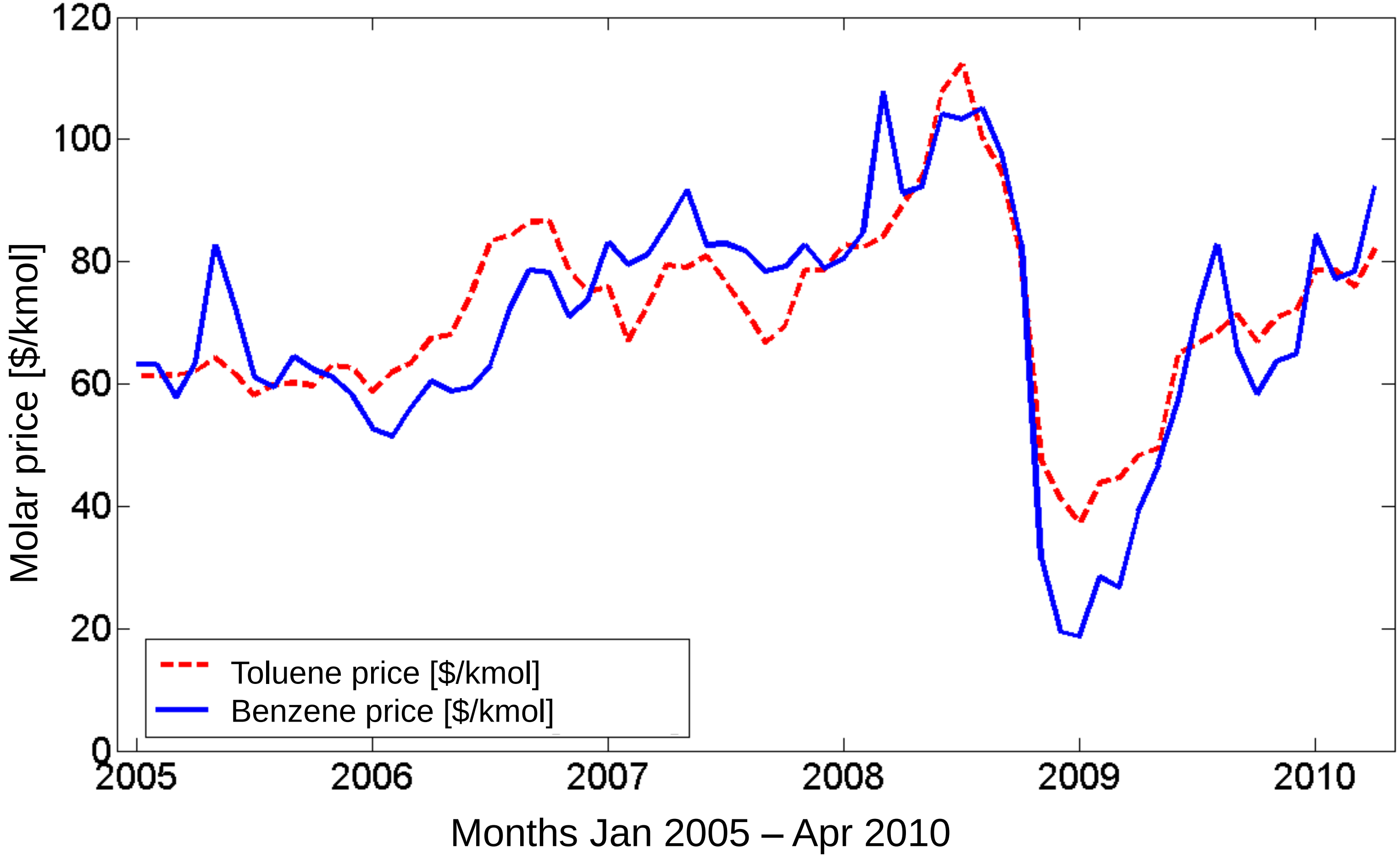
Price/cost of commodities

Modeling the price/cost of commodities

- **We focus on the price/cost of commodities**

- Specifically we consider the HDA process where toluene is *transformed* in benzene:
  - $C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$

Benzene vs Toluene price/cost



The HDA case-study

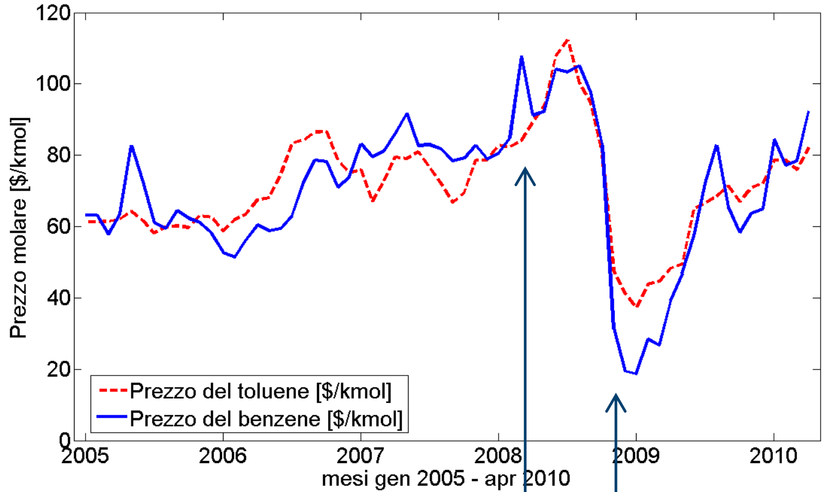
- **Ullmann's encyclopedia of Industrial Chemistry**: *"The amount of toluene in BTX from catalytic reformate is greater than that of benzene. Whether or not hydrodealkylation is used is related directly to the demand and price of benzene relative to toluene. If the relative demand for the two products changes, the dealkylation units may be placed on standby".*

- **Stefan Marcinowski**, BASF: "*The price of benzene has been extremely erratic compared with the prices of other petrochemical raw materials".*

- **Jenny Bouch**, Jacobs Consultancy London: *"The long-term average utilization rate of HDA plants has been around 40% because of the many occasions when the price of the toluene input was higher than that for the benzene output".*

Classic level-2 economic potential

$$EP2\left[\$/y\right] = \left\{ \sum_{p=1}^{NP} C_p \cdot F_p - \sum_{r=1}^{NR} C_r \cdot F_r \right\} \cdot nHoursPerYear$$



	Benzene price	Toluene cost	*EP*2
Average 2005-2010 period	70.16 $/kmol	72.19 $/kmol	**–2.0318 M$/y**
March 2008	107.79 $/kmol	84.18 $/kmol	**51.122 M$/y**
December 2008	19.41 $/kmol	41.17 $/kmol	**–40.589 M$/y**

- It is evident the call for a **dynamic approach** to the evaluation of the economic potential of the plant.

Dynamic economic potential of level-2

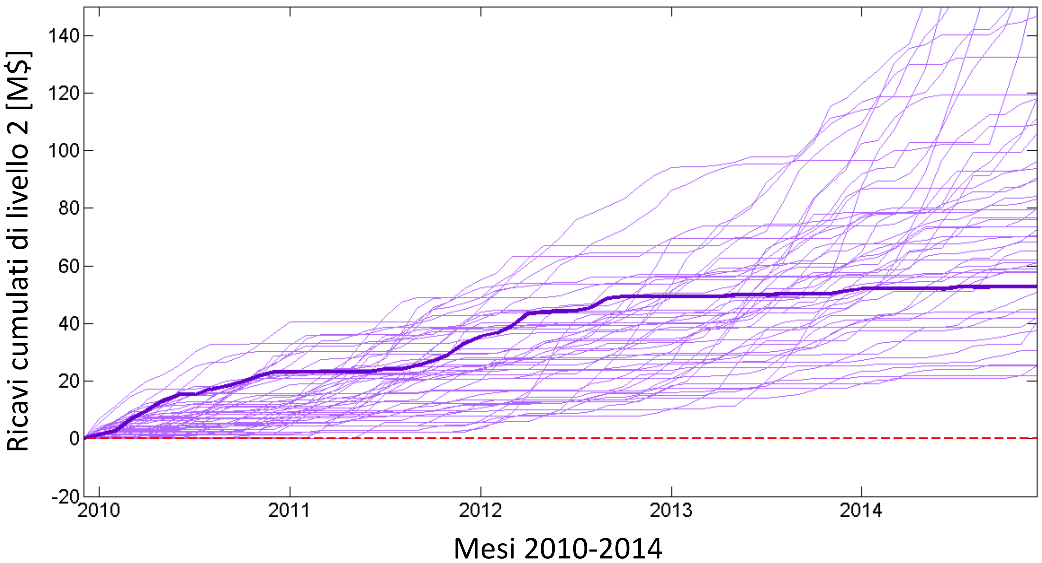
$$DEP2_k\left[\$/y\right]=\frac{\sum_{i=1}^{nMonth}\left(\max\left[0,\left\{\sum_{p=1}^{NP}C_{p,i,k}\cdot F_p-\sum_{r=1}^{NR}C_{r,i,k}\cdot F_r\right\}\right]\cdot nHoursPerMonth\right)}{nMonths/12}$$

$\forall k=1,\dots,nScenarios$

Plant operates only when revenues are positive

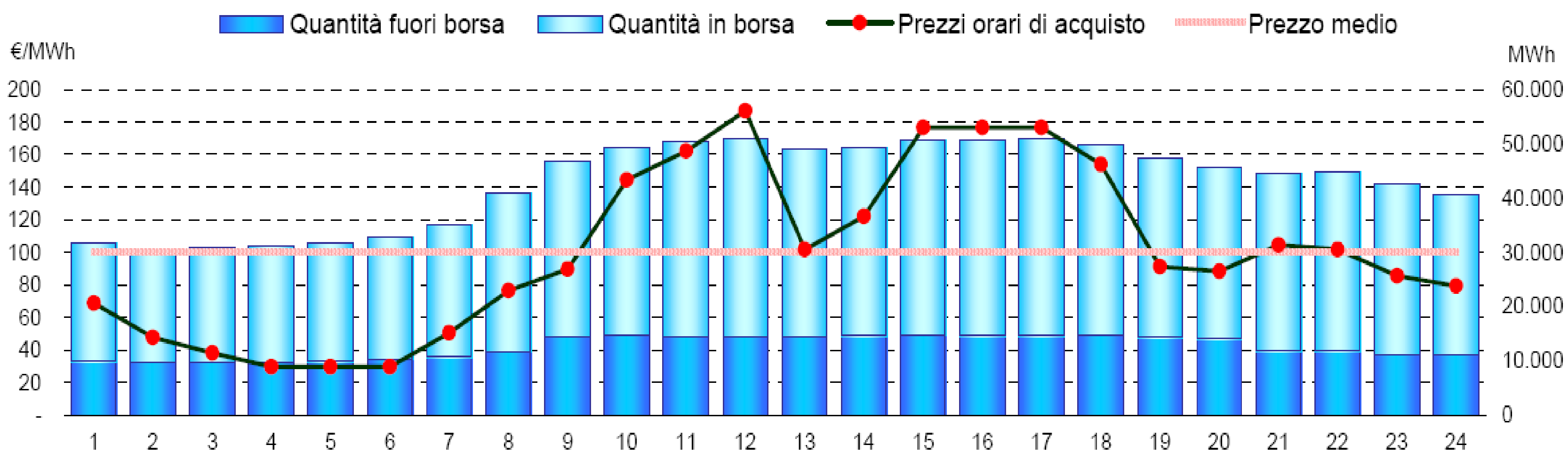
Revenues are the difference between the incomes, from selling the product(s), and the expenses to buy the reactant(s). Revenues are evaluated at month i, for scenario k.

DYNAMIC EVOLUTION OF REVENUES

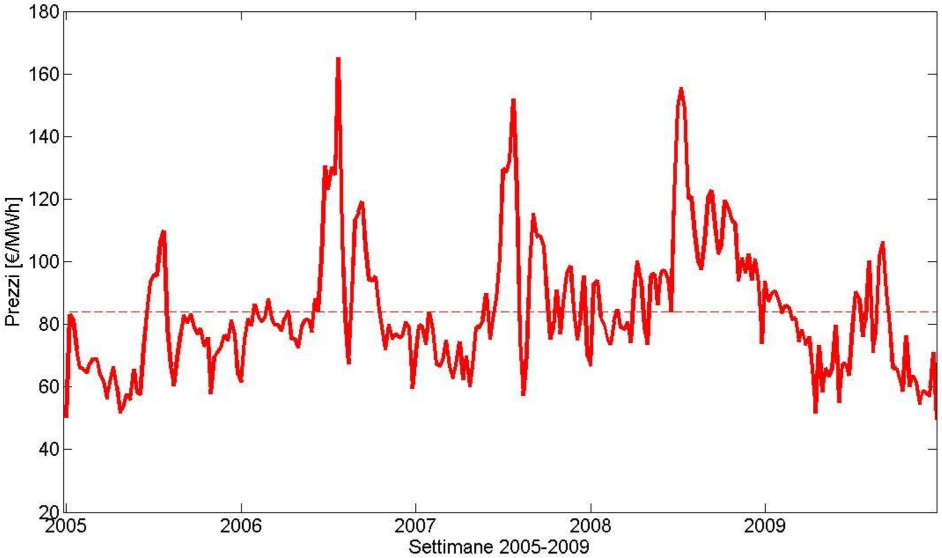


Further dynamic issues

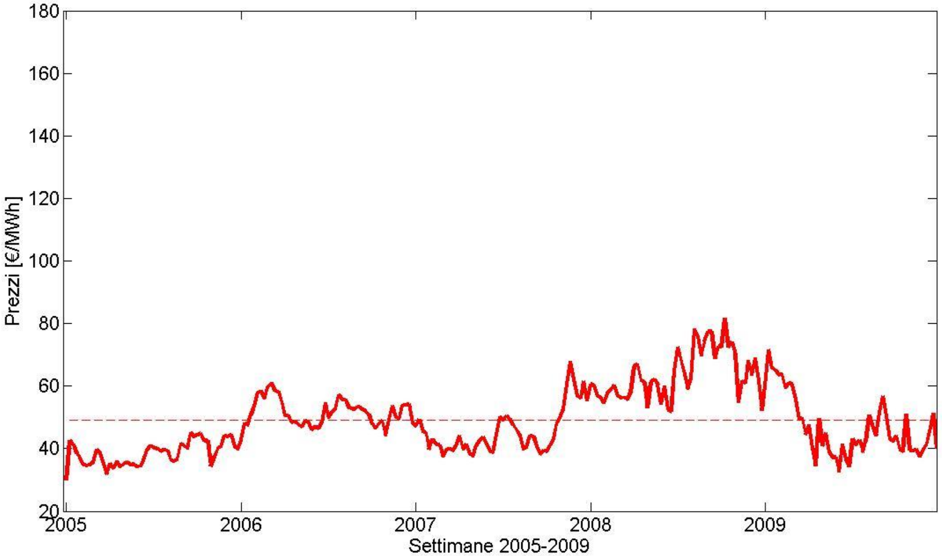
Electric energy quotations



Electric energy quotations



Weekly average of electric energy price in the 2 PM – 5 PM time band for a five-year period



Weekly average of electric energy price in the 10 PM – 9 AM time band for a five-year period

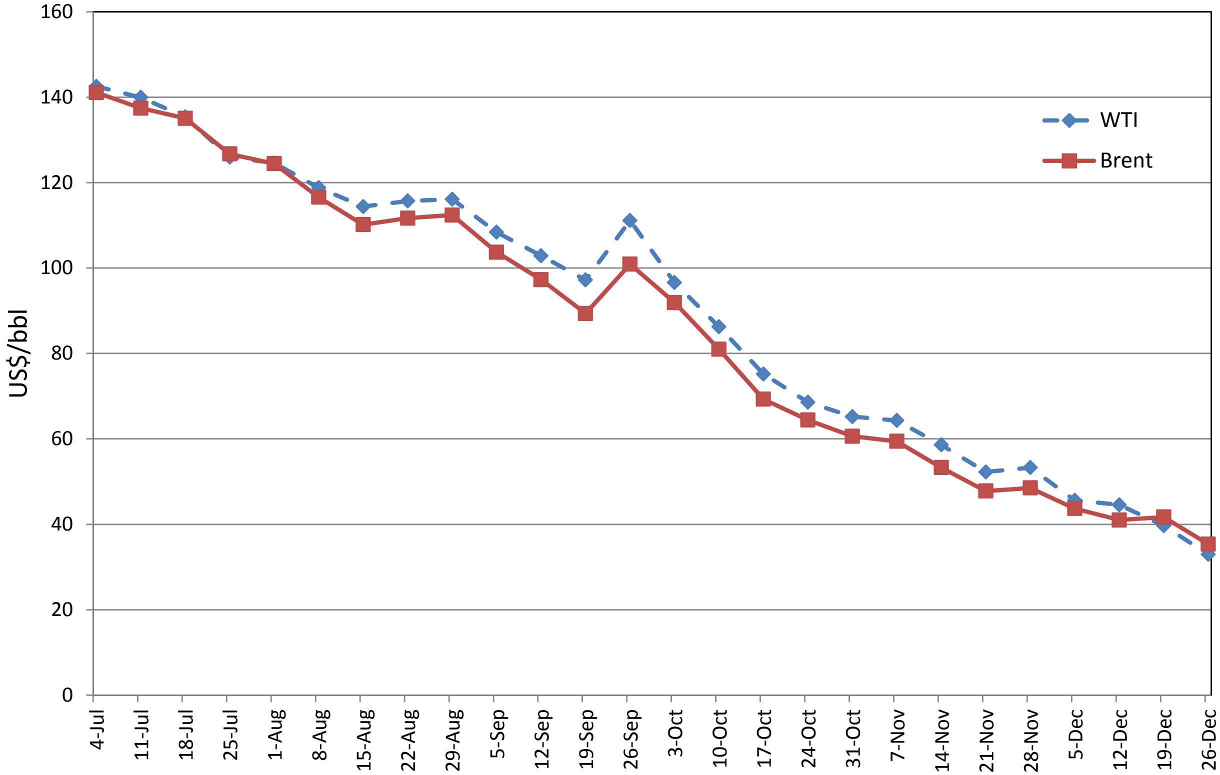
Transport sector

Trends of gasoline (Eurosuper-95) and diesel (Gas Oil) consumption in the most important Eurozone countries during the ten-year period 2002-2011.

The values in parentheses quantify the increments/decrements in consumption for each country.

Eurozone countries	Euro-super 95	Gas Oil
DK, ES, FR, IT, UK	Decreasing (-20%, -14%, -29%, -41%, -29%)	Increasing (+43%, +15%, +15%, +21%, +19%)
DE, FI, PL	Constant (-3%, -4%, -5%)	Increasing (+15%, +30%, + 155%)
GR	Increasing (+31%)	Decreasing (-24%)
AT, CZ, HU, NL	Increasing (+16%, +133%, +12%, +9%)	Increasing (+17%, +353%, +40%, +14%)
BE, PT, SE	Oscillating	Oscillating

Crude oil – Second semester 2008



- Second semester of 2008 saw a tremendous financial and economic calamity that was triggered by the US subprime mortgage crisis
- October-November 2008: 50% reduction in only a 10 week period (from 80 to 40 US$/bbl)
- Reduction of 28% from 140 to 100 US$/bbl in 10 weeks
- Reduction of 42% from 60 to 35 US$/bbl in 7 weeks

Back to the commodities

The reference component

- Instead of tracking the price/cost dynamics of <u>every commodity</u> is it possible to identify a **reference component** and **measure the price/cost of commodities respect to that component**?

- The **reference component** 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

The reference component

- For the <u>Oil&Gas sector</u> a good candidate for the reference component is:

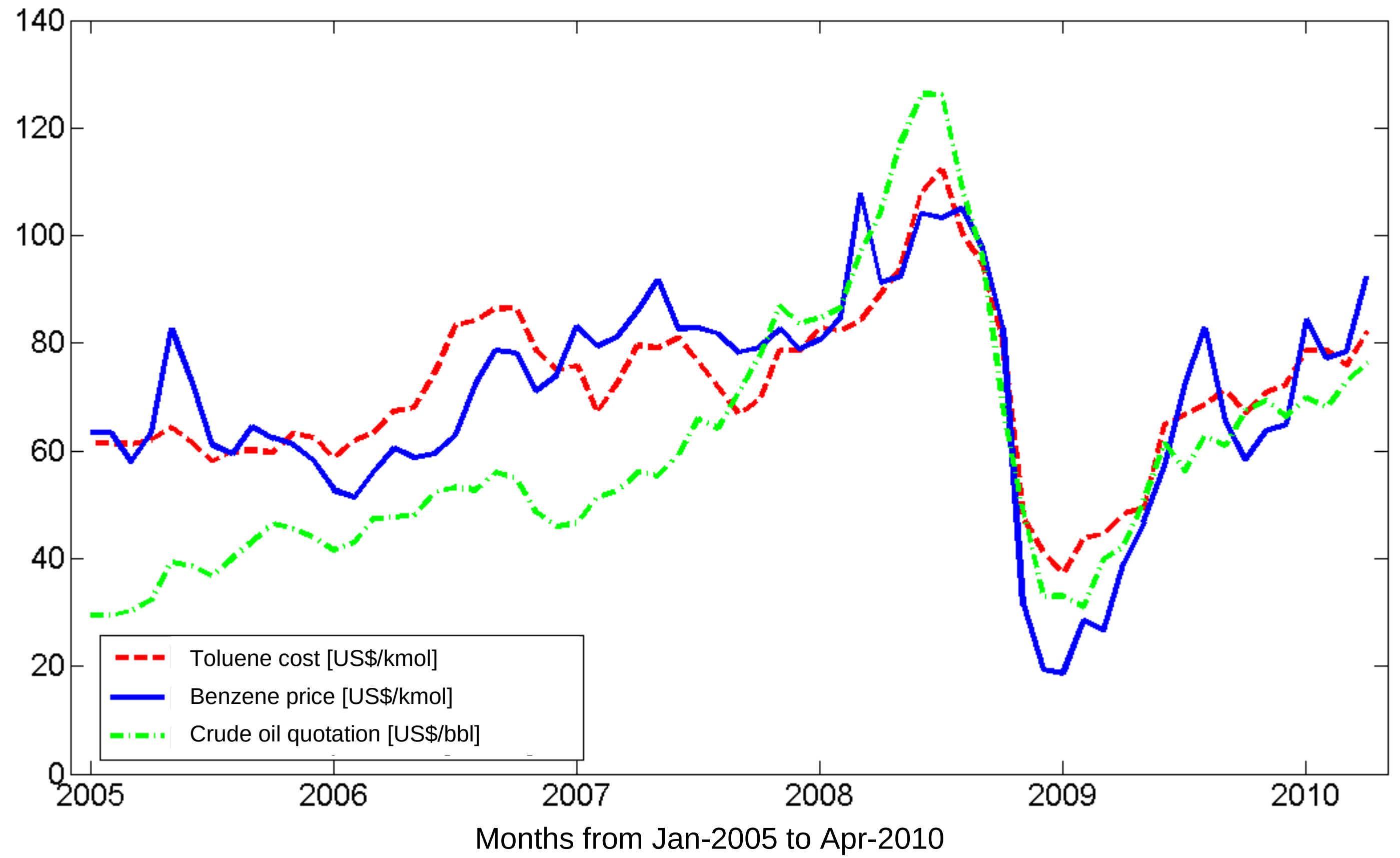
CRUDE OIL

- Consequently, we will refer the price/cost fluctuations of commodities (*e.g.*, toluene, benzene, diphenyl, hydrogen, methane, …) to the cost dynamics of crude oil.

