MODELLING GREEN HOUSE GASES EMISSION IN LP MODELS

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ABSTRACT

The regulations of industrial plants Emissions - existing or foreseen - and the introduction of the Carbon Tax and the Emission Trade are important factors of future refining economics.

All Process and Utility Plants are producer of Emissions that variously contribute to the Green House Effect: a system, integrated in the refinery planning model, that calculates the various Emissions of the planned operation, and compares them with the emission rights, will strongly help to respect the environmental constraints, minimising Rights Purchases in the Emission Trading Market, and foreseeing the Emission Rights that the refinery can instead sell in the same market.

SIMRAF, the Refinery LP optimiser, is equipped to define and calculate for each refinery gas, intermediate stream and products any type of Emission (CO_2 , SO_2 , NO_X , CH_4 , etc) that can be calculated from the processed crude oils quality data: CO_2 emission calculation is included as default. SIMRAF is also equipped to define the Global Green House Impact and one or more refinery Emission Rights and also the Emission purchases and sale, and Prices / Quantity Limits.

The introduction of these additional elements and constraints deeply influences utilities production policy and refinery mode of operation.

BACKGROUND

The sharp economic development of emerging countries in last years has greatly accelerated the environmental impact of the greenhouse gas emissions, as demonstrated by the Arctic Ices melting more rapidly then foreseen by the most pessimistic study, permitting now to reach Tokyo from New York sailing through the North Western passage.

The Kyoto Protocol, an international treaty signed by more than 60 countries including all Europe, commits the underwriters to bring, in the years 2008-2012, almost 5 % below their 1990 values the emission of carbon dioxide and five other greenhouse gases (methane, nitrogen oxides, sulphur exafluoride, hydrofluorocarbons, perfluorocarbon).

The Kyoto Protocol validity period is approaching to the end and the very co-operative approach of the new USA Administration, now similar to the European, and the international common understanding of the urgency to act against the climate change, makes reasonable to foresee that the majority of the industrial countries will soon adopt administrative measures to limit also with fiscal measures the greenhouse gas emissions of their industries.

Currently, the two prevailing fiscal measures options are either a Cap-and-Trade system, such as the one currently favoured by the European Union, or a Carbon Emissions Tax. Both raise the price for carbon and provide economic incentives to lower emission rates, but supporters of each policy seem deadlocked by opposing arguments1.

As explains the U.S. Environmental Protection Agency (EPA), Cap and Trade is a "market-based policy tool for protecting human health and the environment. A cap and trade program first sets a maximum limit, on emissions. Sources covered by the program then receive authorisations to emit in the form of emissions allowances, with the total amount of allowances limited by the cap. Each source can design its own compliance strategy to meet the overall reduction requirement, including sale or purchase of allowances, installation of pollution controls, implementation of efficiency measures, among other options.

Individual control requirements. are not specified under a cap and trade program, but each emissions source must surrender allowances equal to its actual emissions in order to comply. Sources must also completely and accurately measure and report all emissions in a timely manner to guarantee that the overall cap is achieved².

The allowances can be traded, so companies that reduce their emissions can sell surplus allowances to those who would have to pay to comply. Theoretically, this method allows companies to achieve their maximum allowable output at the lowest cost.

¹ Ilya Leybovich, Carbon Tax vs. Cap and Trade, Industrial Market Trends, March 17, 2009

² http://www.epa.gov/airmarkets/cap-trade/index.html

This approach has gained now support in USA Congress and from the Obama administration, with cap-and-trade provisions appearing in the latest Federal budget proposal. Under President Obama's 2010 budget plan, the Government would auction off all emission credits, generating as much as \$650 billion in cumulative Government revenue between 2012 and 2020. Considering that the carbon dioxide emission of USA is presently 6 billion tons per year, 48 billion tons in eight years, the USA Government is foreseeing to obtain an average of 13.5 USD per ton of CO_2 emission, that will be used to Reduce the Taxation of low medium income citizens, to finance Renewable Energy Programs an to reduce the Federal Budget Deficit.