The reference component

- **Crude oil**
  - Being a raw material, it is the precursor of a number of chemical processes
  - Its cost is:
    - well-known,
    - largely available,
    - periodically updated
  - Plays a significant role also respect to a number of industrial utilities (*e.g.*, steam, electric energy)

Price/cost fluctuations



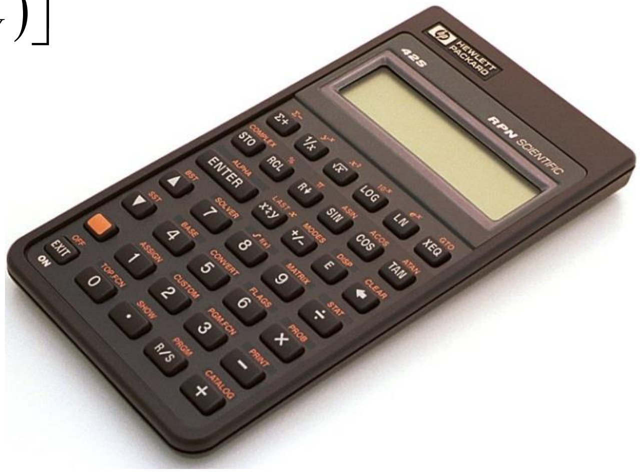
Methodology

The correlation index

- The assessment of the economic dependence of the price/cost of commodities from the reference component is carried out by evaluating the **CORRELATION INDEX**:

$$\mathrm{corr}(X,Y)=\frac{\mathrm{cov}(X,Y)}{\sqrt{\mathrm{var}(X)\,\mathrm{var}(Y)}}=\frac{\sigma_{X,Y}}{\sigma_X\sigma_Y}$$

- Where: $\begin{cases}\sigma_{X,Y}=\mathrm{cov}(X,Y)=E\left[(X-\mu_X)(Y-\mu_Y)\right]\\ \mathrm{corr}(X,Y)\in -1,\ldots,+1\end{cases}$

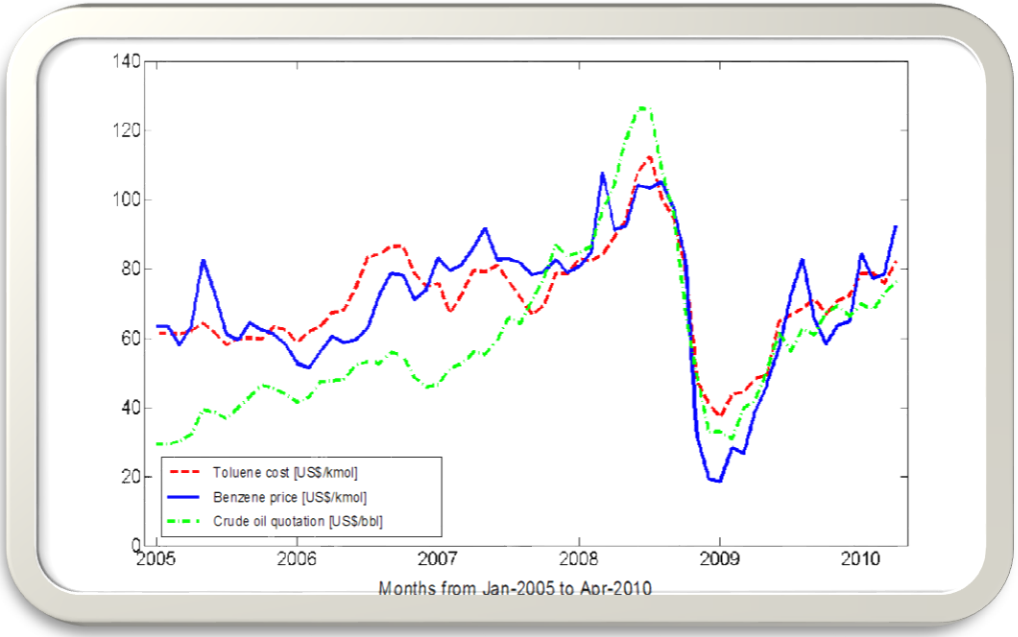


The correlation index

- Specifically we have:

$$\operatorname{corr}\left(CO,T\right)=0.8119$$

$$\operatorname{corr}\left(CO,B\right)=0.7231$$

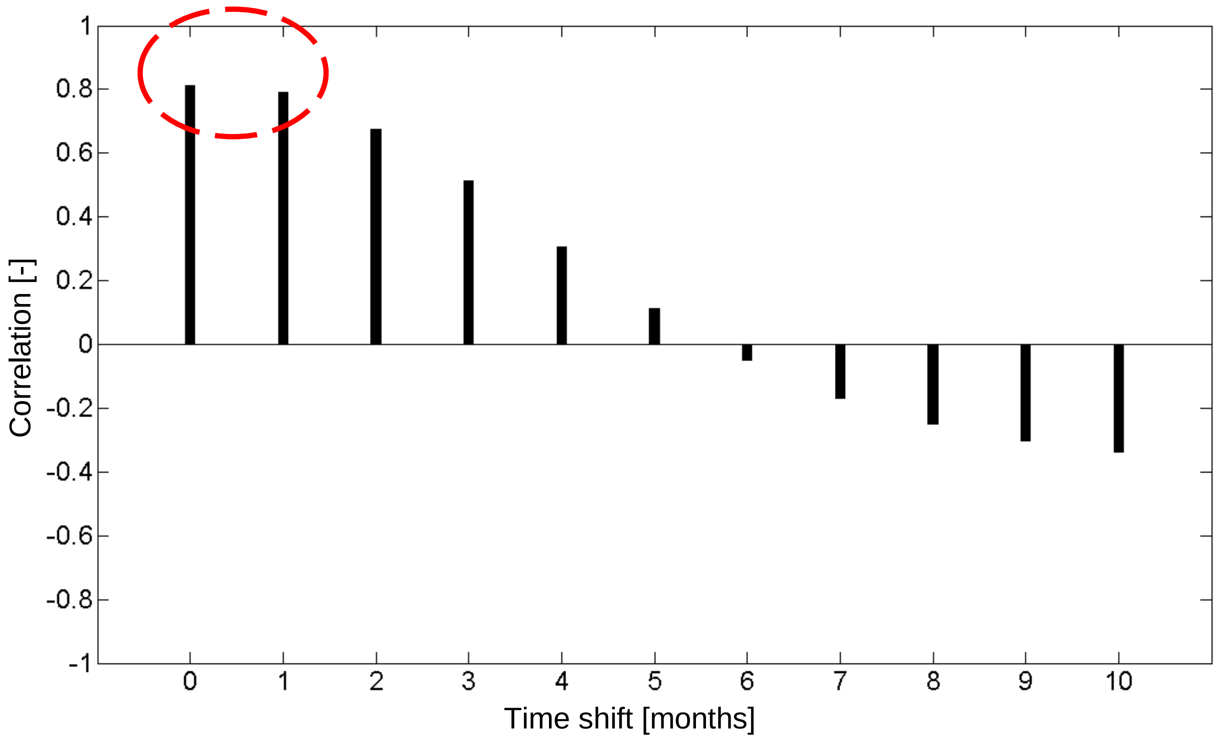


Time dependence

- Are there any **time delays** between the time series of the commodity and reference product?

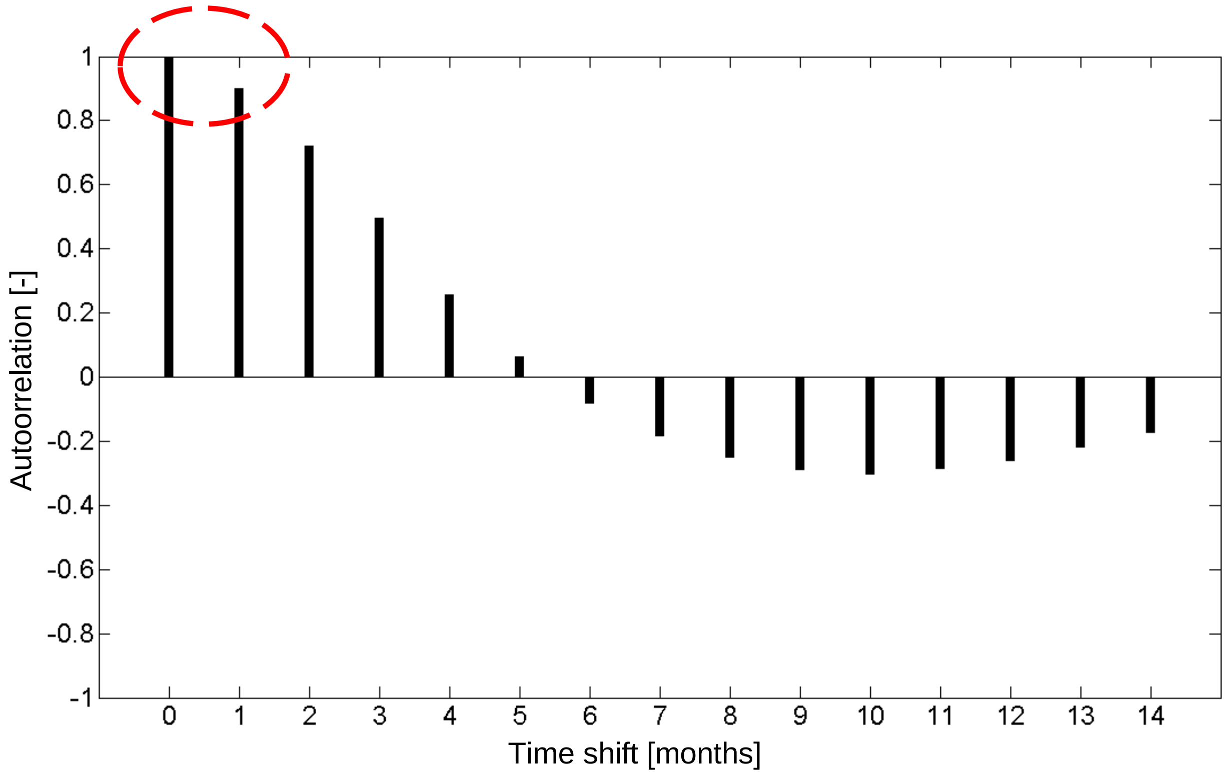
- The **CORRELOGRAMS** can be of real help in identifying the time dependence and any possible delay between the quotation of the reference component and the ones of the depending commodities.

Correlograms



Toluene vs Crude Oil correlogram

Autocorrelograms



Autocorrelogram of Toluene cost

Dynamic model of price/cost of commodities

Dynamic model

- The dynamic model should be as simple as possible, robust and consistent for long periods
- Exploit the functional dependency of T and B from CO
- Maximum time delay of one month → t_i and t_{i-1} for the commodity (in our case B and T)
- No time delay for the reference component (CO)
- Avoid overparameterization

- In econometric terms: mixed autoregressive model and specifically
  - **Autoregressive Distributed Lag** model:

$$ADL(p,q) = c + a_0 x_0 + a_1 x_1 + \ldots + a_p x_p + b_1 y_1 + b_2 y_2 + \ldots + b_q y_q$$

Dynamic model

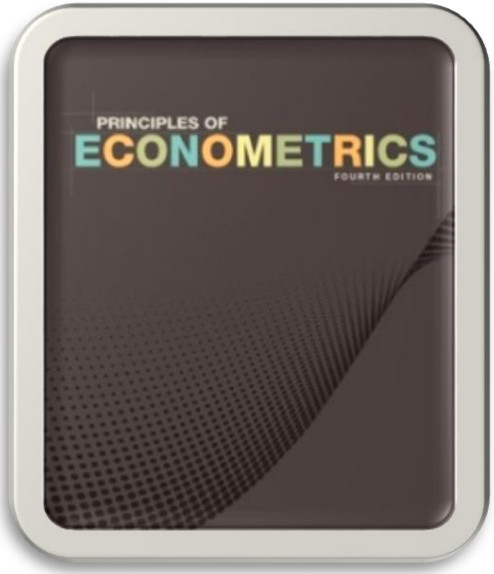
- **Autoregressive Distributed Lag** model (strict analogy with the **ARX** model used in the system identification of dynamic processes):

$$ADL(0,1)$$

$$P_{T,i} = c_T + a_{T,0} P_{CO,i} + b_{T,1} P_{T,i-1}$$

$$P_{B,i} = c_B + a_{B,0} P_{CO,i} + b_{B,1} P_{B,i-1}$$

$$ADL(p,q) = c + a_0 x_0 + a_1 x_1 + \ldots + a_p x_p + b_1 y_1 + b_2 y_2 + \ldots + b_q y_q$$



Parameter identification

- The available input data are the time series for the price/cost of B, T, and CO:
  - from Jan-2005 to Apr-2010 *i.e.* 64 monthly values
  - 50 monthly values used for parameter identification
  - 14 monthly values used for cross-validation
- The regression procedure calls for the minimization of the following objective functions (one minimization at time to determine the parameters c_X, $a_{X,0}$, $b_{X,1}$ for T and B respectively):

$$\min_{c_X, a_{X,0}, b_{X,1}} \sum_{i=1}^{nMonths} \left[\left(c_X + a_{X,0} P_{CO,i} + b_{X,1} P_{X,i-1} \right) - P_{X,i} \right]^2$$

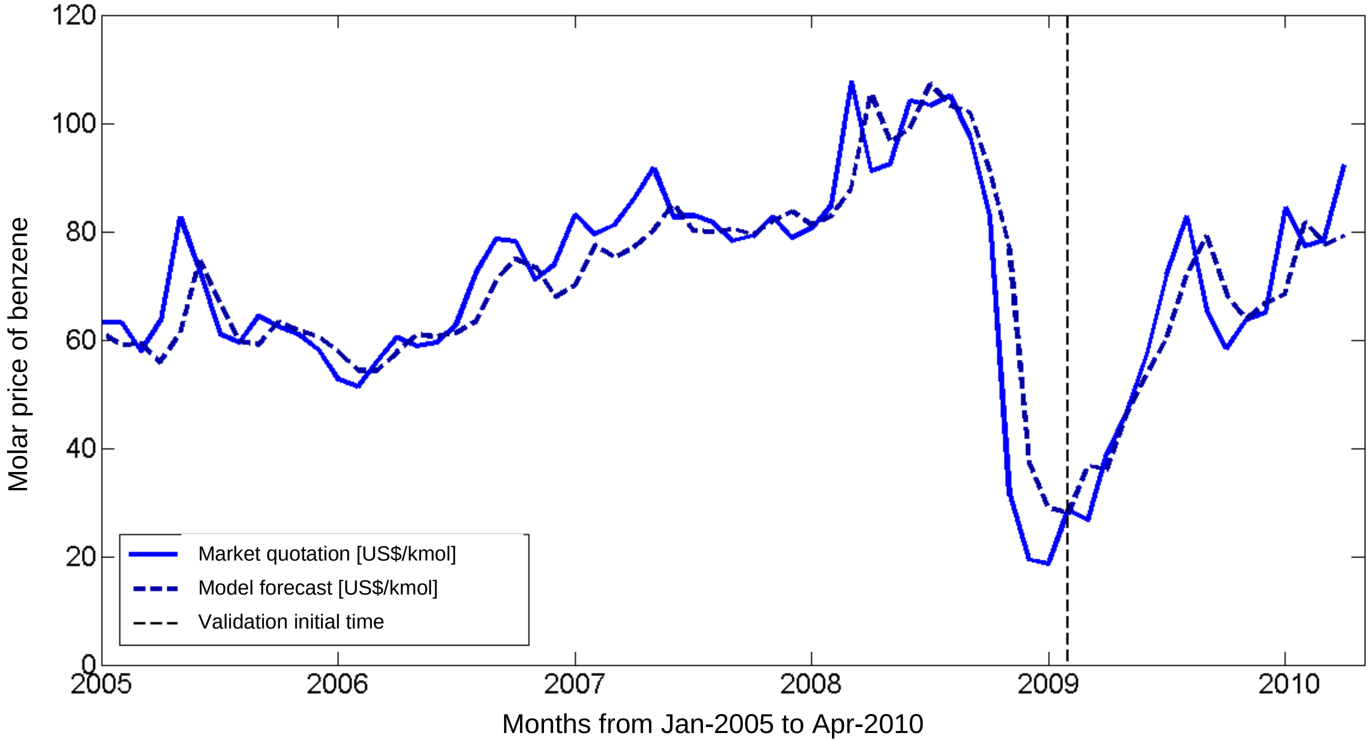
$$\text{where:} \quad X = B, T$$

Parameter identification

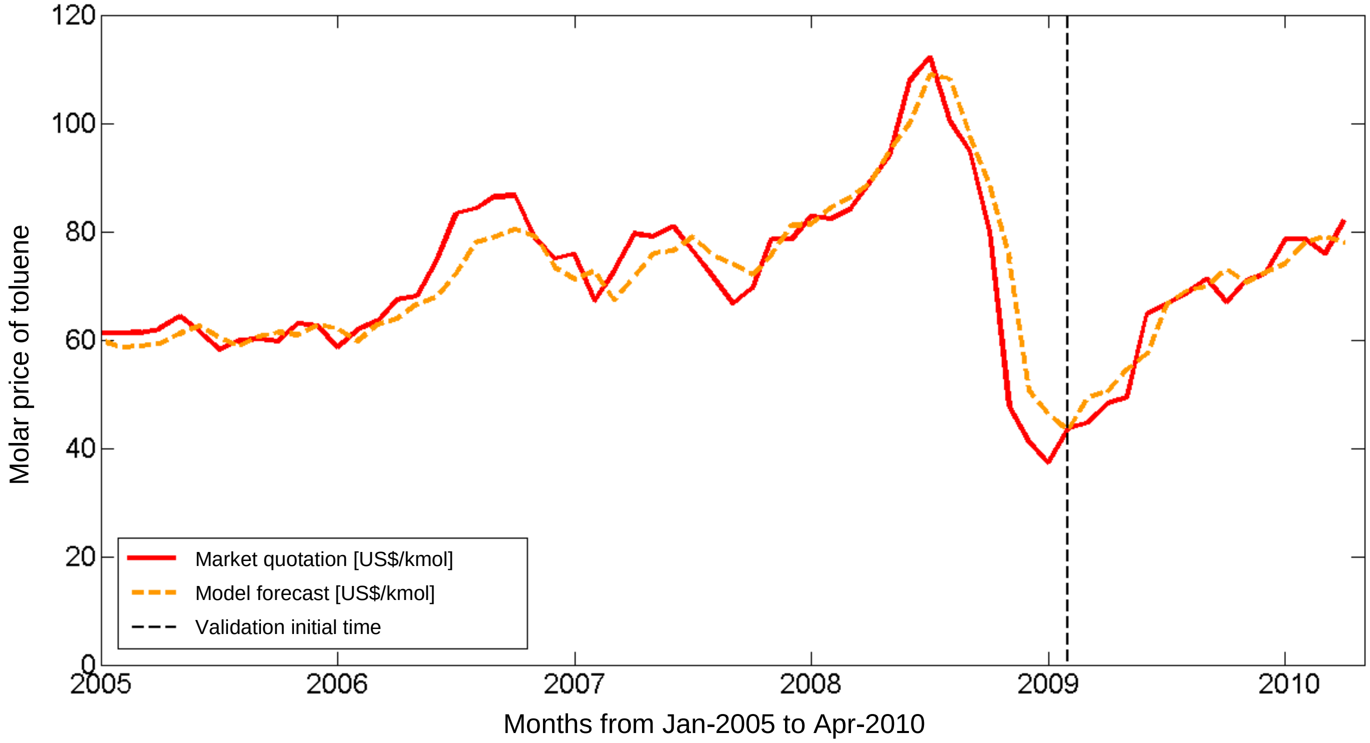
- This is a simple multidimensional unconstrained optimization procedure (for instance in Matlab one can use: *fminsearch* function) that produces the following results:

Benzene		Toluene	
c_B	4.5842 US$/kmol	c_T	12.4068 US$/kmol
$a_{B,0}$	0.3386 bbl/kmol	$a_{T,0}$	0.3824 bbl/kmol
$b_{B,1}$	0.6141 [-]	$b_{T,1}$	0.4636 [-]
R^2	0.7619	R^2	0.8306

Benzene *ADL* model



Toluene *ADL* model



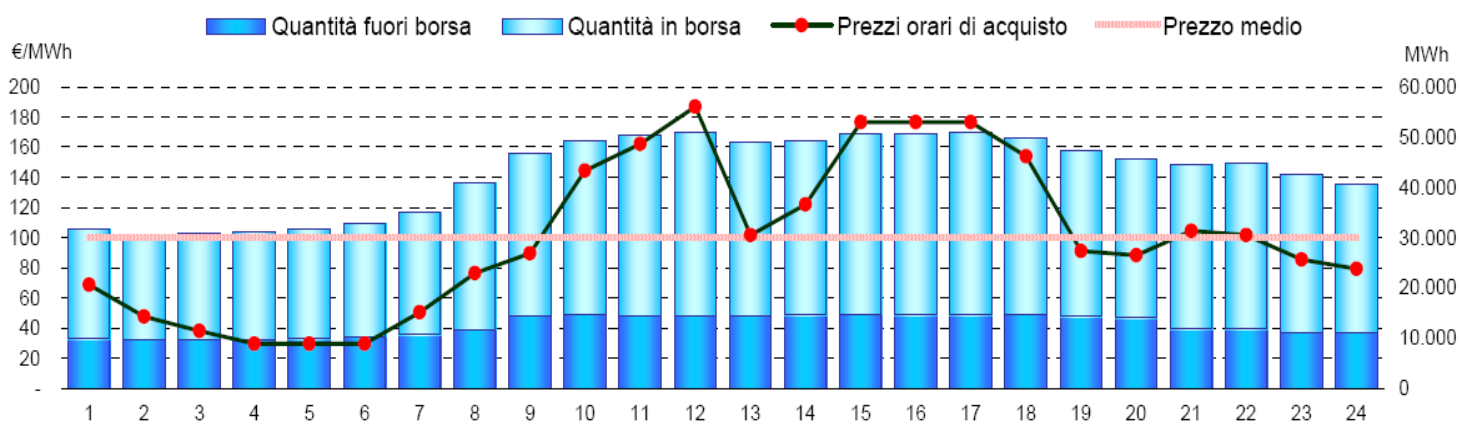
Electric energy price/cost

Electric energy market

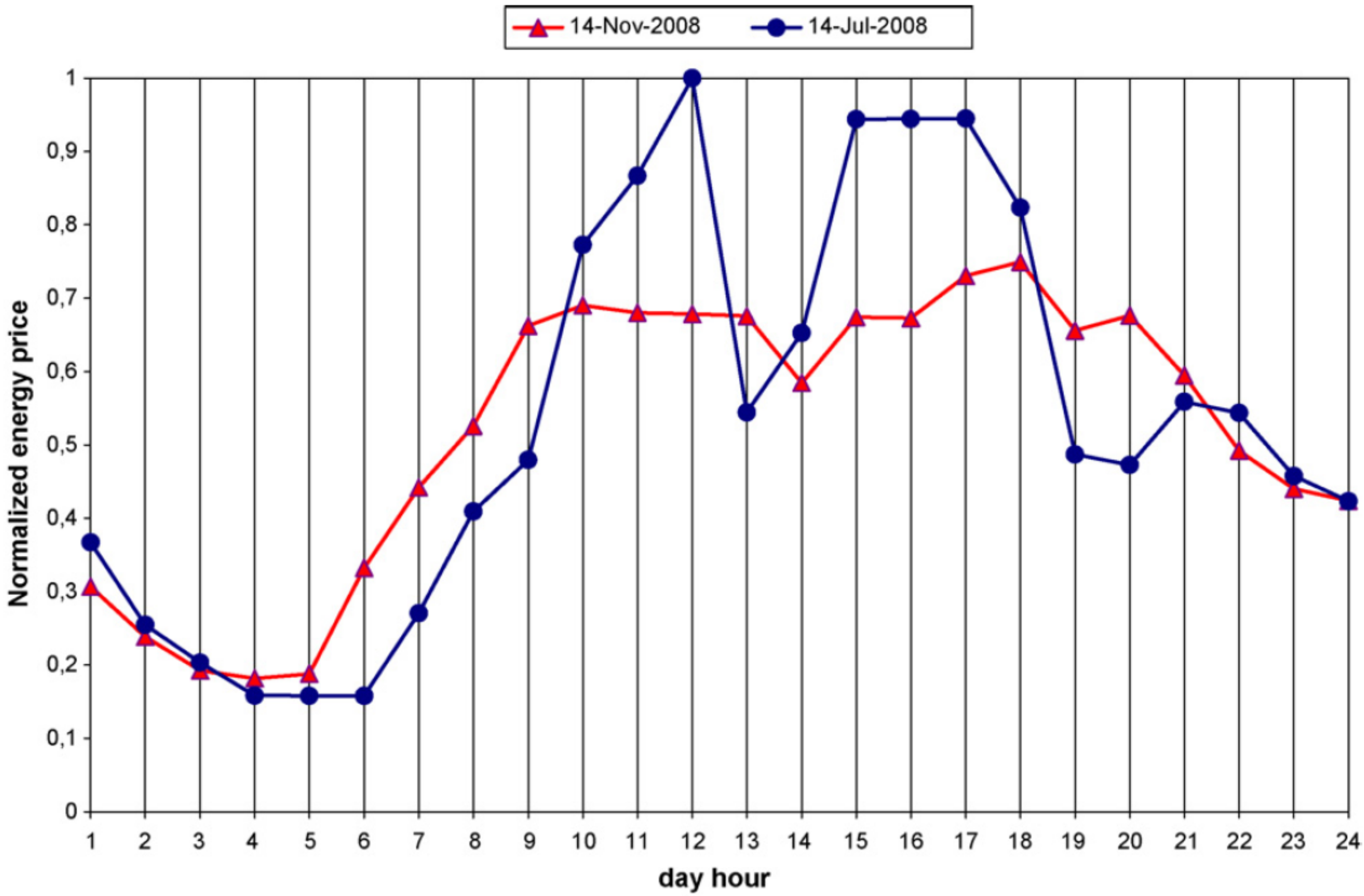
- The price of electric energy is usually controlled by the market.
- The electric market in Italy was introduced by law (D.Lgs. 77/99) to acknowledge the European Community Directive (96/92/CE).
- Since April 2004, the liberalization of the national electric market assigned the economic organization and management of electric market to an independent public company “Gestore del Mercato Elettrico” that allows the producers and consumers to define sell-and-buy contracts on an hour basis.

Electric energy market

- Given a specific day, the electric energy price is characterized by the typical M-shaped curve that comprises two peaks usually positioned in the late morning and in the afternoon.



Electric energy market



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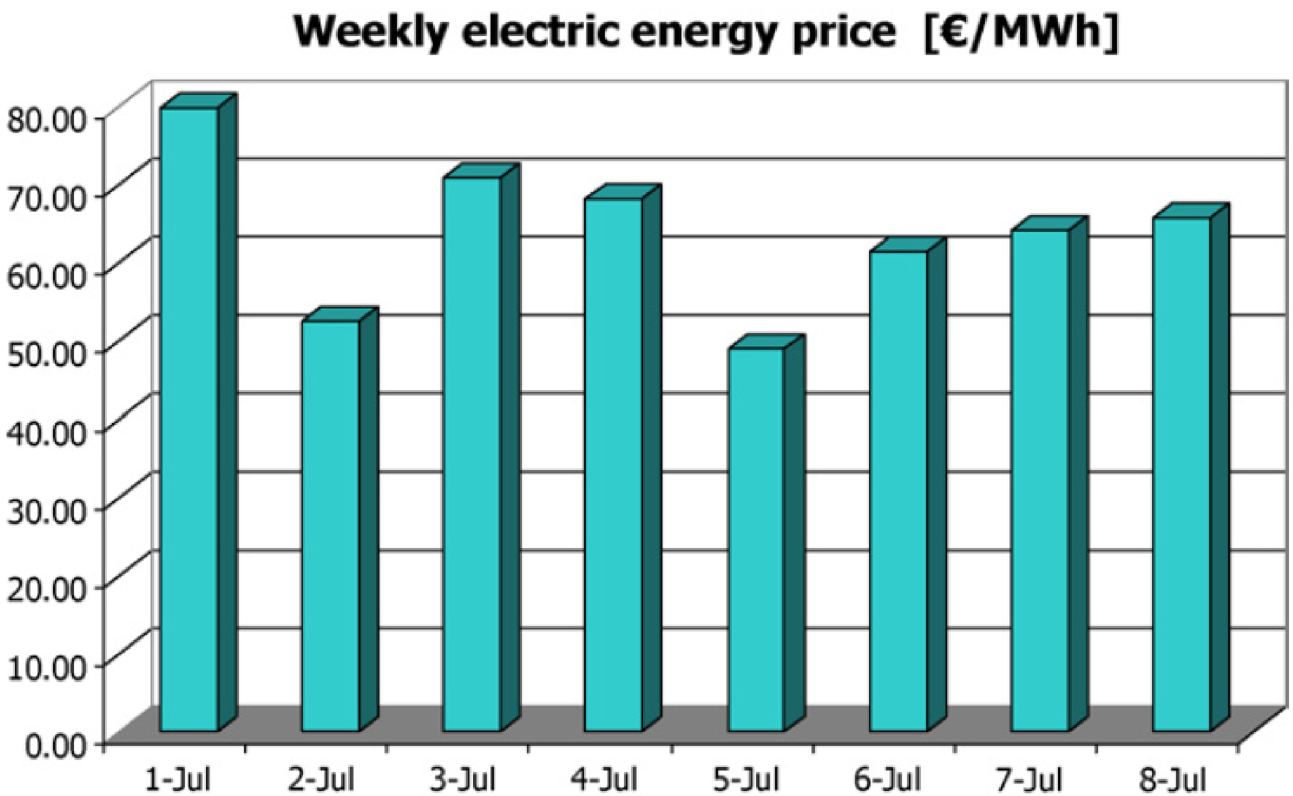
Electric energy market



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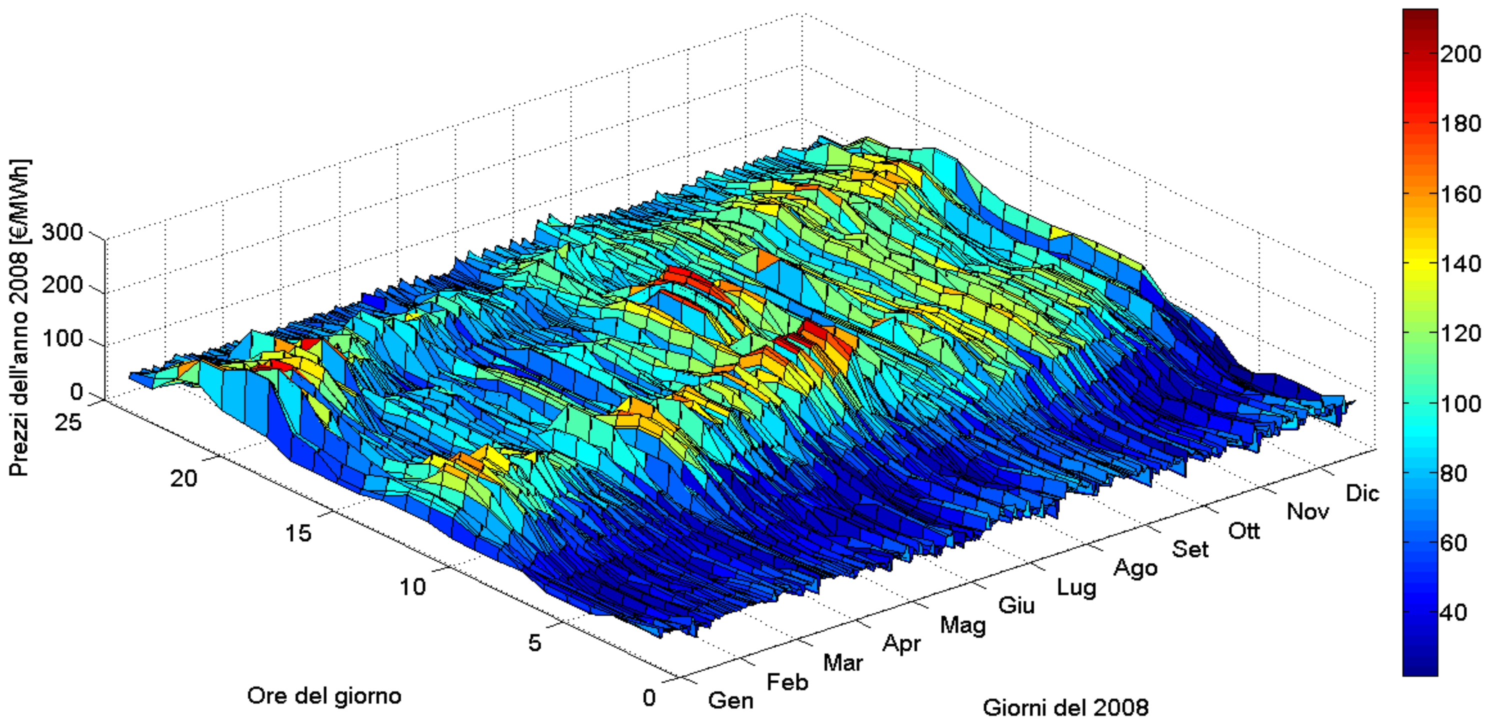
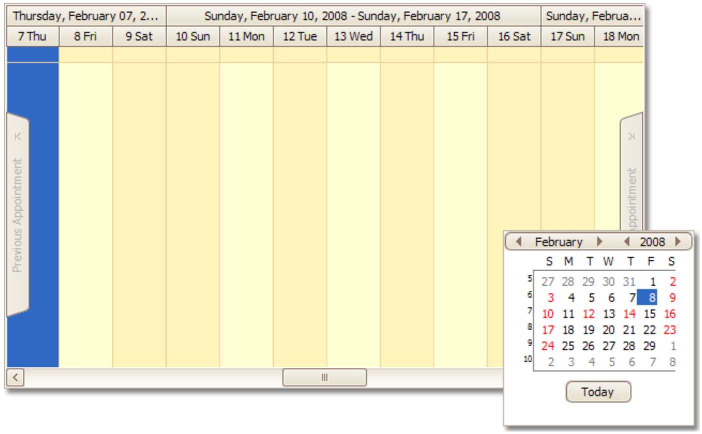
Electric energy market

- If we observe the electric energy price on a longer period (for instance one year) the trend is more complex:



Electric energy market

- We can still observe the typical M-shape for daily quotations but the time of the day and the absolute value of the maxima change from day to day.
- There are differences between working days and holidays and also among seasons.
- Moreover, we can observe stochastic oscillations that by their nature cannot be explained.
- If we enlarge the time interval from one year to five years the noise produced by the stochastic oscillations increases even more.



Methodology

Electric energy market

- We can try to lump the time series by means of a **linear operator** that transforms a y_t series into a new time series x_t by means of properly assigned w_i weights:

$$x_t = \sum_{i=-h}^{k} w_i \cdot y_{t+i}$$

- If the weights of the linear operator respect the condition: $\sum_{i=-h}^{k} w_i = 1$ then we have the so called: **moving average**, which is smoother than the original time series according also to the number of averaged terms in the summation. The more the terms the smoother the averaged curve.
- Since the moving average approach has some drawbacks such as not being applicable to the initial and ending terms, it is advisable to adopt an even simpler approach to smooth the original noise coming from the *experimental* (*i.e.* market) data.

Electric energy market

- We choose to average the single hour-values of the quotations of the electric energy over a weekly time interval:

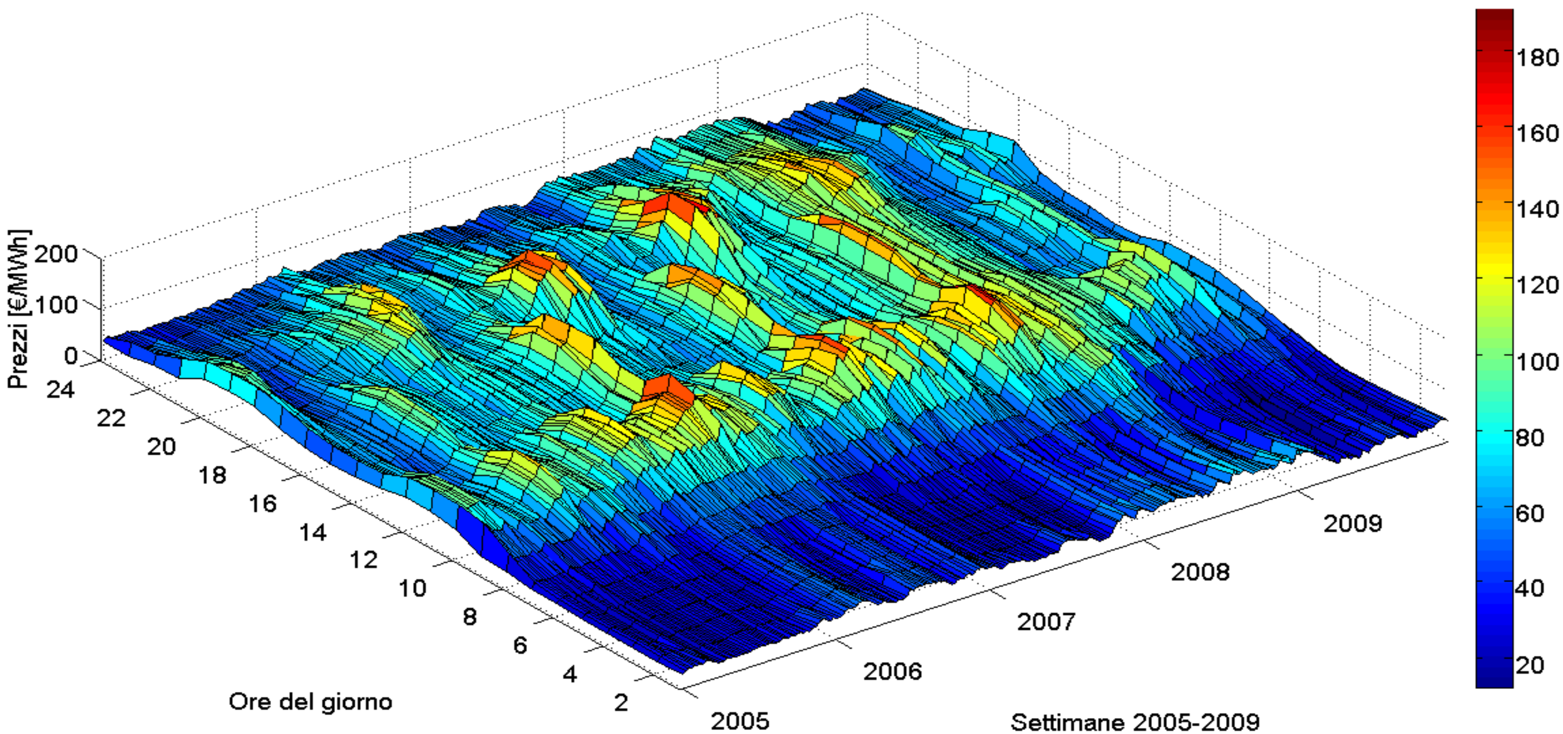
$$p_j = \frac{\sum_{i=1}^{7} p_{7j+i}}{7}$$

where j is the week index and i the day index.

- This assumption allows contracting the total number of data to be analyzed for every year (thus reducing the noise). Eventually, on an annual basis we have 24 hour-values of the electric energy price that are averaged (*i.e.* sampled) on 52 week-values.

Electric energy market

- For the five-year period we have:

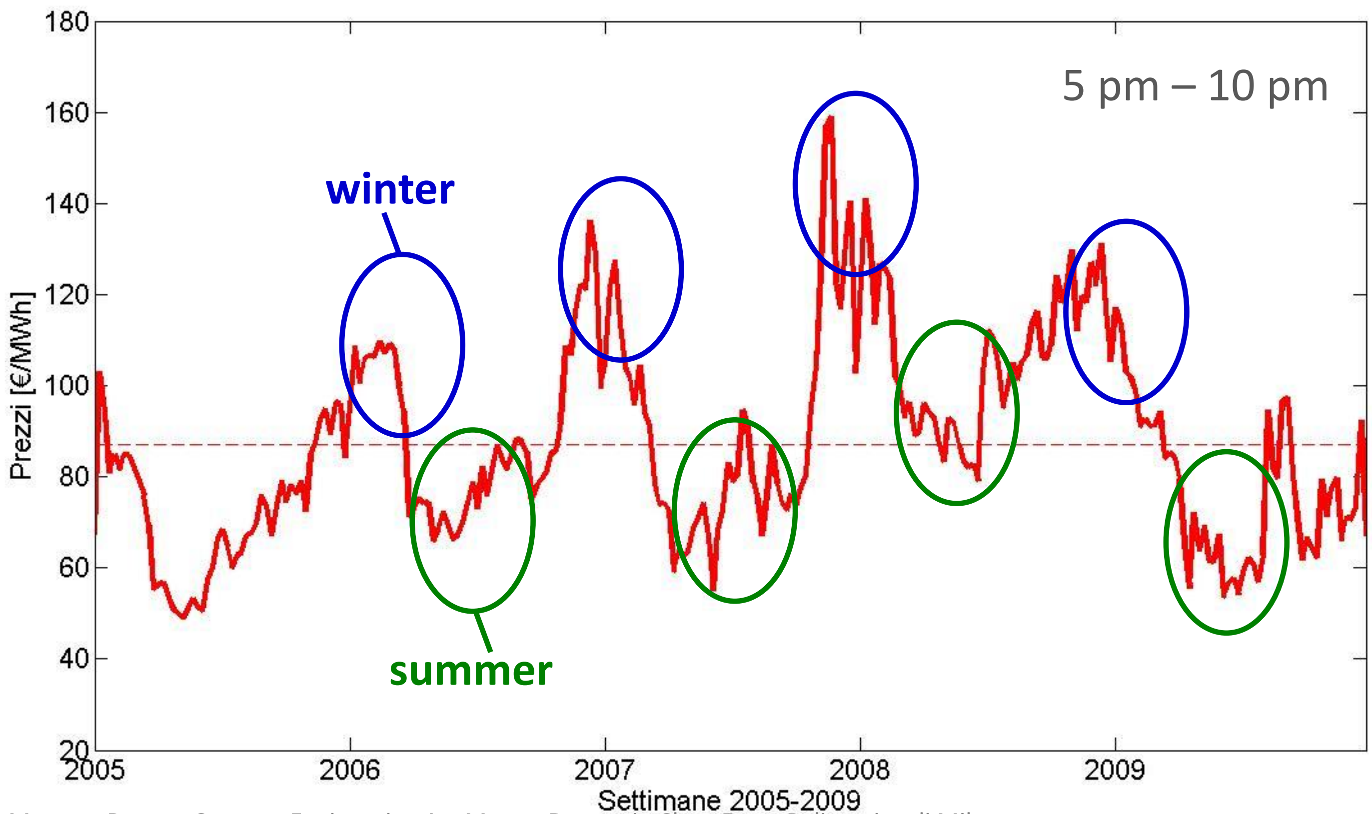


Electric energy market

- We can observe that:
  - the daily maxima are higher during the summer months
  - The second maximum changes with time according to a seasonal trend:
    - In summer months the second maximum is in the 2 PM – 5 PM interval
    - In winter months the second maximum is in the 5 PM – 10 PM interval
  - The explanation to previous point is due to the fact that in summer the peak for energy production (and therefore its price) occurs during the hottest period of the day whilst in winter the peak is due to the request for artificial lighting.