Supporters of the cap-and-trade system claim it provides greater investor certainty by enabling businesses to estimate allowance prices needed for their work, offers greater environmental benefits by placing a fixed cap on emissions and may create a useful economic shock absorber because carbon allowance prices could be adjusted according to changing economic conditions³.

It could also promote broad international participation: developing countries would most likely become sellers in a global carbon allowances market and could expect to earn substantial profits. Meanwhile, because advanced economies can set the terms of access to their own markets, they would have considerable leverage to persuade those other countries to take on binding emissions targets.

The Environmental Defense Fund (EDF) claims that turning pollution reduction into marketable assets will also encourage technological and process innovations, citing the success of the Acid rain cap-and-trade program of the 1990s to support the new policy⁴.

The Carbon Tax is a less complex option that asks carbon dioxide emitters to pay a tax for every ton of pollution they produce. Proponents of the carbon tax argue it offers a direct profit incentive for the development of emission-reduction technology and encourages scaling back carbon pollution. According to carbon tax proponent Carbon Tax Centre, a first-year tax rate of \$15 per ton of carbon dioxide coupled with incremental rate increases of \$10 per ton each year would lower emissions to 25 percent below 2005 levels by 2022⁵.

³ http://whatmatters.mckinseydigital.com/the_debate_zone/carbon-tax-vs-cap-and-trade

⁴ http://www.edf.org/page.cfm?tagID=1085

⁵ http://www.carbontax.org/blogarchives/2009/03/06/new-larson-bill-raises-the-bar-for-congressional-climateaction/

CAP AND TRADE IN EUROPE

In May 2002 the European Community ratified the Kyoto Protocol committing to reduce globally of 8 % its green house gases emissions against the 1990 values assigning different % reduction to each country, according to its industry conditions and emissions at that time, assigning for example to Italy the goal of a 6,5% reduction.

The Kyoto Protocol became operative in February 2005, foreseeing flexible arrangements to favour the objectives achievement, otherwise too much expensive for the European Union countries.

The European Community Instruction 2003/87/CE on Emission Trading started between its countries an exchange system of EUA, *European Unit Allowances* to emit 1 ton of Carbon Dioxide correspondent to 1 ton of Green House gases.

In the European Cap and Trade System each Government allocates yearly to the industries linked with energy production or consumption the total EUA assigned to the country by the European Community.

The national amount of EUA is distributed free of charge, following rules agreed in each country between Government and Industry Organisations.

The application to be submitted for an emitting industry depends as well on national rules and can be long and complicated: for instance in Italy, each emitting industry needs to declare in advance the amount of foreseen emissions, measurement systems and errors, each source involved by the process (in case of refineries furnaces, flares but also maintenance operations like catalyst regeneration). Any procedure must be approved by the Ministry of Environment and the declared emissions are to be certified yearly by an organisation authorised by the Government.

Usually the EUA assigned are lower then the real emissions of each industry, so at the end of the year, if they have not provided to reduce its emissions burning alternative fuel or buying instead of producing utilities as Electric Energy or Steam or Hydrogen, the industries have to buy on the Emission Trade Market the quantity of EUA necessary to match his emission allowance, from industries that dispose of EUA in excess because they are producing renewable energy, or because they did not use their EUA for different reasons. If the industry will not find the necessary EUA on the market, starting from 2008 they will pay a fine of 100 Euro for each lacking one (previously the fine was 40 Euros).

During the year it is possible to trade EUA may be selling them when the market is high and trying to buy when the market is down, for example when the emission allowances expiration date it is approaching and some industry can find to dispose of past year EUA in excess: in the last years the EUA market value ranged between 30 to 10 Euros.