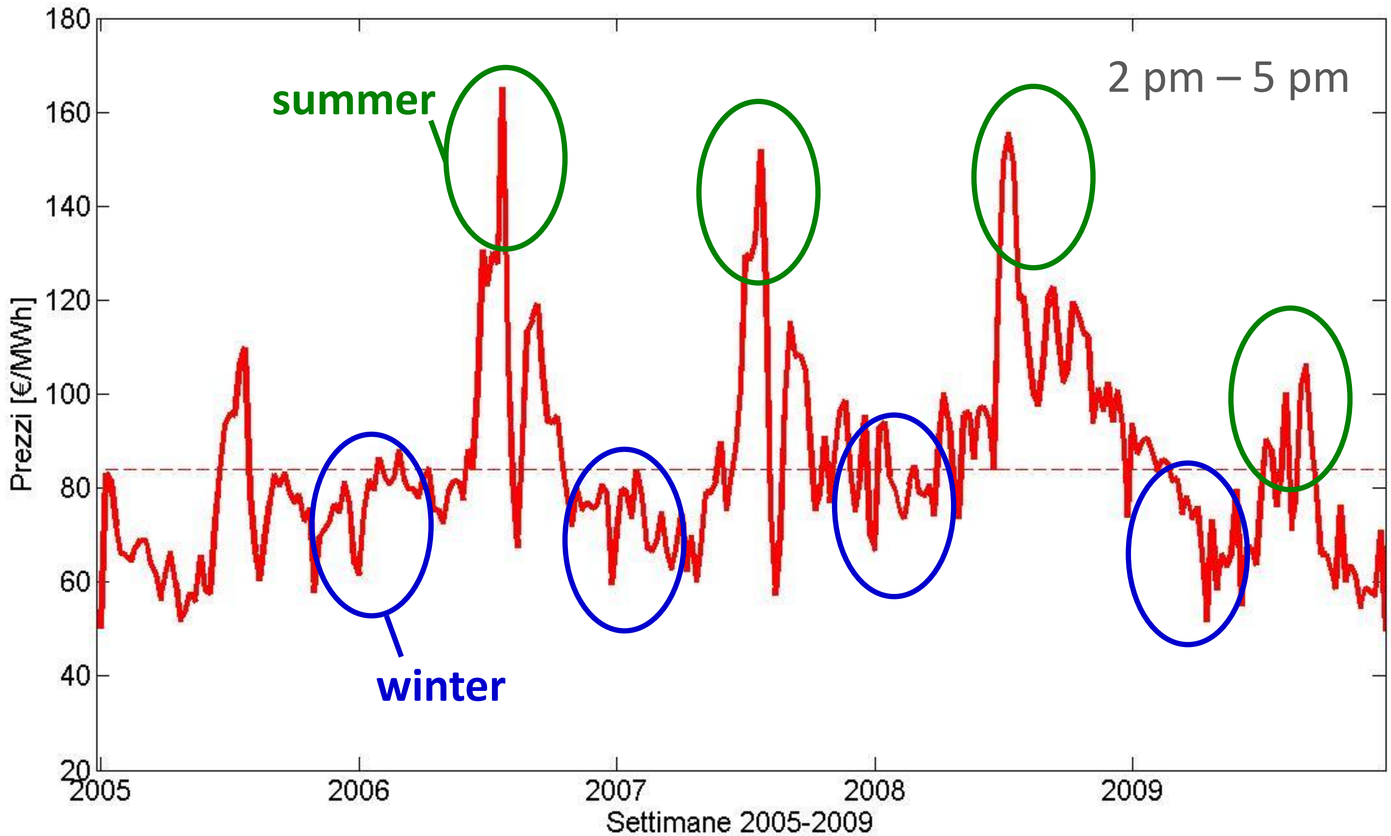
Qualitative analysis of electric energy price

- Let us first analyze qualitatively the diagrams of the energy price.
- The evening band (from 5 pm to 10 pm) complies with some periodic patterns. During the winter months the price is significantly higher than the average value whilst during the summer months the price is lower.



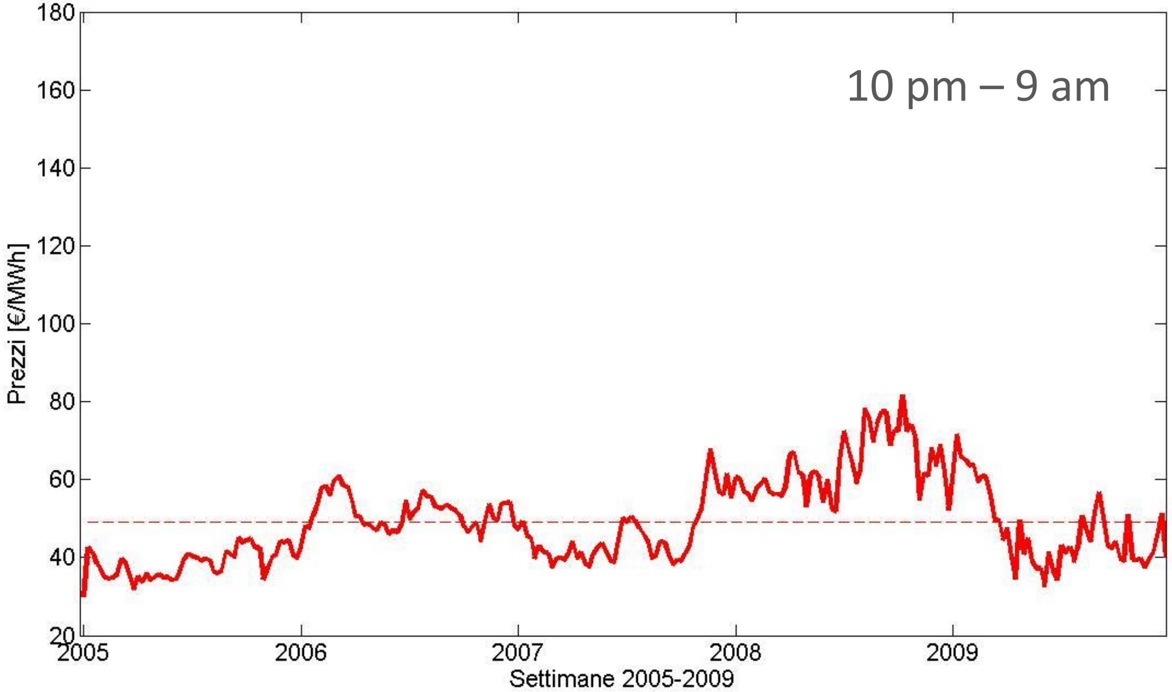
Qualitative analysis of electric energy price

- The afternoon band (from 2 pm to 5 pm) is characterised by other periodic patterns. During the summer months the price is significantly higher than the average value due to the higher energy request for conditioning/cooling purposes (both civil and industrial).



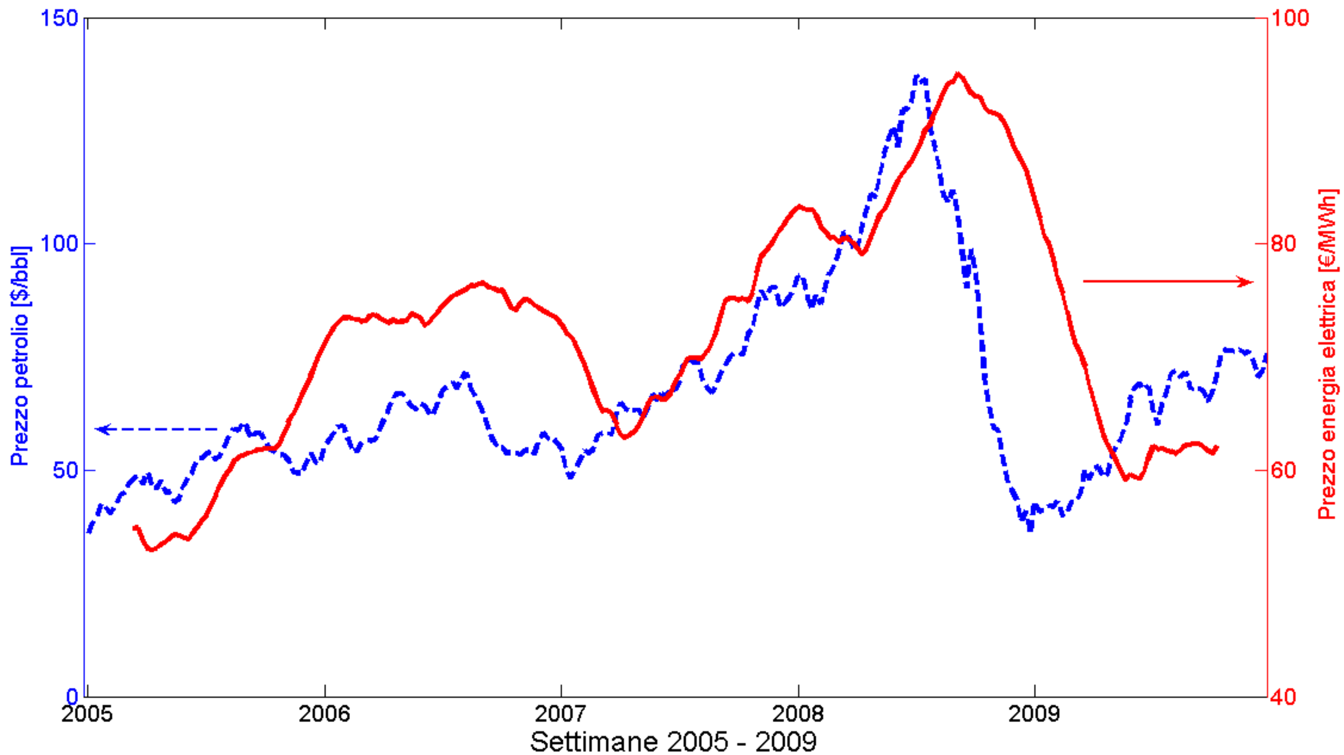
Qualitative analysis of electric energy price

- Conversely, in the morning band (9 am – 1 pm), it is more difficult to outline a periodicity. The highs and lows of energy price occur both in summer and in winter.
- The night band (10 pm – 9 am) is characterized by a very low average value and by reduced seasonal oscillations due to the reduced energy demand. We can observe a *bull trend* (increase) in the 2007-2008 period and a *bear trend* (decrease) in the 2008-2009 period.



Quantitative analysis of electric energy price

- As for the commodities case, the idea is to refer the price of electric energy to the crude oil price that plays the role of reference component.
- To better visualize the possible dependency of energy price from crude oil it is recommended to remove the *stochastic* noise and obtain a smoothed profile by means of a moving average of 17 weekly elements (about 4 months).



Quantitative analysis of electric energy price

- We can observe how the electric energy price is significantly influenced by the crude oil quotations.
- There is a time delay between the EE and CO quotations that can be visually estimated into 10-15 weeks.
- Back to the modeling issue, we have observed that the EE price depends dynamically on:
  - the time bands of the day
  - a seasonal component

Quantitative analysis of electric energy price

- To model the seasonal component we can introduce a suitable sinusoidal dependency. Consequently, the proposed **model for the EE price** is:

$$P_{EE,i,j} = a_j + b_j \cdot P_{CO,i-t_{d,j}} + c_j \cdot \sin\left(\frac{2\pi \cdot i}{T_j} + \varphi_j\right)$$

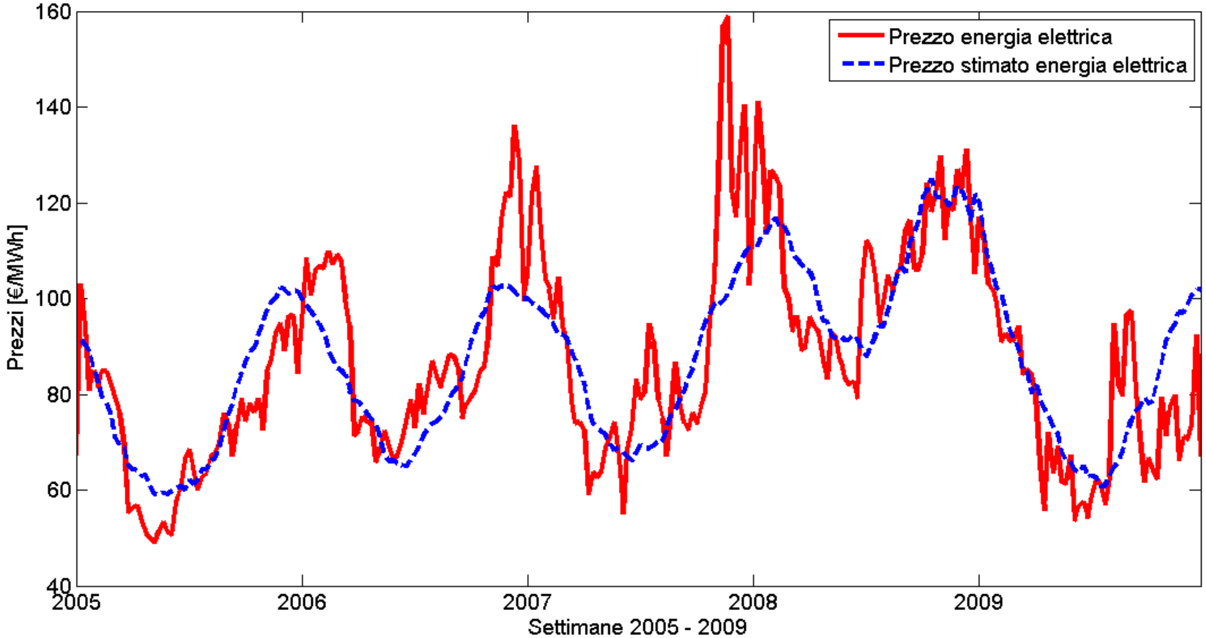
- Where:
  - i: the i-th week
  - j: the time band (there are <u>four</u> bands in a day: morning, afternoon, evening, night)
  - a: reference value of EE price [€/MWh]
  - b: coefficient for the dependency of EE price from CO [€ bbl/$ MWh]
  - t_d: time delay [week] (*i.e.* number of weeks of delay between the EE and CO prices)
  - c: parameter of the periodic component [€/MWh]
  - T: period of the sine-wave function (the period is expected to be comparable to a season) [week]
  - φ: phase of the sine-wave function [-]

Quantitative analysis of electric energy price

- There are six parameters (a, b, c, t_d, T, φ) to be identified by optimizing the following problem:

$$\min_{a_j,b_j,t_{d,j},c_j,T_j,\varphi_j} \left\{ \sum_{i=1}^{nWeeks} \left[\left(a_j + b_j \cdot P_{CO,i-t_{d,j}} + c_j \cdot \sin\left(\frac{2\pi \cdot i}{T_j} + \varphi_j \right) \right) - P_{EE,i,j} \right]^2 \right\} \qquad j = 1,\dots,4$$

- With reference to the evening band (5 pm – 10 pm) we obtain:



Quantitative analysis of electric energy price

- For the evening band we have the following regression parameters:

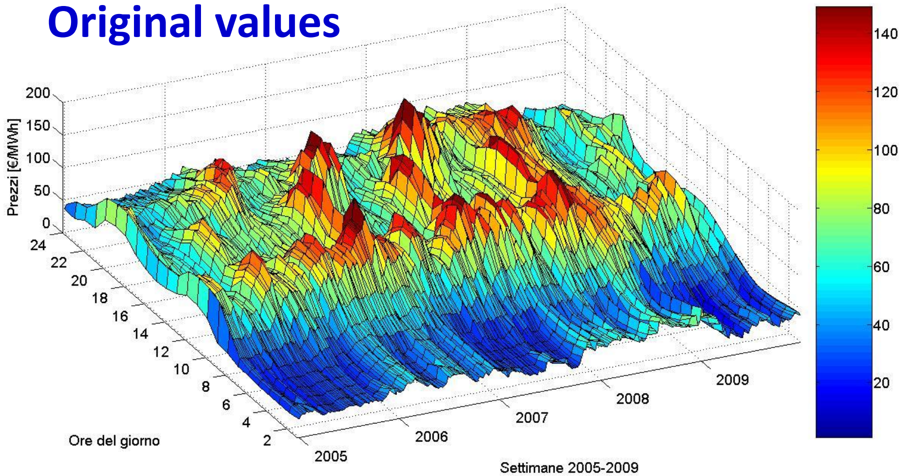
a [€/MWh]	b [€ bbl/ $ MWh]	t_d [week]	c [€/MWh]	T [week]	φ [-]
52.3741	0.5385	13	17.9956	53.6492	1.9022

- It is interesting to observe that the **time delay** is **13 weeks** in line with the qualitative observations. **13 weeks** are equivalent to about **3 months** that is a **season**.
- In addition the **period of the sine-wave** function is **53.65 weeks** that is quite similar to **52 weeks** *i.e.* **a year** (in line with the preliminary remarks).
- A further improvement of the model consists in assigning a constant value to the time delay t_d as it is reasonable assuming that the EE price cannot depend on the CO price with different time delays.
- Any further regression procedure will work on 5 parameters only.
- We can now pass from the time band regressions to 24-hour regressions.

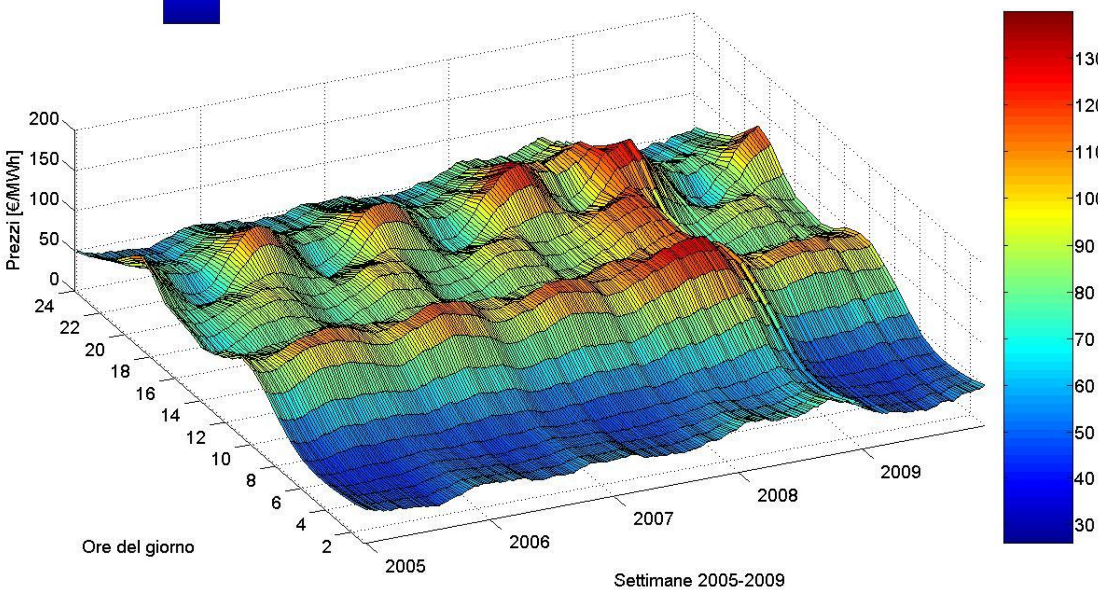
Quantitative analysis of electric energy price

- Performing the regression procedure for every hour of the day we finally obtain:

Original values

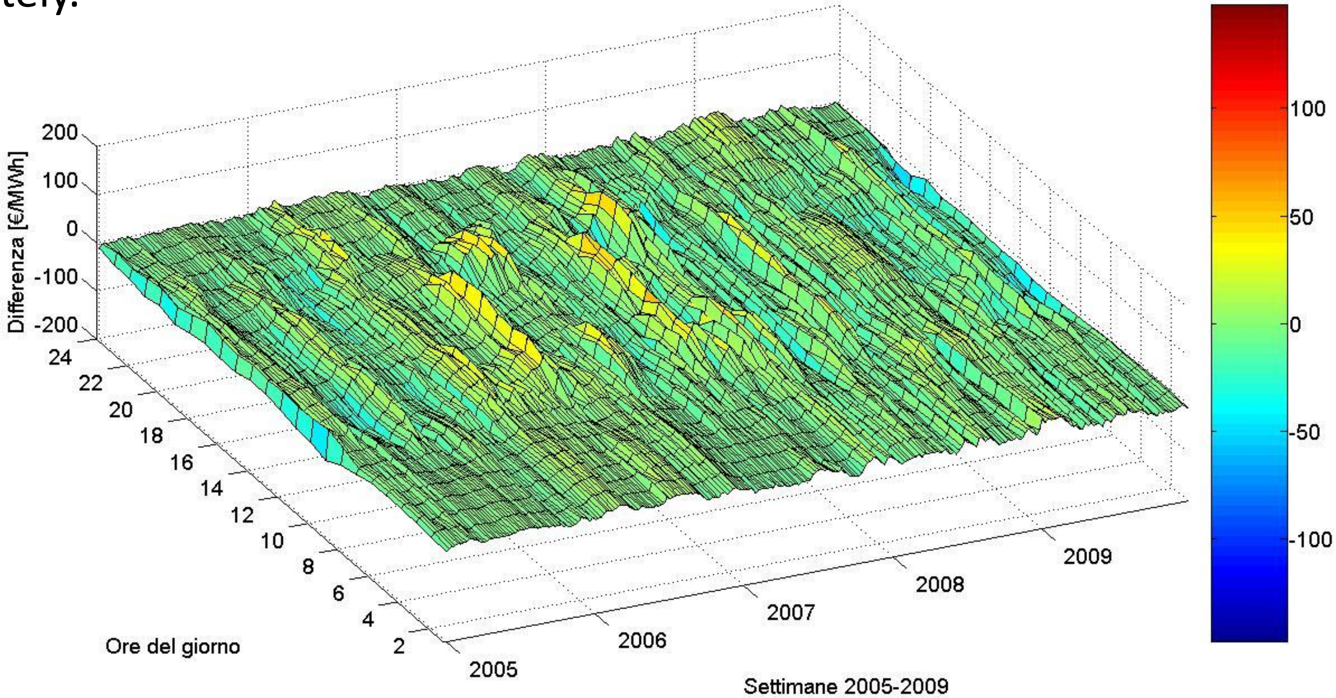


Identified model



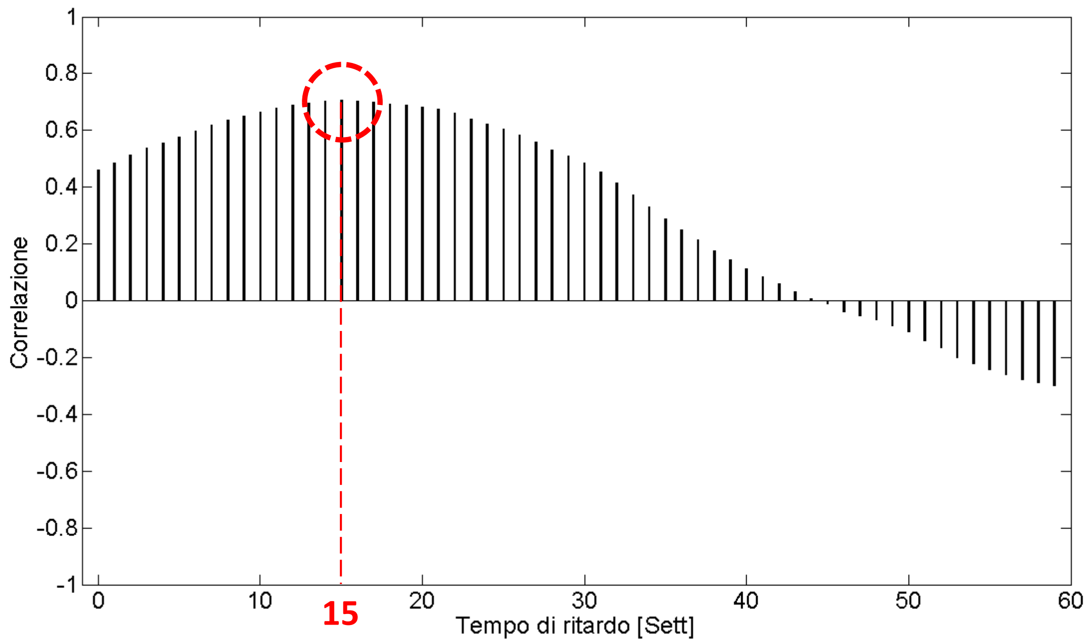
Quantitative analysis of electric energy price

- The model is capable of describing both the daily oscillations and the dependency from the CO quotations.
- Here following are the residuals, *i.e.* the difference between the original EE prices and the identified ones (model predictions).
- the residuals are due to the stochastic component that cannot be modeled adequately.



Evaluation of the optimal time delay

- As aforementioned, the delay time existing between the CO quotations and the following EE price should be assumed constant due to the characteristics of the market.
- The correlogram between the time series (*i.e.* EE and CO) can be used to determine the delay time (*i.e.* time shift) that maximizes the correlation of those series:



Crude oil quotations: modeling and forecast

Crude-oil models classification

1 – Time horizon

Depending on the specific problem to be solved, the economic assessment of a chemical plant can cover a time horizon that is:

- **Short**: from hours to days (scheduling);
- **Medium**: from weeks to months (planning);
- **Long**: up to several years (Conceptual Design).

2 – Time granularity

This criterion deals with the time discretization (*aka* sampling time) of the dataset of input variables, *i.e.* daily, weekly, monthly, quarterly, or yearly values.

Crude-oil models classification

3 – Typology

This criterion distinguishes between **economic** and **econometric** models, which differ for both the mechanism used to generate future prices and the fundamentals used to model their trend.

- **Economic models**: based on physical, economic, and financial features
- **Econometric models**: based on the statistical analysis of past price shocks

Econometric vs Economic

Econometric models do not take into account the forces that cause **price fluctuations**, but are focused only on the **price trends**.

- Follow the historical fluctuations of prices;
- Can cover short-, medium-, and long-term horizons;
- Neglect the dependency of economic terms from the time-varying market oscillations.

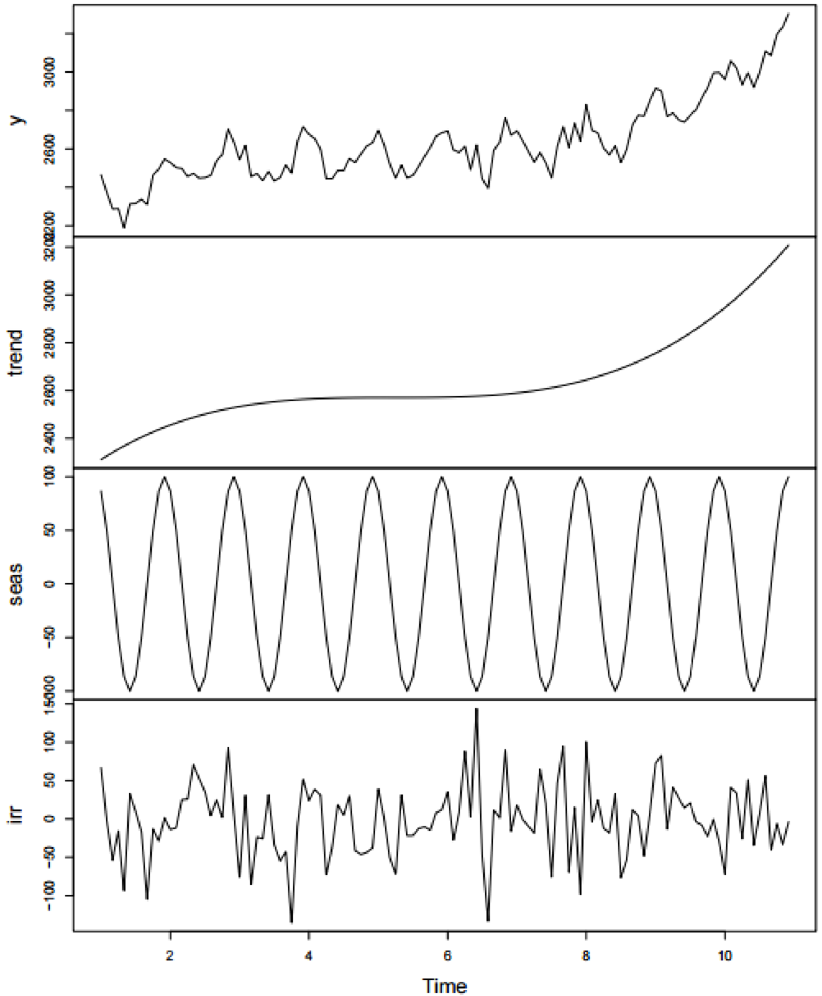
Economic models account for **economic real variables** and simulate the fluctuations of crude oil price according to the **supply and demand law**.

- Take into account "physical" variables (*i.e.* supply-and-demand law);
- Follow the historical market price trend;
- Problematic long-term forecast of the involved variables.

Crude oil econometric model

Crude Oil: Autoregressive Model

The historical time series of crude oil can be decomposed into **three terms**:



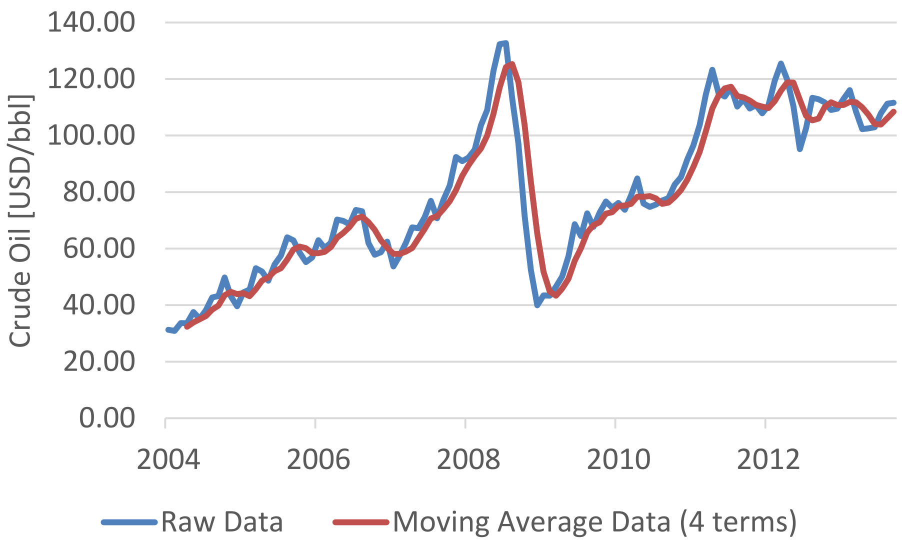
$$y(t) = T(t) + S(t) + I(t)$$

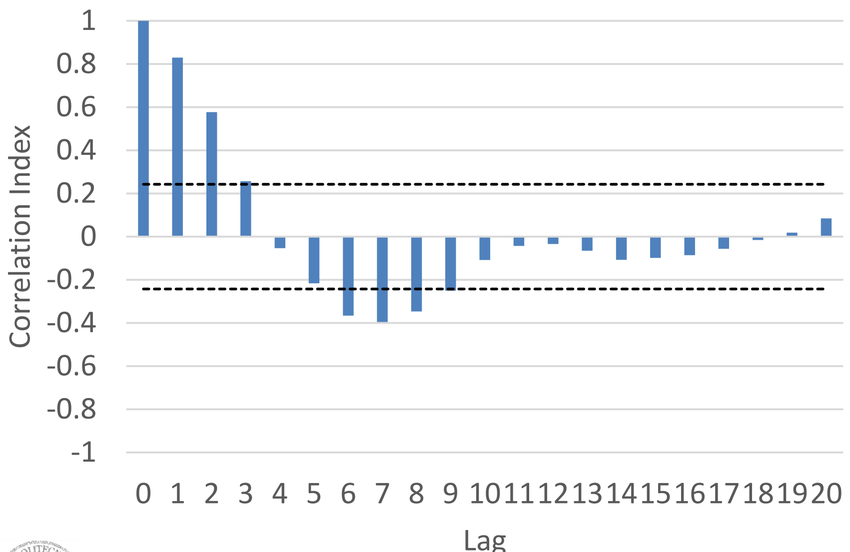
Trend: a trend exists when there is a long-term increase or decrease in measured data. The trend does not have to be necessarily linear.

Seasonal: a seasonal pattern exists when a time series is influenced by seasonal factors.

Irregular: the variations caused by neither trend nor seasonal terms are assimilated to stochastic contributions.

Crude Oil: Autoregressive Model



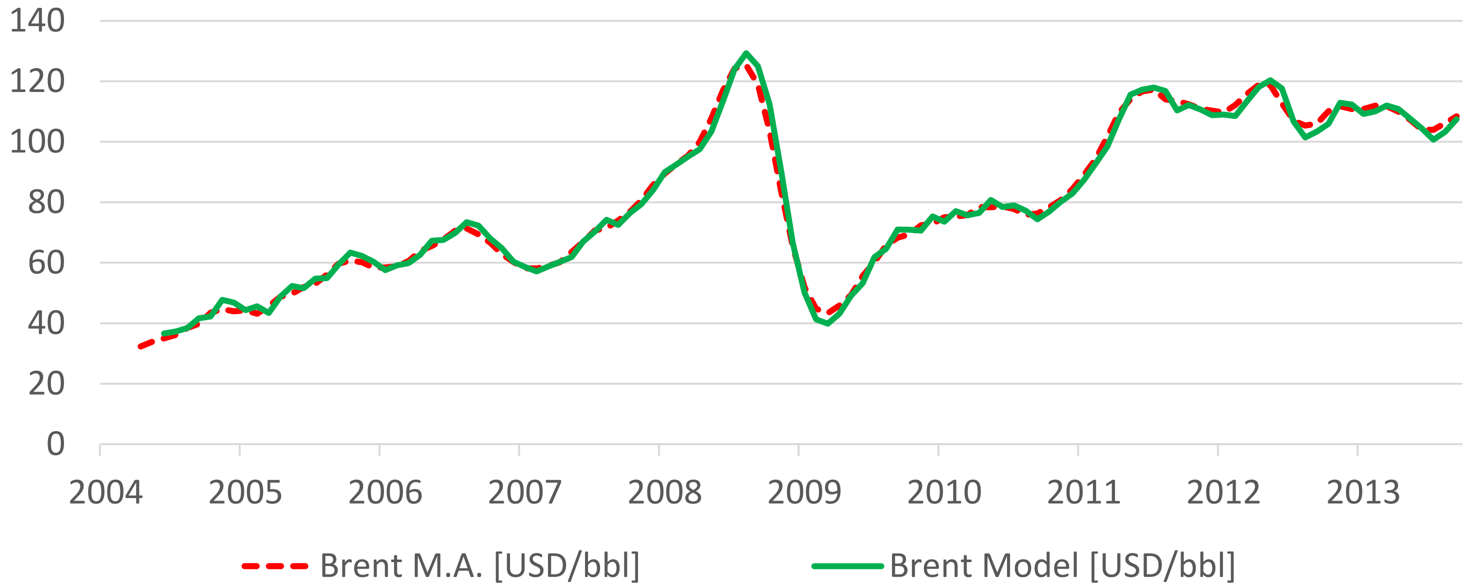


- A **4-term Moving Average** (M.A.) allows evaluating the **trend** component of CO time series;
- the M.A. operator introduces a **lag** in the averaged data. This lag (*i.e.* time delay), estimated in 2 months, is **negligible** for **Conceptual Design** applications.
- The **shock correlogram** shows how the shocks **depend** from previous values;
- the correlation is **high** for time delays equal to $\boldsymbol{t-1}$ and $\boldsymbol{t-2}$;
- the correlations at times $t-6$, $t-7$ and $t-8$ are not considered due to the risk of model overparametrization.

Crude Oil: Autoregressive Model

- By applying the information provided by the shock autocorrelogram, an **Autoregressive Model** of three parameters is eventually proposed:

$$P_{CO}^{Trend}(t) = A + B\,P_{CO}(t-1) + C\,P_{CO}(t-2)$$



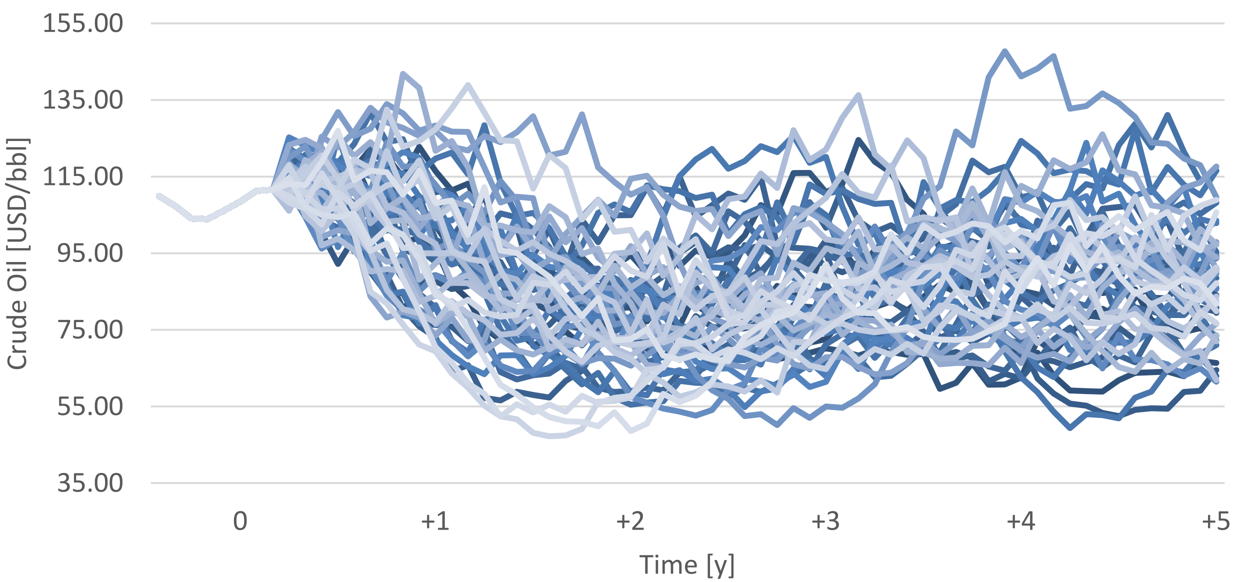
A	B	C	R^2
2.32898	1.82382	-0.85178	99.2%

The **correlation index** (R^2) is **99%**

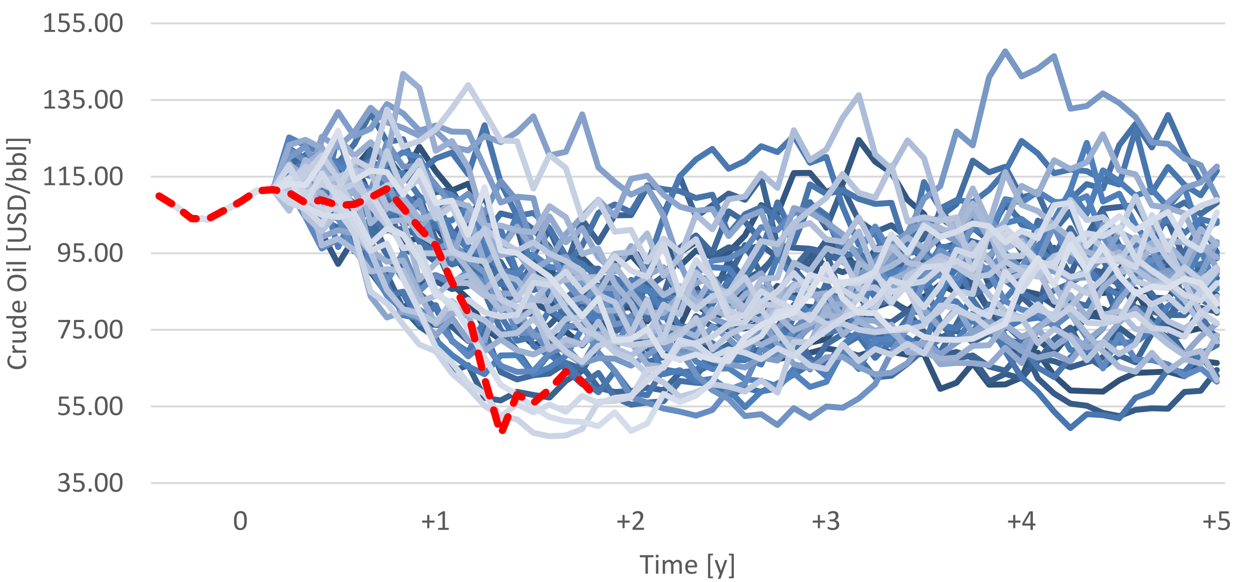
Crude Oil: Autoregressive Model

- The CO **trend scenarios** are generated according to the following formula:
- $P_{CO}^{Trend}(t) = [A + B\, P_{CO}(t-1) + C\, P_{CO}(t-2)] \cdot (1 + StdDev \cdot Random + Mean)$
- the **seasonal component** is not present in the CO time series;
- the **irregular component** $\varepsilon(t)$ is added to each scenario.

$$P_{CO}(t) = P_{CO}^{Trend}(t) + \varepsilon(t)$$



Crude Oil: Autoregressive Model



The Autoregressive model **is suitable** for PSE/CAPE applications

Future price scenarios

Future scenarios of commodity prices

- Once we have built the models for the price of commodities and we have also quantified their stochastic fluctuations, we can use these models to forecast the future prices and quantify possible scenarios.

$$P_{B,i} = \left(c_B + a_{B,0} \cdot P_{CO,i} + b_{B,1} \cdot P_{B,i-1}\right) \cdot \left(1 + RAND \cdot \sigma_B\right)$$

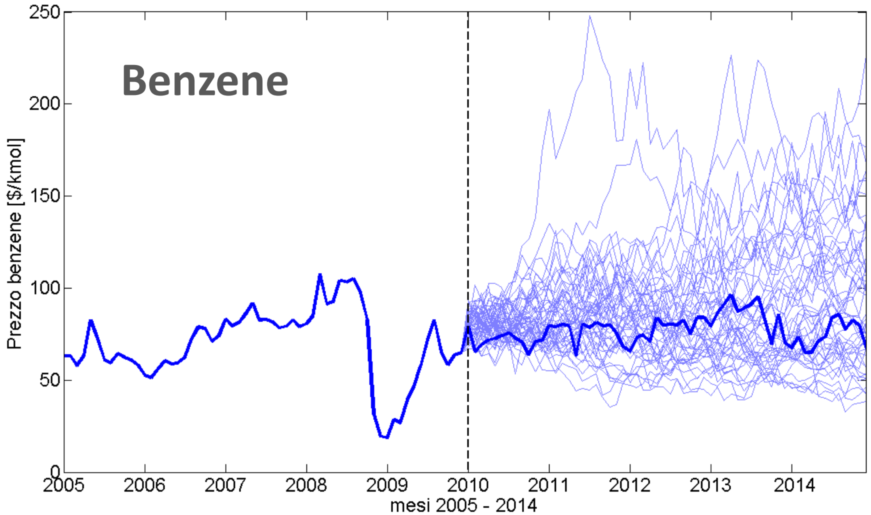
$$i = 1, \dots, nMonths$$

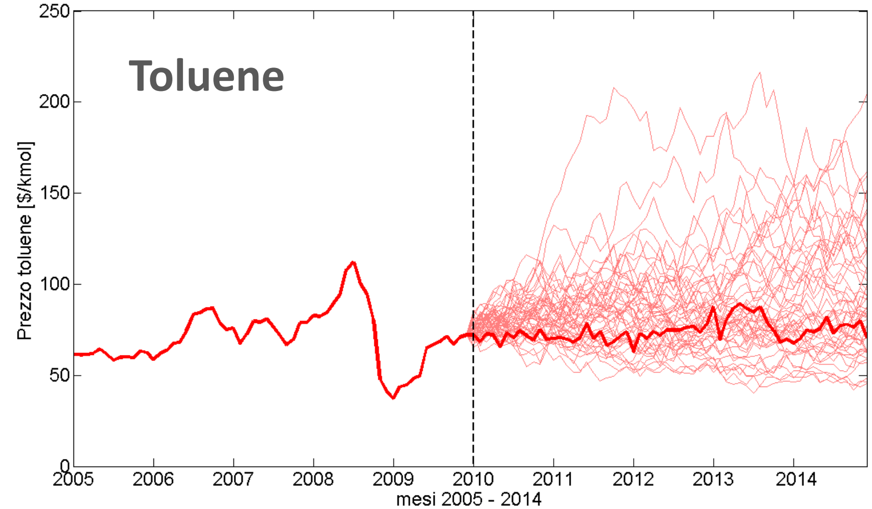
$$P_{T,i} = \left(c_T + a_{T,0} \cdot P_{CO,i} + b_{T,1} \cdot P_{T,i-1}\right) \cdot \left(1 + RAND \cdot \sigma_T\right)$$

- **N.B.**: it is worth observing that the price of commodities is forecast by means of **two distinct stochastic contributions** from **CO** and the **commodity** itself (*i.e.* $\sigma_{B,T}$ and σ_{CO}).

Future scenarios of commodity prices

- Here following are reported 50 distinct scenarios of the benzene and toluene price in the 2010-2014 purely forecasting period:





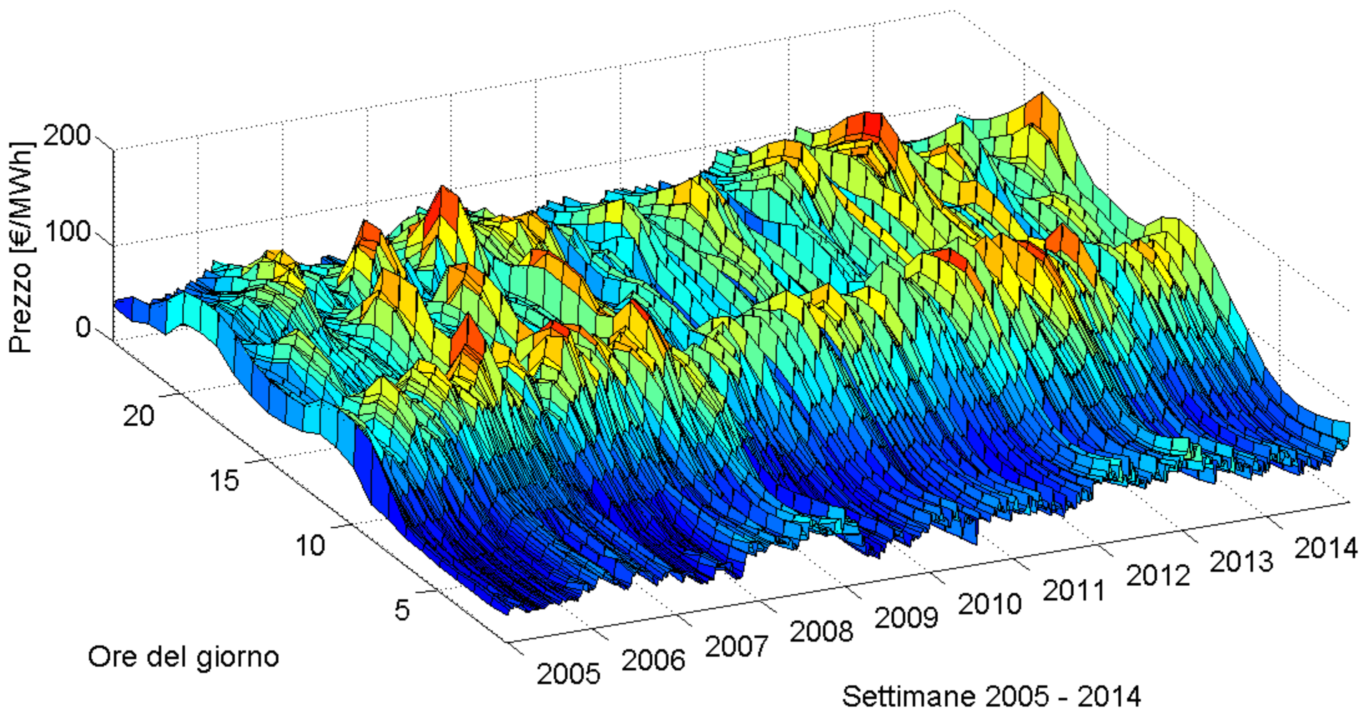
- **N.B.**: every forecasting scenario has a common basis represented by the same CO forecast scenario. Nonetheless, an additional source of stochasticity is introduced by the random contribution of the specific commodity that multiplies its standard deviation.