The emission allowances for a country are agreed with the European Community each year, in a progressive trend of reduction: as an example the EUA assigned to Italy for the period 2008-2012 are the following:

Industry Sectors	Millions EUA per Year
Thermal Electric Energy Production	85.29
Other combustion Plant (Tele-heating, etc.)	17.89
Oil Refineries	19.06
Metals Production	22.72
Minerals Production (Cement, glass, ceramics, etc.)	34,65
Other	5,09
New Plants	16,93
Total	201,63

Table 1: EUA distribution over industry sectors in Italy period 2008-2012

For the Italian Refining System are then available 19,06 million EUA per year, 25 % less of the previous allowances, and each refinery has its allowance calculated according with well defined formulas of the Allocation National Plan (ANP)⁶.

Figure 1 reports an excerpt of the Italian Allocation Plan detailing the distribution of the Cap assigned to the refining sector.

⁶D.lgs. 4 Aprile 2006, Decisione di assegnazione delle quote di CO2 per il periodo 2008-2012, 20 Febbraio 2008

D.lgs 4 aprile 2006, n. 216 - Decisione di Assegnazione 2008-2012

Elenco settoriale 3: Implanti di raffinazione

N Aut	Ragione Sociale Del Gestore	Denominazione Impianto	Quote 2008 - 2012 ²⁴ [t CO ₂]
42	ESSO ITALIANA S.r.L.	RAFFINERIA DI AUGUSTA	1.716.530
54	S.A.R.P.O.M S.p.A.	S.A.R.P.O.M S.p.A.	1.070.012
99	Alma Petroli Spa	Raffineria di greggi e oli pesanti	19.107
103	IPLOM S.p.A.	IPLOM S.p.A Raffineria di Busalla	219.997
223	ENI SpA - DIVISIONE REFINING & MARKETING - RAFFINERIA DI SANNAZZARO	ENI SpA - DIVISIONE REFINING & MARKETING - RAFFINERIA DI SANNAZZARO	1.718.236
231	TAMOIL RAFFINAZIONE S.P.A.	RAFFINERIA DI CREMONA	407.187
240	IES-Italiana Energia e Servizi SpA	Raffineria di Petrolio	316.479
335	Eni S.p.A. Divisione Refining & Marketing Raffineria di Venezia	Eni S.p.A. Divisione Refining & Marketing Raffineria di Venezia	646.114
561	Api raffineria di ancona S.p.A.	Raffineria api di Falconara Marittima	462.932
613	ENI SpA Divisione Refining & Marketing Raffineria di Livorno	Eni SpA Divisione Refining & Marketing Raffineria di Livorno	505.694
674	Raffineria di Roma S.p.A.	Raffineria di Roma	369.270
759	Eni S.p.A. Divisione Refining & Marketing - Raffineria di Taranto	Raffineria di Taranto	848.673
802	Raffineria di Milazzo S.C.p.A.	Raffineria di Milazzo	1.528.028
808	Raffineria di Gela S.P.A.	Raffineria di Gela S.P.A.	2.938.704
822	ERG RAFFINERIE MEDITERRANEE S.p.A.	RAFFINERIA ISAB IMPIANTI NORD	795.692
823	ERG Raffinerie Mediterranee SpA	Raffineria Isab Impianti Sud	1.024.193
826	ERG NUOVE CENTRALI SpA	ERG NUOVE CENTRALI - IMPIANTI NORD	1.748.226
827	ERG NUOVE CENTRALI SpA	ERG NUOVE CENTRALI - IMPIANTI SUD	587.543
841	Saras S.p.A	Saras SpA	2.137.383
Totale			19.060.000

²⁴ Assegnazione media annua per il periodo 2008-2012

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Figure 1 – EUA Distribution in Italian Refining Sector

PROBLEM DEFINITION

An average modern European refinery processing 5 million tons per year of crude oil, has an internal consumption for oil processing and energy production ranging around 5 % of the processed crude oil, that is 250.000 tons per year of oil products and gases, corresponding to about 720.000 tons of Carbon Dioxide emission.

Assuming that the Government will assign to the refinery 600.000 EUA, corresponding to 83 % of the consumption, to avoid to buy EUA on the market the refinery will have to reduce its Carbon Dioxide Emissions of 120.000 tons per year, or instead buy EUA at a total cost ranging between 1.2 to 3.6 Millions Euros per year; in case it will not succeed to find a EUA seller, the refinery would have to pay a fine of 12 million Euros per year.

The available ways to reduce the emissions other than increasing the heat exchange or furnaces efficiency, are various, for example to burn Natural Gas that to produce the same heat emits less Carbon Dioxide than Fuel Oil, or reducing the utilities internal production buying more Electric Energy and Steam from external sources, etc.

The economic convenience to adopt different alternative decisions is linked to the availability and the market price of crude oil, fuel oil, natural gas, electric energy and also EUA, market prices that are continuously changing: for this reason it will be useful to dispose of a technical and economical model able to optimise the technical and economical variables, but also to optimise the global emission that now with the EUA of the Cap and Trade System has also a market price.

To model in a simple way all these aspects, it will be necessary to calculate the emissions linked to each crude oil processing, plant by plant, and to each utility production and to oblige the model to respect the global limit assigned by the public administration: the Prometheus Decision Support System, has been upgraded to reach these goals with the amicability that is one of its main characteristics.

PROMETHEUS APPROACH

The Prometheus Decision Support System is a user-friendly suite of applications for refinery planning and scheduling activities covering the entire supply chain from crude oil logistics to finished products distribution.

Differently from other commercial applications, SIMRAF has been specifically designed to assist Oil Industry Professional to achieve reliable modelling and complex systems optimisation with no need of specific Linear Programming expertise.

To create this software, many years experts in process refining, information technology and operational research have been utilised, trusting that a real efficiency improvement will be obtained when the refinery managers and operators will be able to calculate autonomously the impact of thousands of variables (technical and economical), that affect every day refining profitability: too many to be accounted for, at the same time, without this type of tools: now also the emission variables.

Now are available software tools using the same database, the same plant simulators and blending methods, that all together form a Decision Support System.

For the Emission Modelling two DSS tools are useful: CUTS, for Crude Oil Characterisation and SIMRAF, the Refinery Linear Programming Optimiser

CRUDE OIL CHARACTERISATION WITH CUTS

CUTS is a crude oil quality data base builder able to provide a very accurate crude oil qualities distribution in narrow cuts starting from the available data bases, and also starting from a limited number of laboratory analysis data, and then providing to the crude oil recutting as requested.

CUTS characterises every Crude Oil as a mix of pure components (C5 minus) and "pseudo-components" (C6 plus), which overall cover the entire crude boiling range. Each pseudo component envelops pure components boiling in a narrow range of 10/30 °C. This type of characterisation is quite "unusual" for planning and scheduling commercial applications, but permits to embed shortcut plant simulators into the models: the level of characterisation that is normally available from a typical crude assay does not permit to calculate with reliable results the properties of the crude oil fractions different from the ones analysed: CUTS' elaborates the crude assay data, finding an harmonic and consistent distribution of property values to pseudo-components. Once the pseudo-components property values are available, it is possible to estimate the properties of any fraction of the crude oil, keeping the results consistent with the crude assay data.

CUTS property values calculation is based on a multidimensional regression on assay data. The software distributes properties of the original assay, finding the best agreement between the natural curve shape and the input data. The algorithm is designed to calculate consistent values for contiguous pseudo components, while special operating parameters are available to harmonise the shape of the resulting curve, if necessary.

CUTS also provides proper user calibration and takes care of reliability of input data: if the original assay is consistent, fraction and global balances will be always satisfied, otherwise inconsistent input data will be highlighted. The curves are always validated by comparison with original input values.

Accurate crude oil characterisation is fundamental for the reliable simulation of each element involved with refinery operation, including the prediction of refinery emissions: the amount of EUA associated to refinery processing is intimately connected to crude oil quality which affects quality, type, composition and amounts of the material burned and flared.

REFINERY LP OPTIMISATION WITH SIMRAF

SIMRAF is a refinery modeller, including plant simulators based on the crude oil narrow cuts available in its internal library and fully customisable to actual plants' performances, makes easy to build every refinery processing and utilities production: specifying the crude oils choice, products specifications and prices, it allows fast and accurate analysis of refinery's profitability in alternative operating conditions and marketing scenarios. Linear Programming and recursive methods for stream pooling and investment studies are bundled together in a easy to use interface.