Future scenarios of electric energy prices

- The price scenarios of electric energy are generated by the following formula:

$$P_{EE,i,j} = \left[a_j + b_j \cdot P_{CO,i-t_{d,j}} + c_j \cdot \sin\left(\frac{2\pi \cdot i}{T_j} + \varphi_j \right) \right] \left(1 + RAND_i \cdot \sigma_j \right)$$

$$i = 1, \ldots, nWeeks \qquad j = 1, \ldots, nHours$$



Dynamic Economic Potentials

Dynamic economic potentials

- The same hierarchical approach to conceptual design proposed by Douglas in 1988 can be applied to the dynamic assessment of the economic potentials proposed by that methodology.
- We can coin a new paradigm for the design of industrial plants: the **Dynamic Conceptual Design** methodology. **This is based on the dynamic evolution of OPEX terms according to a set of economic scenarios that finally produce a distribution of economic potentials (at the different levels of the hierarchy)**.
- In the same way, we will have a set of dynamic economic potentials.
- Douglas (1988) proposed a hierarchy of 5 economic potentials, EPs.
- The level-1 economic EP remains the same also in the dynamic framework since it only discriminates and provides a criterion to choose between continuous and batch processes.
- Therefore, by placing before a **D** for the "**dynamic**" attribute, we state that:

DEP1 = EP1

Dynamic economic potential of level-2

- Proceeding with Douglas' hierarchical approach we have the level-2 EP, *i.e.* DEP2.
- It does not make sense anymore to assume the OPEX terms fixed for years (even decades).
- We also saw that the EP2 of HDA process changes completely according to the period when the commodities price is referred to.

	Benzene price	Toluene cost	**EP2**
Averaged 2005-2010 period	70.16 \$/kmol	72.19 \$/kmol	**–2.0318 M\$/y**
March 2008	107.79 \$/kmol	84.18 \$/kmol	**51.122 M\$/y**
December 2008	19.41 \$/kmol	41.17 \$/kmol	**–40.589 M\$/y**

- Therefore, we can introduce a new DEP2:

$$DEP2_k\left[\$/y\right]=\frac{\sum_{i=1}^{nMonth}\left(\max\left[0,\left\{\sum_{p=1}^{NP}C_{p,i,k}\cdot F_p-\sum_{r=1}^{NR}C_{r,i,k}\cdot F_r\right\}\right]\cdot nHoursPerMonth\right)}{nMonths/12}$$

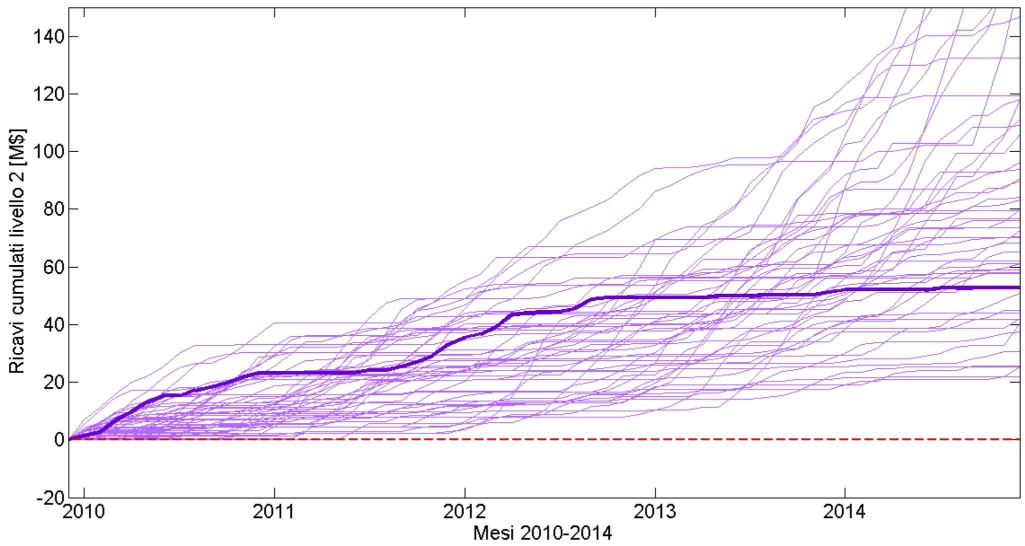
$$\forall k=1,\ldots,nScenarios$$

Dynamic economic potential of level-2

- **N.B.**: the DEP2 is not a single value. It is a distribution of values produced by a set of stochastic scenarios produced by the methodology presented and discussed before.
- The DEP2 suggests running the plant only when the revenues from selling the products are higher than the expenditures for reactants.
- One drawback or better one weakness of the DEP2 formulation is that it does not take into account the feasibility of running and stopping the production both in terms of **economic allocation of resources** and **physical stress and impact on the plant equipment**. It does not even take into account the transients due to switching on and off the production. These transients (*i.e.* start-ups and shut-downs) reduce the real periods of operation of the plant when the production specifications are respected (*i.e.* normal operating conditions).

Dynamic economic potential of level-2

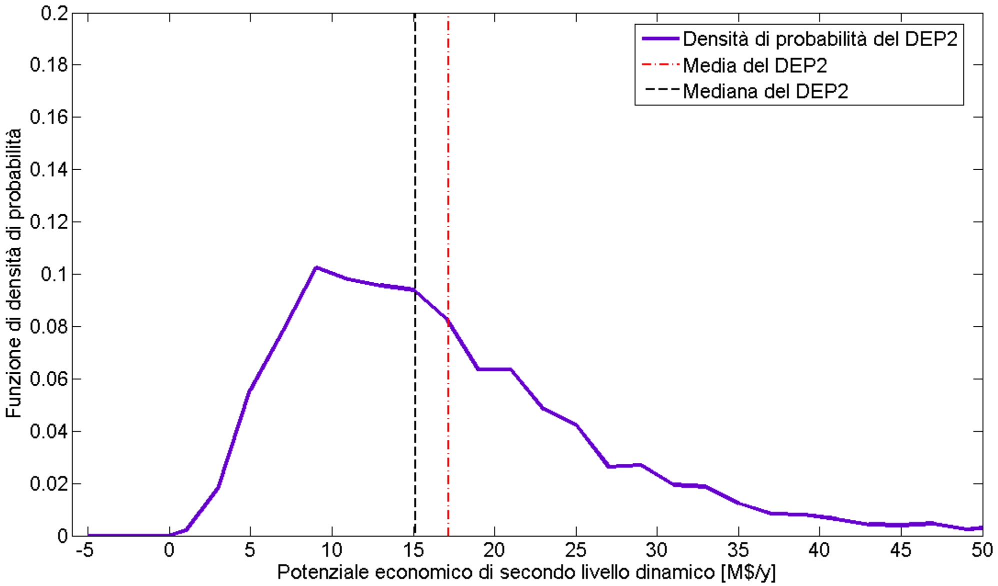
- The DEP2 formulation produces for any forecast scenarios a **monotonically increasing** trend of the <u>cumulative revenues at level-2</u>:



- **N.B.**: the periods when the cumulative revenues of level-2 are constant correspond to the periods when the overall OPEX terms of level-2 would be negative. The $\max$ function of DEP2 allows avoiding any reductions of the cumulative revenues.

Dynamic economic potential of level-2

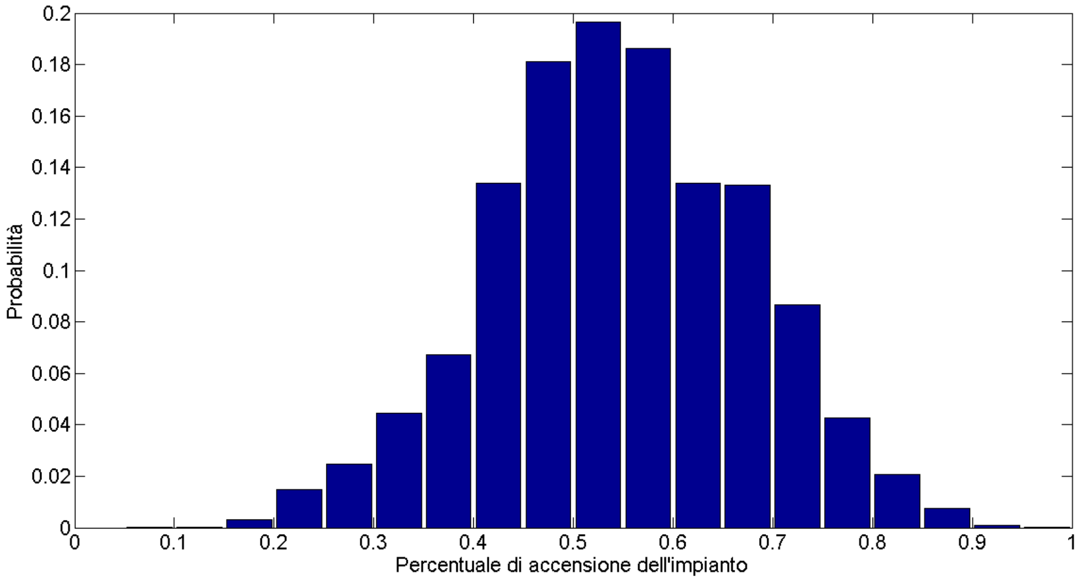
- By running a large number of simulations based on stochastic scenarios and by evaluating accordingly the DEP2 terms, we obtain the following distribution of DEP2 (the diagram summarizes 3000 distinct scenarios):



Mode [M$/y]	9.00
Median [M$/y]	14.80
Mean [M$/y]	17.31

Dynamic economic potential of level-2

- It is worth observing that the DEP2 value evaluated for the 2005-2009 period (with real values) is 8.81 M$/y which is consistent and coherent with the forecasts produced by the DCD methodology.
- In addition, it is also possible to evaluate the **fraction of the year when the HDA plant should be run** according to the forecast scenarios:



Mean	0.5418
Median	0.5333
Standard deviation	0.1271

Dynamic economic potential of level-3

- Increasing the detail of the hierarchical approach to economic assessment we propose the following formula:

No OPEX for the HDA reactor

$$Revenus3_{i,k}\left[\$/h\right] = \max\left[0, \left\{\sum_{p=1}^{NP} C_{p,i,k}\cdot F_p - \sum_{r=1}^{NR} C_{r,i,k}\cdot F_r - W_{compr}\cdot C_{EE,i,k}\right\}\right]$$

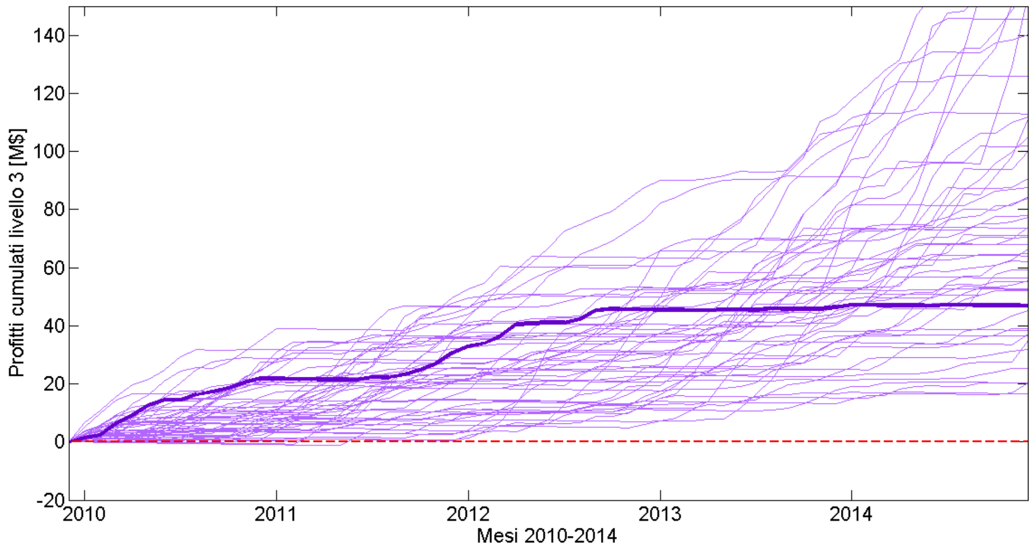
IC = installation cost

$$DEP3_k\left[\$/y\right] = \underbrace{\frac{\sum_{i=1}^{nMonths}\left(Revenus3_{i,k}\cdot nHoursPerMonth\right)}{nMonths/12}}_{\textbf{OPEXs}} - \underbrace{\frac{\left(IC_{react}+IC_{compr}\right)}{nMonths/12}}_{\textbf{CAPEXs}} \qquad k=1,\ldots,nScenarios$$

- The EE price, $C_{EE,i,k}$, is averaged for every time-band over a whole i-th month for every month of the k-th forecasting horizon.
- Since the currency of C_{EE} is in € whilst the DEP3 is in US$, a fixed €/US$ exchange rate can be assumed throughout the forecasting horizon (thus avoiding any further uncertainties on the financial side).

Dynamic economic potential of level-3

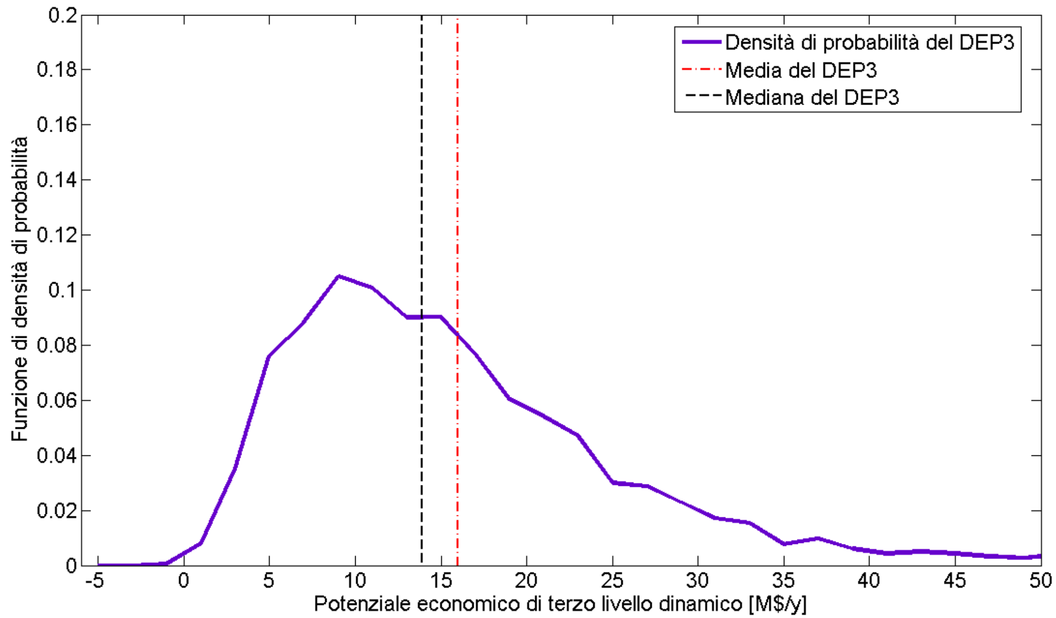
- A set of forecast scenarios allows evaluating the corresponding cumulative profit curves derived by the DEP3 assessment:



- As it happened at level-2, the plant is operated only when the revenues from selling the product(s) are higher then the OPEX term.
- Nonetheless, the negative contribution of CAPEX terms must be taken into account throughout the life of the plant. Consequently, <u>some scenarios can produce negative values of DEP3</u>.

Dynamic economic potential of level-3

- By increasing the number of simulated scenarios to 3000 we get a distribution of the cumulative DEP3 revenues that accounts also for some negative values:



Mode [M$/y]	9.00
Median [M$/y]	13.60
Mean [M$/y]	16.09

N.B.: in compliance with Douglas' theory, the dynamic economic potentials are monotonically decreasing.

Dynamic economic potential of level-4

- The DEP4 accounts also for the furnace and the separation system both in terms of CAPEX and OPEX terms:

$$Revenues4_{i,k}\left[\$/h\right] =$$

$$= \max\left[0, \left\{ \sum_{p=1}^{NP} C_{p,i,k}\cdot F_p - \sum_{r=1}^{NR} C_{r,i,k}\cdot F_r - \sum C_{EE,i,k}\cdot W_{electr} - \sum C_{steam}\cdot F_{steam} - \sum C_{H_2O}\cdot F_{H_2O} - C_{FuelOil,i,k}\cdot F_{FuelOil} \right\}\right]$$

$$DEP4_k\left[\$/y\right] = \frac{\sum_{i=1}^{nMonths}\left(Revenues4_{i,k}\cdot nHoursPerMonth\right)}{nMonths/12} - \frac{\sum_{e=1}^{nEquip}\left(IC_e\right)}{nMonths/12} \qquad k = 1,\ldots,nScenarios$$

- *nEquip* are all the pieces of equipment designed in the process flowsheet
- W_{electr} is the electric power absorbed by compressor and toluene recycle pump
- F_{steam} is the steam flowrate required by any of the heat exchangers (the plant works with high pressure (70 bar) and low pressure (30 bar) steam)
- F_{H2O} is the water flowrate required by any of the heat exchangers

Dynamic economic potential of level-4

- The furnace is heated with a fuel oil flowrate, $F_{FuelOil}$ whose cost depends on that of CO. From an econometric analysis of time series of CO and fuel oil prices it is possible to derive the following functional dependency:

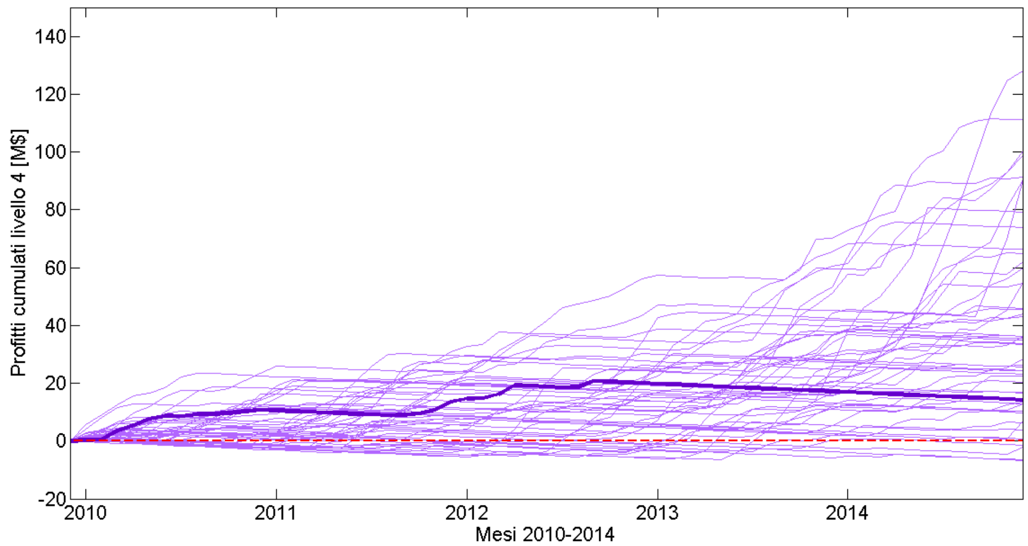
$$C_{FuelOil,i,k}\left[\$/kg\right] = 0.008329 \cdot C_{CO,i,k}$$

where C_{CO} is expressed in US$/bbl.

- Therefore, the cost of fuel oil depends directly on the economic scenarios considered for crude oil.

Dynamic economic potential of level-4

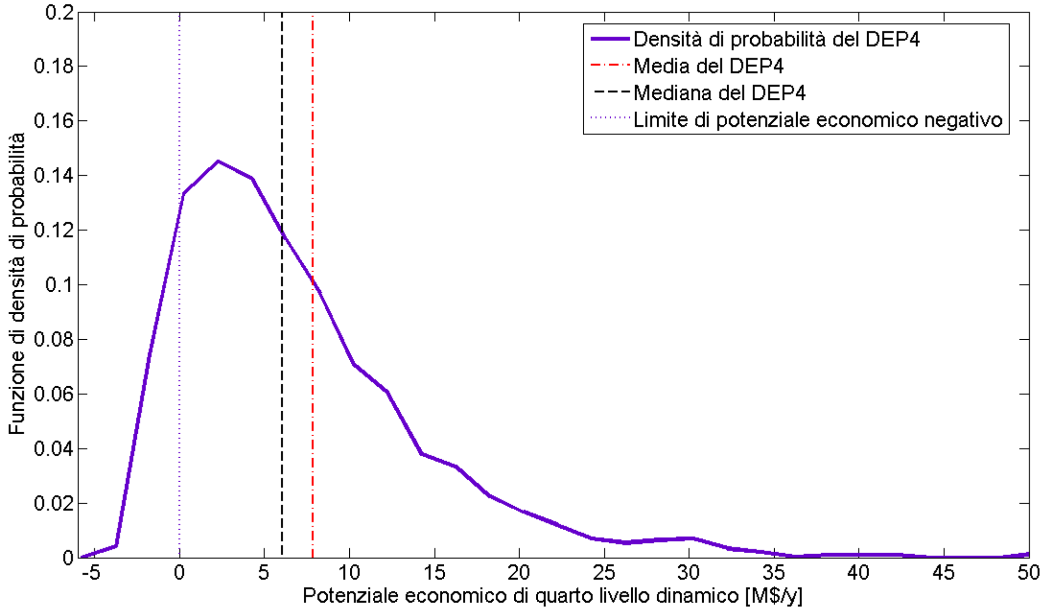
- Finally the cumulative values of the DEP4 forecast scenarios are the following:



- Respect to level-3, even with only 50 scenarios, the number of negative DEP4 values, over a five-year period, is rather high.