SIMRAF accurately calculates yields, qualities, fractionation tails, using consolidated Blending Methods, and easy to consult reporting, now extended also to Emissions. Methods for solution analysis, model diagnostic, ranges inspection and infeasibilities management are available.

SIMRAF can be used also for multi period simulations, defining for each period different economics, plant capacities, raw materials and also emissions; in this option the intermediate tanks stock capacity controls the transfer of streams, products and crude oils from one period to another.

It is possible also to simulate a group of refineries sharing raw materials and product markets, including crude oil and product distribution to demand areas, pipelines and other means of transportation and loss control. What makes SIMRAF particularly adequate for Emissions calculations is the complementary application of simulation and optimisation technologies that permits to calculate and update the quality database used for matrix generation and optimisation according to Crude Oil quality and Plant Operating Conditions.

To predict the EUA emitted by a refinery processing it is necessary to estimate the Specific Emission (EUA produced per each ton burned) to be considered for each refinery stream (intermediates produced by crude oil processing, intermediates imported and finished products): this parameter is used within the matrix generation process to set the coefficients related to the Emissions Constraints which account automatically Heat Production (Fuels burning to Furnaces) and Flaring (Plant Losses) Operations.

This is a general approach that can be used to model any type of Emission (CO_2 , SO_2 , NO_X etc.), and specific objects have been designed to account also for the combined effect of different Emissions.

Physical Properties Management

Fundamental physical properties (e.g. Density, Viscosity, Evaporates, Sulphur, Antiknock, Cold Properties, Metals) are natively known and managed by the system, and are automatically calculated for each intermediate stream produced by Refinery Units. Depending on the specific property calculations are based either on Crude Oil pseudo component property values (Fundamental Properties) or correlated (Derived Properties).

To predict the amount of CO_2 emission a new Derived Property (Specific CO_2 Emission, CO2E) has been added in order to calculate the amount of CO_2 produced burning a ton of intermediate product. Depending on the type of stream and on data availability, this property is correlated to product Molecular Weight, Density and Carbon Content.

Generic (52)	Generalities Blends	
- TINI - TFIN - RTFI - DENS - MOLW - RIDX - SULP - V050	Generalities Name: CO2E Description: CO2 Emission Units Type: GENERIC Unit: Mix type: Mix in weight ✓ Derived: ✓ ✓	isu 💌
V100 VIDX ACID PAFI NAFI ARFI OLEF	Use volume factor: - Library - Pure Comp.: Image: Sector Comp.: Pseudo Comp.: - Light streams: -	on]
- BENZ - PAGC	Crude Oils: Heavy streams: Pormat: ##0.000 Pormat: ##	+36

Figure 2 – Generic Properties Definition Tab

Moreover it is possible to manage and define additional User Properties, through which it is possible to define the Specific Emission linked to other type of emissions: Figure 3 shows for example a Derived Property added to calculate the Sulphur Dioxide emission involved by the burning of each oil fraction; once the property is defined, the systems calculates its value for each intermediate stream permitting to set and manage constraints useful to model the emission limits.

🛓 Formula Generator)	×
[SULP]*2						lear All	
						ear Last	
						Test	
1						-	
B-Generic (52)	Add	Property	,			log	
RTIN (*C) RTFI (*C)	7	8	9	•	ехр	log	
DENS [kg/dm3] MOLW [Kg/mol] BIDX [1]	4	5	6	+	^	sqr	
	1	2	3	×	sin	COS	
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<u></u>				<u>E</u> xit		Apply	

Figure 3 – Derived Properties Formula Generation

Shortcut Plant Simulators

As previously mentioned, SIMRAF embeds Shortcut Plant Simulators able to calculate Yields and Properties of plant effluents as function of feed quality and operating conditions. Plant Simulators can be fine-tuned to reproduce the actual performance of refinery units. The number of input parameters needed to fine-tune and operate the simulators is limited and depends on the type of process modelled.

Developed by internal research and field-validated data, shortcut simulators are used to set plant operating conditions fitting the specific simulation needs.

The following refining processes are available:

- CDU and other distillation processes
- Desulphurisation and Hydro Treatments
- Catalytic Conversions (Naphtha Reforming, FCC, Mild Hydro Cracking)
- Thermal Conversions (Visbreaking, Thermal Cracking, Delayed Coking)

Depending on the refining process represented, different input parameters are available to configure the Plant Simulator to reproduce the real behaviour of actual units; besides calculating plant effluents yields and quality, shortcut simulators permit to manage various parameters strictly involved to Emission Calculations such as:

- Plant losses: used to estimate the amount of material flared; each processing option calculates for each feed quality the plant emissions as the difference between feed and output streams quantity, multiplied by the emission obtained theoretically burning the feed: the result will be for a process plant the emissions due to plant losses and for an utility plant the emissions of the fuel burned.
- Hydrogen Chemical Consumption and Downgrading: used to estimate the amount of hydrogen sent to Fuel Gas Network for Downgrading Losses. Differently from the hydrogen consumed for Chemical Reactions (that being absorbed by plant effluents improves plant product yields), hydrogen losses for Downgrading effect are included in the Fuel Gas balance permitting to better estimate the emissions involved by fuel gas burning. Figure 4 shows an example detailing the hydrogen distribution calculated by the LP model: in this case nearly the 26% of the hydrogen produced or imported by the refinery is sent to Fuel Gas Network to be burned.

Naturally, the correct prediction of the amount of hydrogen burned or flared is important because of the null impact of this combustible on CO_2 Emissions (Specific Emission equal to zero).

Imperiod "1												
-	NaftaHydr	KeroHydr	HP GoHydr	LP GoHydr	Isomerisation	Reforming	Mild Hydr	F. Gases	H2 Rec.	IMPORT	EXPORT	
Imported H2							-7485.1		-1299.3	8784.3		
H2 a Fuel Gas								-5195.5	5195.5			
Reforming H2	-2949.8	-1162.7	-4515.5	-4208.9	-801.0	10789.7			2848.4			
Desulphurization treatment	127.0	261.0	2032.9	920.2			1639.8					
Denitrogenation treatment	8.8						0.1					
Olefines saturation treatment	1258.4		1237.0	994.7			162.3					
Conversion - DHA treatment	85.4	494.4	765.1	453.4	406.6		3527.0					
Downgrading losses	1470.2	407.3	480.5	1840.7	394.4		2155.9					
? Add	Dyplical	e	Dejete	E <u>x</u> port	Įmpo	t		Pre	view	<u>E</u> xit		Apply

Figure 4 – Hydrogen Balance

• Plant Effluents Specific Emissions: as previously mentioned each simulator calculates the Specific Emission associated to each effluent (see example in Figure 5); this information is calculated for each feed and for each crude and is used to predict the emissions due to plant losses in the following units.