Dynamic economic potential of level-4

- The distribution of cumulative values of DEP4 is:

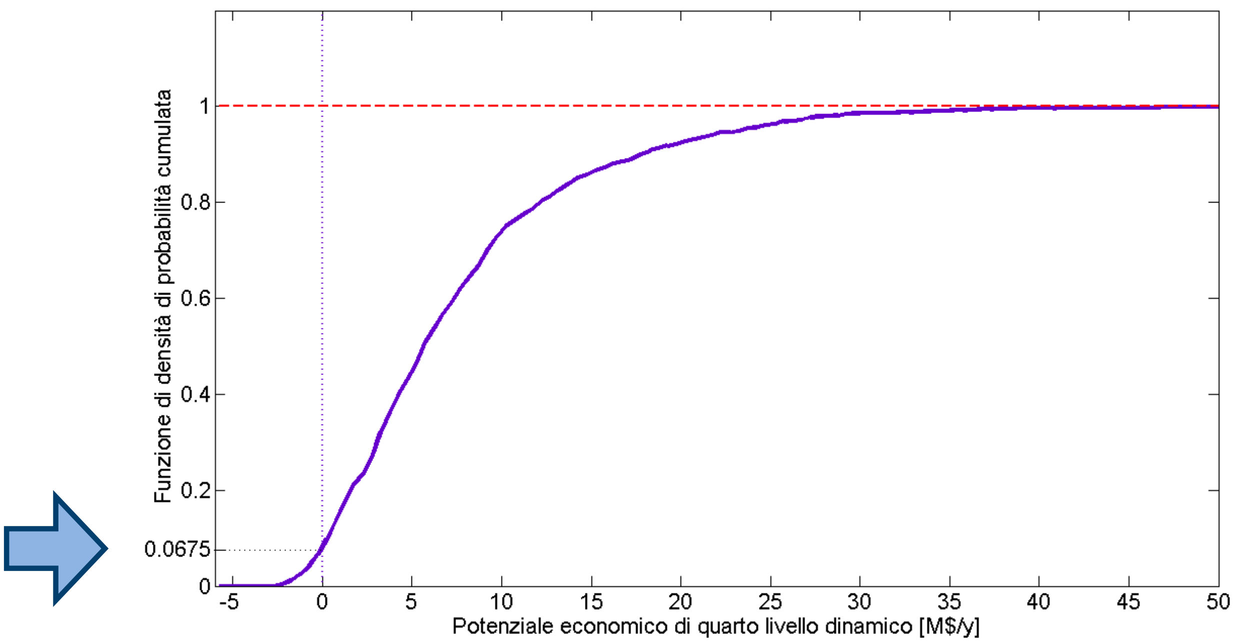


Mode [M$/y]	2.50
Median [M$/y]	6.12
Mean [M$/y]	7.59

N.B.: all the economic indicators of the probability distribution function have significantly decreased.

Dynamic economic potential of level-4

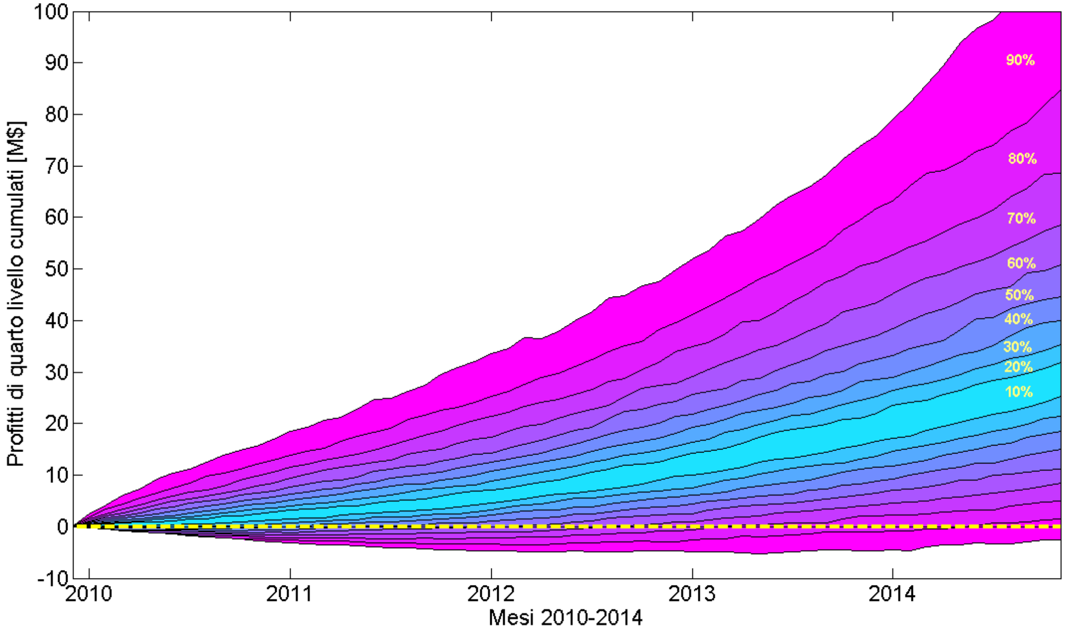
- Previous diagram showed a not negligible probability to get negative DEP4 values. This would mean that the HDA process is unfeasible and should be neither built nor operated.
- To quantify the probability to have an economically unfeasible HDA plant we can draw the cumulative probability density function:



N.B.: 6.75% of forecast scenarios show a negative DEP4, which means that in those circumstances the HDA plant is economically unfeasible

Dynamic economic potential of level-4

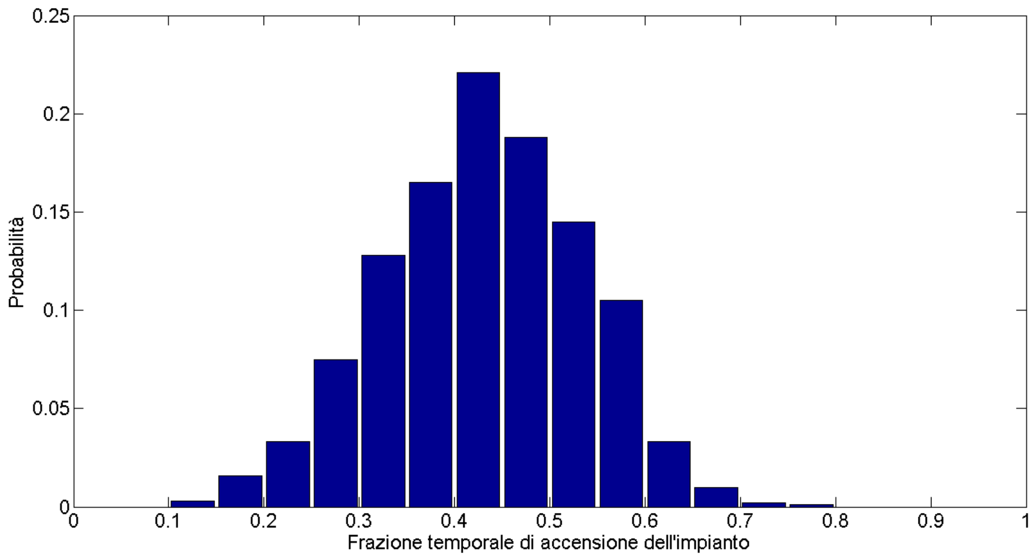
- The fan chart (also known as "*river of blood*" diagram) shows the same contents for the DEP4 scenarios in a different way:



- It is worth observing that the percentage of scenarios, which bring to a negative value of DEP4, decreases with time. Indeed, after one year of operation 35% of scenarios brings to negative values of DEP4. After five years such a percentage decreases to 6.75%. This is because in the very first years of operation the shutting-down of the process due to the $\max$ function does not allow recovering from the capital expenditures.

Dynamic economic potential of level-4

- Also for level-4, it is possible to evaluate the fraction of the year when the HDA plant should not be operated:

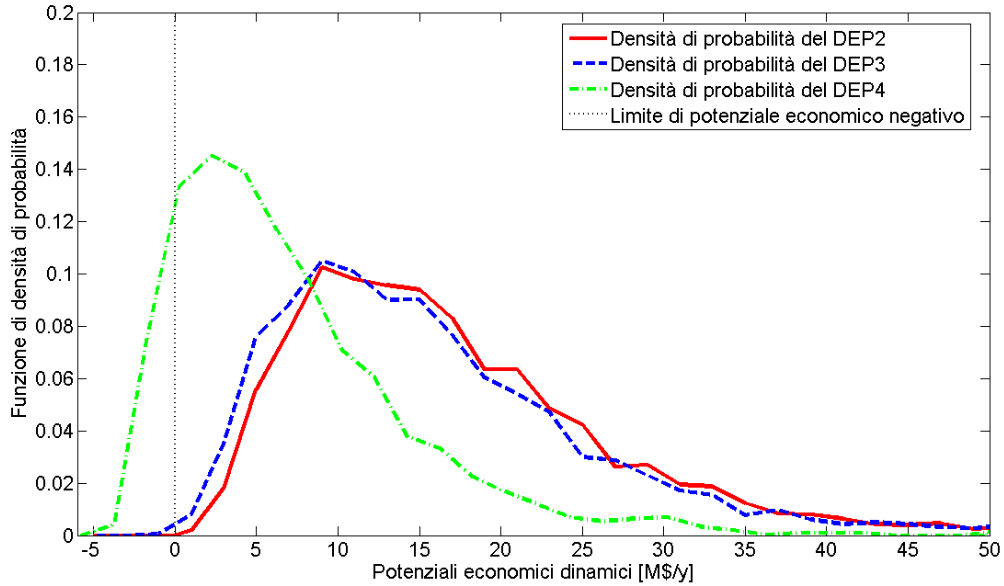


Mean	0.4212
Median	0.4196
Standard deviation	0.1126

- It is interesting to observe that according to DEP4 the plant should be operated for about **42%** of the time. This is perfectly in line with Milmo's (2004) comments: "*The long-term average utilization rate of HDA plants has been around **40 percent** because of the many occasions when the price of the toluene input was higher than that for the benzene output*".

Comparison of level-2, -3, -4 DEP estimates

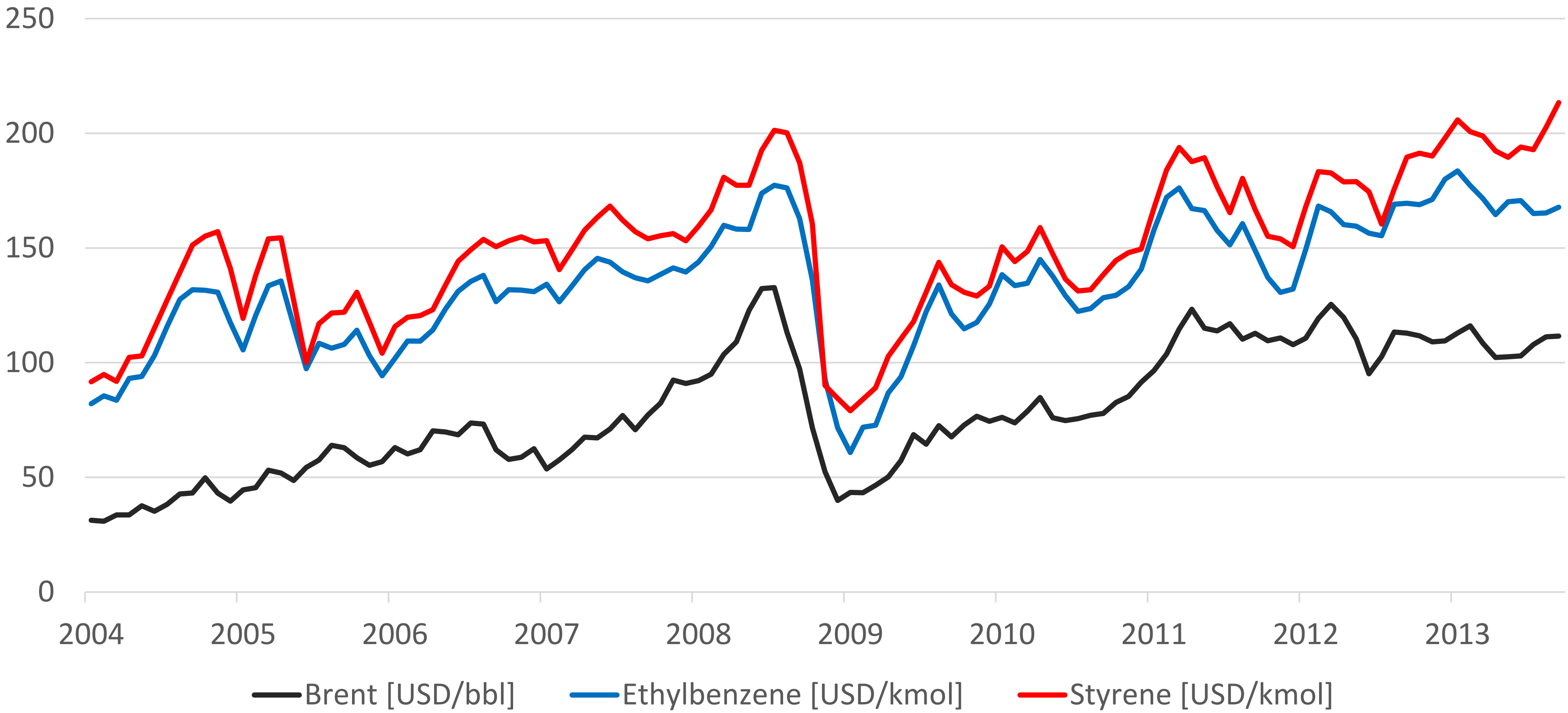
- The comparison of distributions of cumulative DEP2, DEP3 and DEP4:



- The increase of detail in the CAPEX and OPEX estimates of the hierarchical approach to dynamic assessment of forecast scenarios shows a progressive decrease of the economic feasibility of the HDA plant. In addition, the distribution of the cumulative DEP4 being narrower than that of DEP2 and DEP3 means a more reliable assessment of the economic potential of the plant due to the higher detail of investigation.

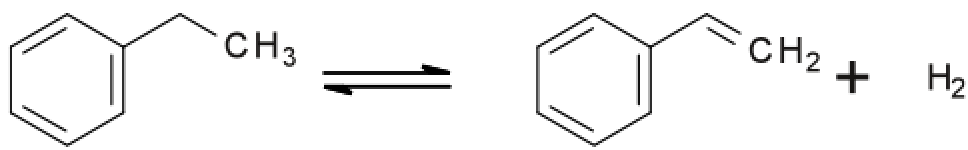
Case study
Styrene monomer plant

Market Variability



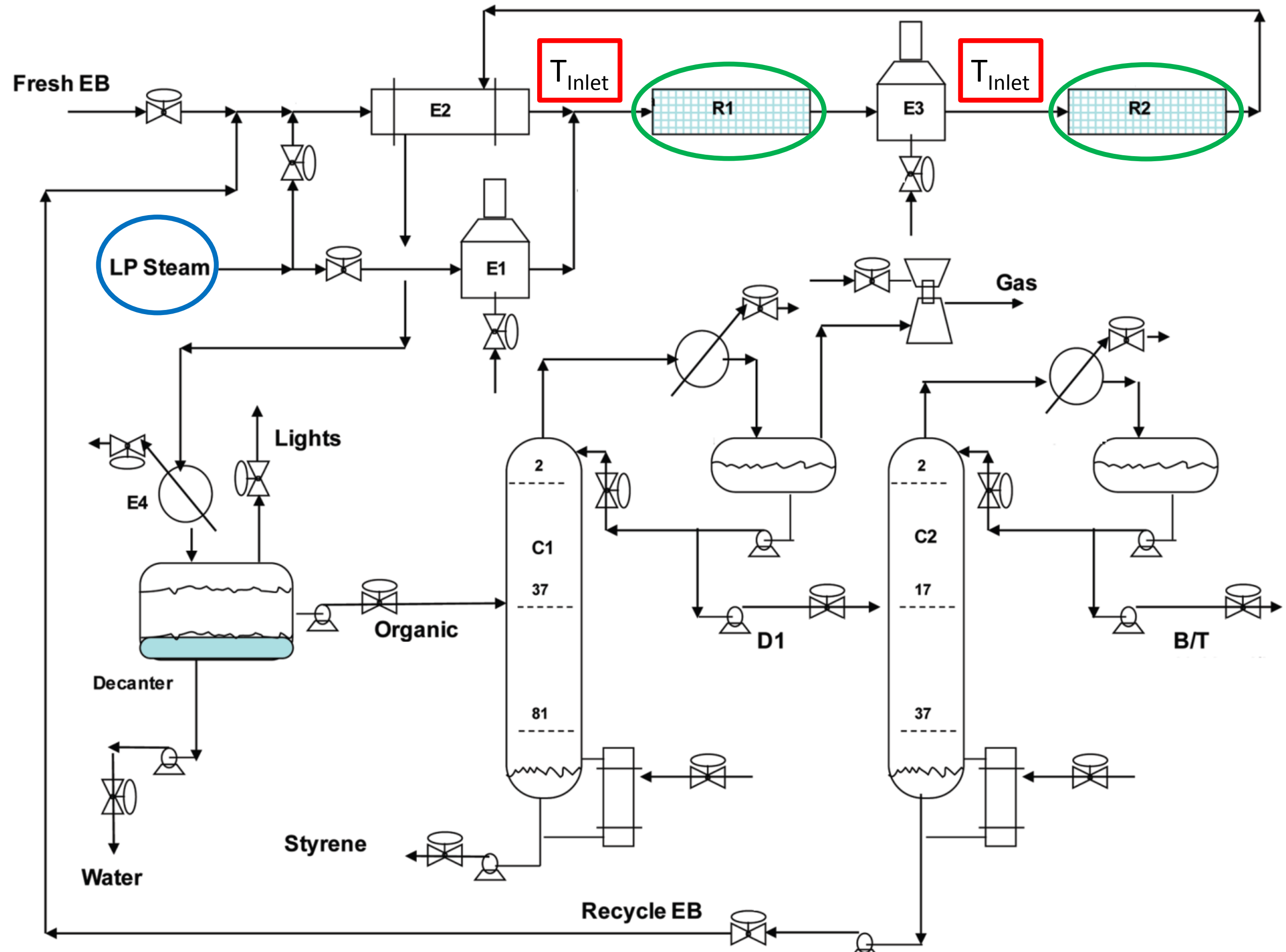
Do the price fluctuations affect the optimal design of chemical plants?

Styrene monomer plant: overview

- **Styrene monomer** is the most important aromatic compound;
- approximately **26.4 million tons** of styrene were produced in 2012;
- it is an intermediate to produce plastics and elastomers (*e.g.,* polystyrene, ABS resin, SBR rubber);
- the process from **ethylbenzene** accounts for 90% of global production;
- Catalysts: Fe_2O_3, Cr_2O_3, K_2CO_3;
- **Synthesis reaction**:
- 

$\Delta H_R = 29\ kcal/mol$
- **Side reactions**:
  - production of benzene and ethylene:
    $$C_6H_5 - CH_2CH_3 \rightarrow C_6H_6 + C_2H_4$$
  - production of toluene and methane:
    $$C_6H_5 - CH_2CH_3 + 2H_2 \rightarrow C_6H_5 - CH_3 + CH_4$$

Styrene monomer plant: overview



Optimization variables:

Steam flowrate; Reactor Volumes; Inlet Temperatures

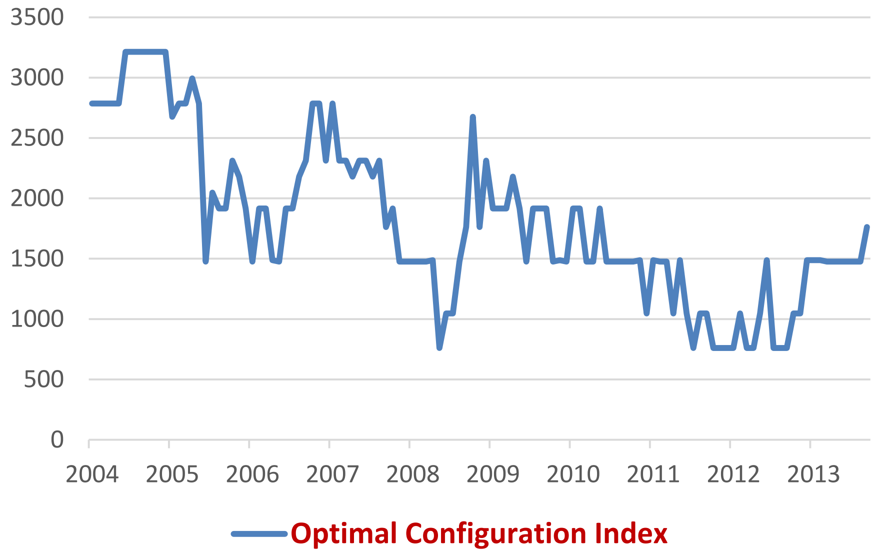
Luyben, W. (2011). Design and Control of the Styrene Process. Industrial and Engineering Chemistry Research. Vol. 50(3), 1231-1246.

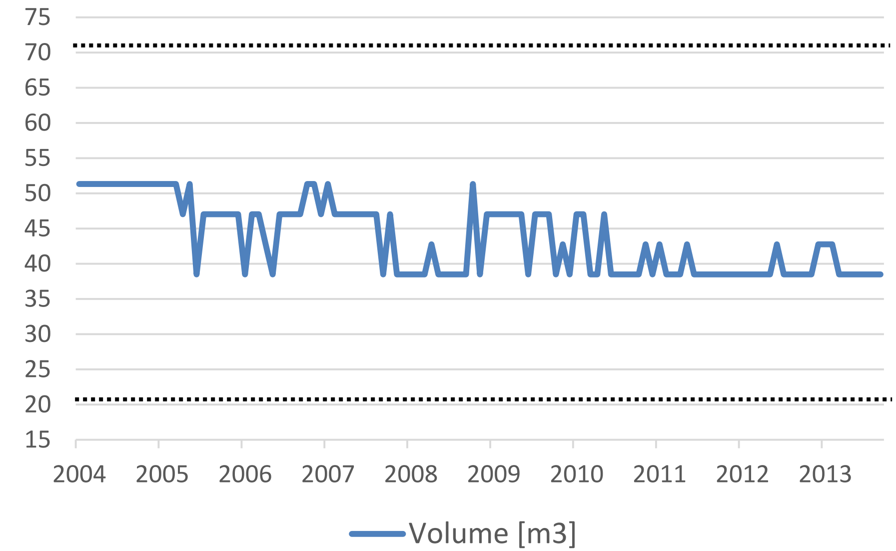
Operative Expenses Evaluation

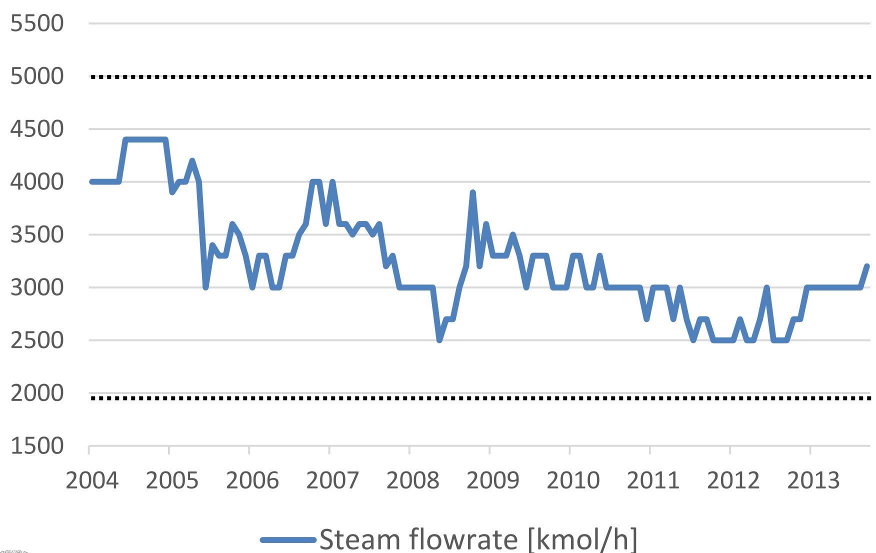
- **OPEX** terms vary according to Crude Oil (**CO)** fluctuations;
- **fuel oil** price is assumed proportional to **CO** price:
- $P_{Fuel\ Oil}(t) = 0.008329\ P_{CO}$

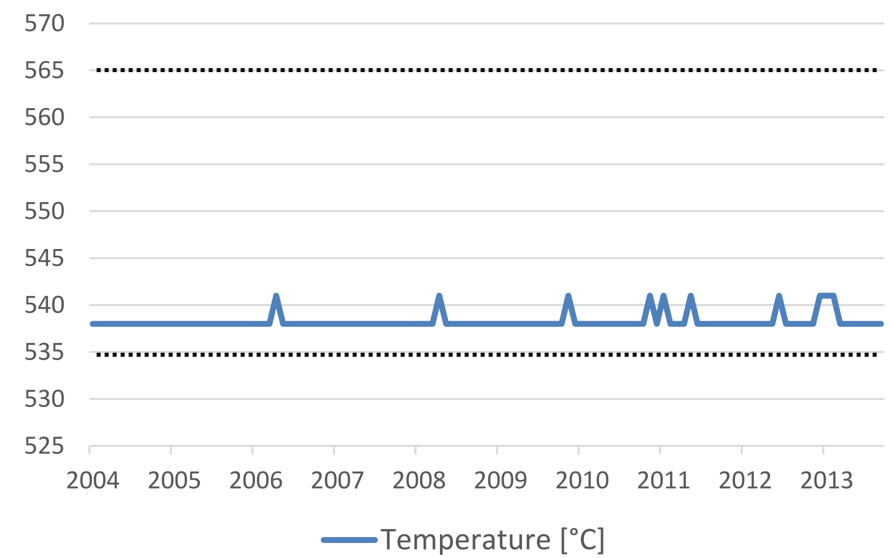
  with $P_{Fuel\ Oil}$ in USD/kg and P_{CO} in USD/bbl.
- the proportional constant (0.008329) is calculated from an analysis of fuel-oil historical price series;
- **low pressure steam** price (*i.e.* 200 °C, 4 bar) is evaluated by considering a boiler heated with fuel oil (with a heat of combustion of 10,000 kcal/kg)
- $P_{Steam}(t) = 0.009762\ P_{CO}(t)$
- with P_{Steam} in USD/kmol.

Effects of price fluctuations

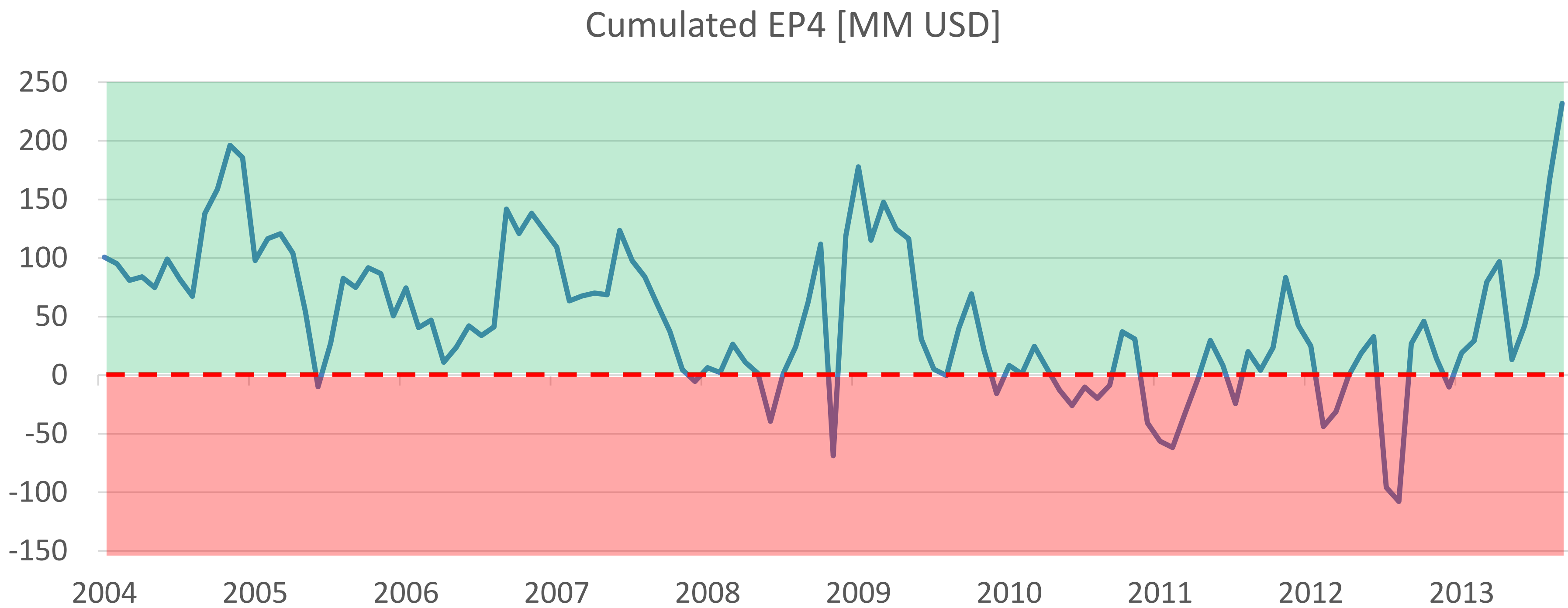








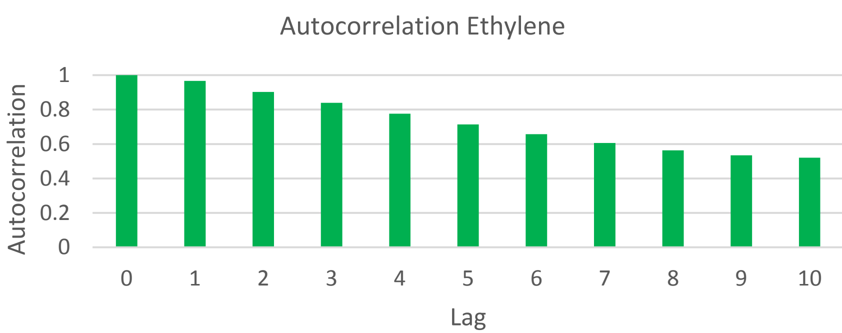
Effects of price fluctuations

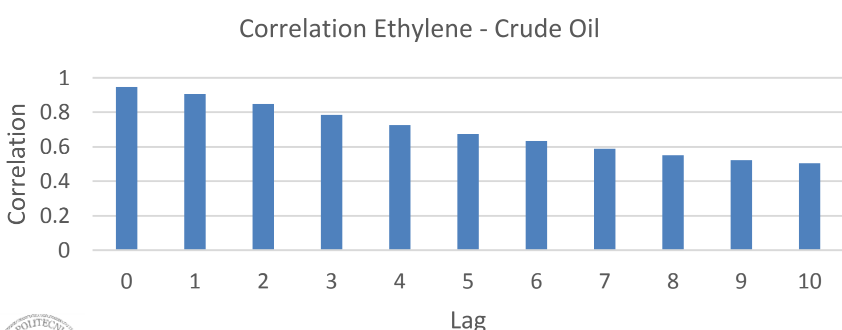


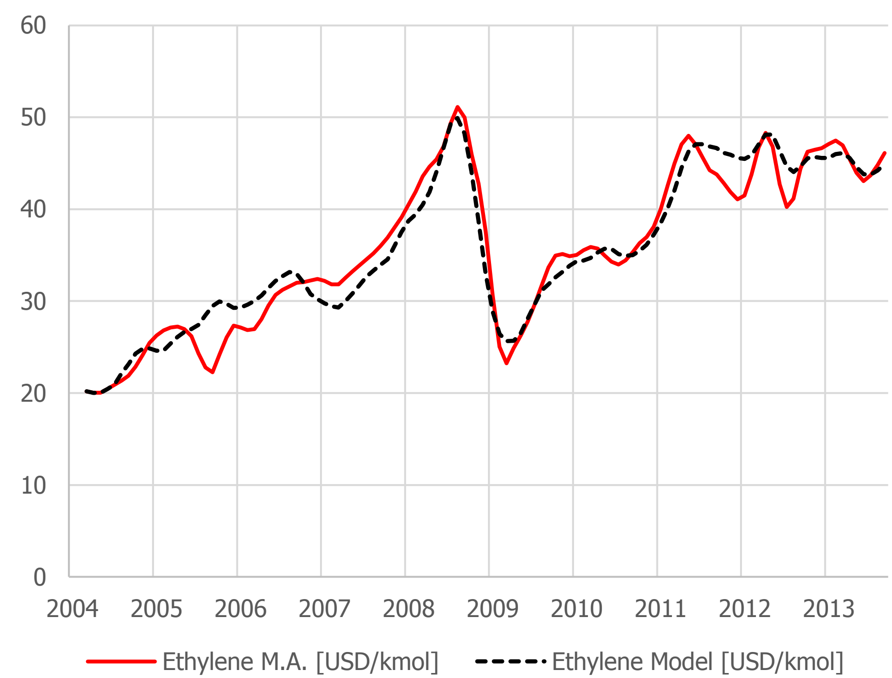
- **Optimal Configuration Index** varies considerably with price fluctuations;
- **Cumulated EP4** is an economic indicator that measures the process profitability and changes significantly with price fluctuations;
- → Conceptual Design **is not a reliable method** to perform process optimization.

Ethylene: Autoregressive Model

- The analysis of ethylene historical prices allows estimating the price of ethylbenzene;
- the **autocorrelogram** shows an autocorrelation of ethylene price series;
- a correlation with **CO** quotations is confirmed by the corresponding **correlogram**.
- $P_{Et}(t) = A + B\ P_{CO}(t) + C\ P_{Et}(t-1)$



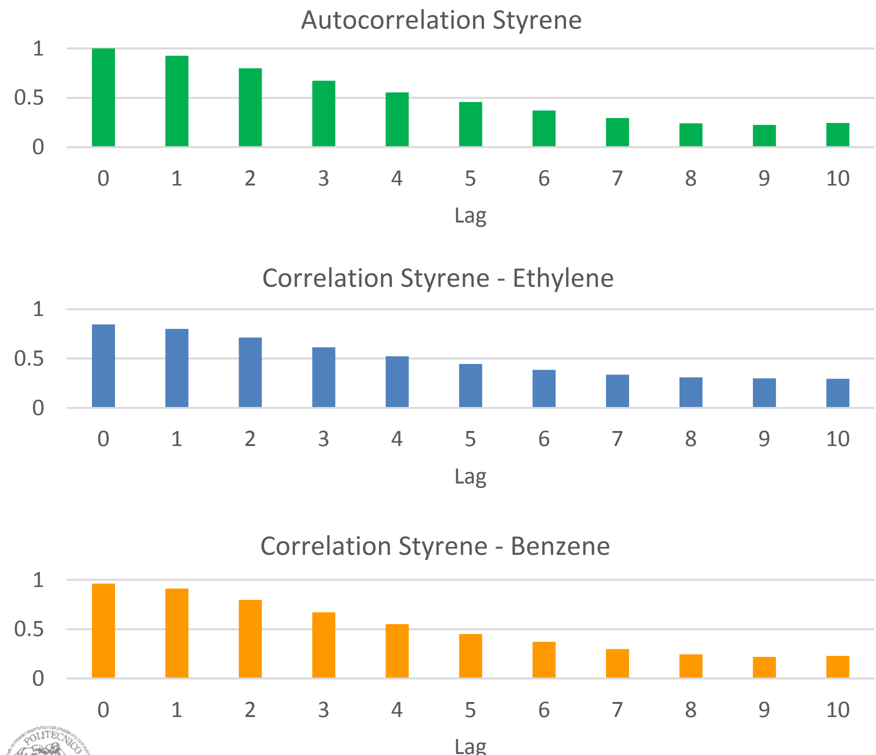


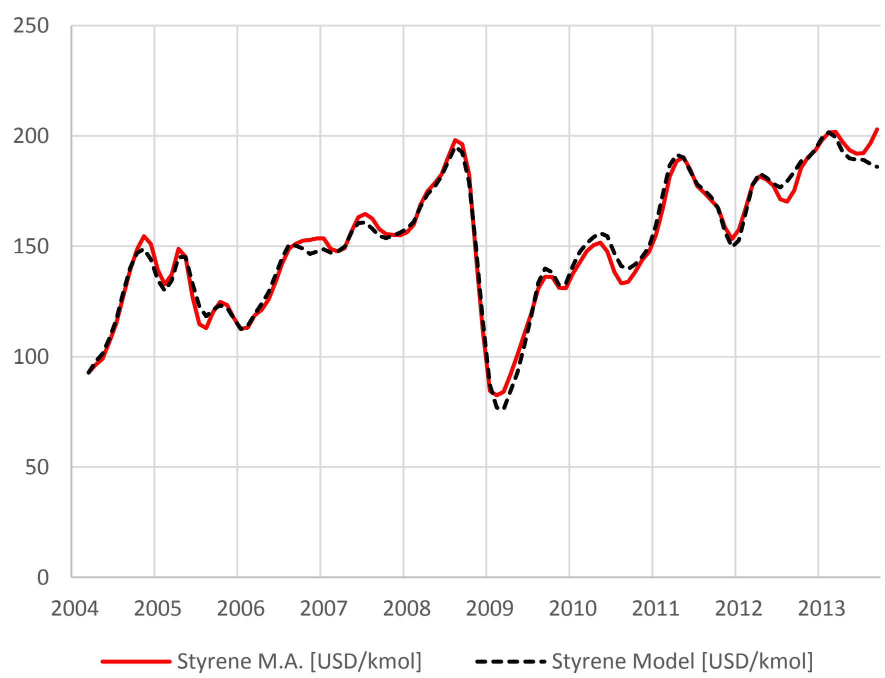


Styrene: Autoregressive Model

- The ethylbenzene process accounts for 90% of global styrene production. Ethylbenzene is largely produced by alkylation of benzene with ethylene;
- the **autocorrelogram** shows an autocorrelation of styrene price series;
- a correlation with **Ethylene** and **Benzene** quotations is also confirmed:

$$P_{Styrene}(t) = A + B\ P_{Styrene}(t-1) + C\ P_{Et}(t) + D\ P_{Benz}(t)$$

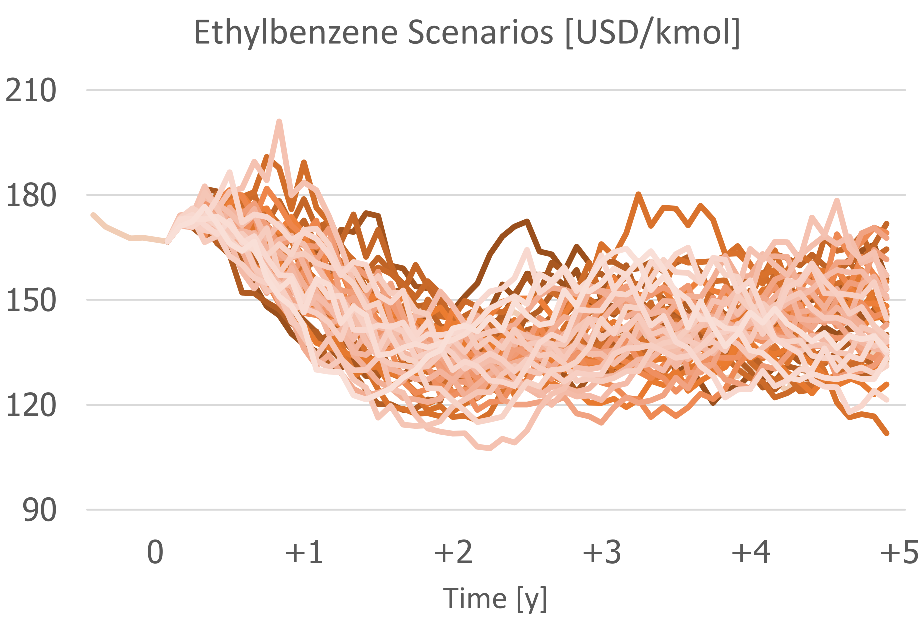


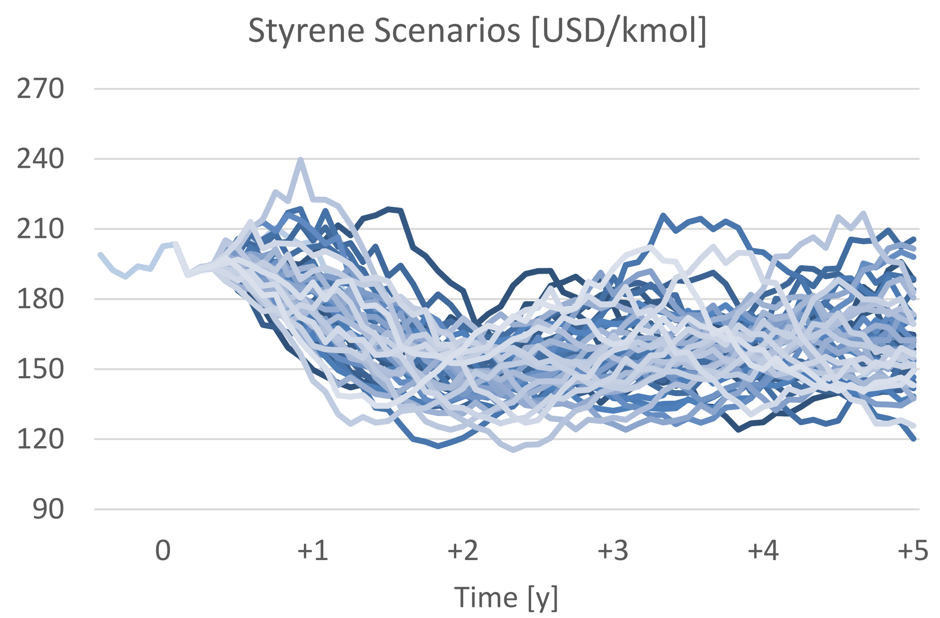


Ethylbenzene and Styrene scenarios

- **Ethylbenzene** historical price series is not available in the literature. Therefore, its price is estimated as the sum of **Benzene** and **Ethylene** molar prices with the addition of production costs (*i.e.* 20 USD/kmol according to the scientific literature*);

- Crude Oil price scenarios allow evaluating a set of corresponding price scenarios of **Ethylbenzene** and **Styrene**.





*MacDonald, J. (2005). Liquid Phase Alkylation of Benzene with-Ethylene. Dalhousie University.

Styrene monomer process optimization

- **Dynamic Conceptual Design**: an optimization of both geometric and nominal operating conditions is performed for every scenario of commodity prices;
- different scenarios lead to **different optimal points**.

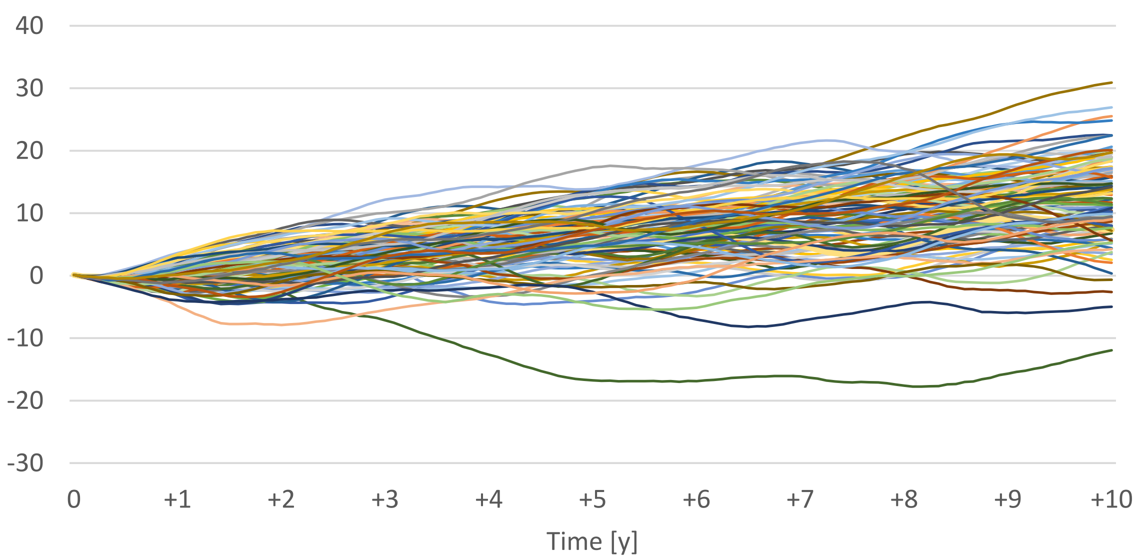
Configuration Index	Steam Flowrate [kmol/h]	Reactor Volumes [m^3]	Inlet Temperatures [°C]
#1488 [80.0%]	3000	42.76	541
#1784 [18.3%]	3200	47.04	538
#1916 [1.3%]	3300	47.04	538
#1498 [0.3%]	3000	47.04	538
#1047 [0.1%]	2700	38.48	538

- Configurations **#1488** and **#1784** optimize more than **98%** of scenarios.

Styrene monomer process optimization

- A **feasibility study** is performed for the most probable optimal configuration (*i.e.* #1488);
- the results show that the **economic potential** can vary significantly among different scenarios;
- the risk of **economic losses** is estimated to be about 5% (*i.e.* having a negative Cumulated DEP4).

Cumulated DEP4 for the optimal configuration #1488 [MM USD]



Mean	13.4	MM USD
Median	13.9	MM USD
Std Dev	7.56	MM USD
Skewness	-0.42	
Maximum	33.6	MM USD
Minimum	-25.5	MM USD

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