Name	Description	Unit	FG	VNVVT1	KEVVT1	GOVVT1	GPVVT1	B1WT1	VNGST1	KEGST1	GOGST1
RFI	Aromatics FIA	%v	0.00	7.22	15.00				5.73	15.00	
LEF	Olefins	%v	0.00	0.00					0.00		
ENZ	Benzene	%v	0.0	2.0	0.0				2.0	0.0	
AGC	Paraffins GC	%w	100.00								
IAGC	Naphthenes GC	%w	0.00								
RGC	Aromatics GC	%w	0.00								
ION_	Motor Octane		98.0	40.0					56.1		
IONE	MON 0.5 TEL		105.1	58.0					58.0		
IONM	MON 0.5 TML		105.1	58.0					58.0		
ION_	Research Octane		105.4	46.0					62.3		
ONE	RON 0.5 TEL		112.6	64.0					75.7		
IONM	RON 0.5 TML		112.6	64.0					75.7		
ID1_	RON rec.@100°C		105.4	60.0					68.5	54.6	
RD1E	RON 0.5 TEL rec.@100°C		112.6	75.0					79.8	65.3	
RD1M	RON 0.5 TML rec.@100°C		112.6	75.0					79.8	65.3	
IVP_	Reid Vapour Pressure	bar	28.827	0.976					1.000		
ROM	Bromine Number	g/100g	0.0	0.0	0.0	0.0			0.0	0.0	0.1
AND	Paraffins ndM	%w			63.51	58.75	55.13		-	64.05	59.9
IAND	Naphthenes ndM	%w			24.23	23.56	28.55			24.21	23.4
RND	Aromatics ndM	%w			12.27	17.69	16.32			11.74	16.5
LSH	Flash point	°C			48.0	118.7	192.4	221.5		48.0	118.
NIT	Total Nitrogen	ppm	-	53.0					53.0	1.9	99.
INIT	Basic Nitrogen	ppm	-								
NIL	Aniline Point	°C									
CETA	Cetane Index				52.0	50.4				52.0	52.
бмок	Smoke Point	mm	-		23.0					23.4	
REZ	Freezing point	°C									
LOU	Cloud Point	°C			-65.0	2.7	31.1			-46.3	2.
POUR	Pour Point	°C	-		-50.0					-50.0	-3.
DIES	Diesel Index				58.3	56.1				58.3	58.
ASPH	Asphaltenes	w.fraction									
CONR	Conradson Carbon	%w			0.0	0.0	0.0	14.4		0.0	0.1
PENE	Penetration	mm									
VICK	Nickel	ppm			0.0	0.0	0.7	58.4		0.0	0.
/ANA	Vanadium	ppm			0.0	0.0	0.5	168.7		0.0	0.
NAX_	Waxes	%w							-		
SH	Ashes	w fraction		2		0.005				0.000	0.00
:02E	CO2 Emission	ton/ton	2.983	3.090	3.114	3.127	3.136	3.152	3.091	3.114	3.12
070	Hec.@/UTC	%v	100.0	32.8	U.U	U.U	U.U	0.0	26.3	0.0	U.
100	Rec.@100°C	%v	100.0	65.6	0.0	0.0	0.0	0.0	60.9	0.0	0.
117	D00 D1 + 11500	6,	1 400.0	01.0			0.0	î	70 5	0.0	21

Figure 5 – Plant Effluents Quality

• Utility production and Consumption: Plant simulators give great flexibility evaluating alternative processing options considering different process parameters and also alternative utilities consumption that can be useful to optimise the emissions; for each Utility defined in the simulation it is possible to define the consumption associated to each operating mode end eventually to put in competition alternative operating modes characterised by a different consumption profiles (for example choose whether to use steam or electricity to drive unit main items). Figure 6 reports an example of the optimal utility balance calculated by the model.

💑 Utilities Balanc	ž Utilities Balance								
period '1									
_	Heat from Fuels MKcal	Electric Energy MWh	Refinery H20 m3	Hot Oil MKcal	Tele Heating MKcal	HP Steam ton	MP Steam ton	LP Steam ton	Oxigen m3
Marginal Value	-38.2 \$/MKcal	-80.0 \$/MWh	0.0 \$/m3	-47.9 \$/MKcal	-1.9 \$/MKcal	-31.9 \$/ton	-31.9 \$/ton	-23.8 \$/ton	-0.1 \$/m3
Crude Oil Unit	-613765.6	-18,054.000	-4667500.0		78000.0		59000.0	7500.0	
Nafta Splitter		-3,318.843	-2951335.0	-137531.3				-13165.9	
DeisoC5		-376.891	-8129736.0		-28671.2				
NaftaHydr	-32638.8	-3,277.452	-1761841.0						
KeroHydr		-3,051.532	-486808.6	-18953.6					
HP GoHydr	-48648.6	-15,948.930	-3330413.0	-30630.6			-14242.8		
LP GoHydr	-37605.9	-9,655.576	-1379070.0		15347.3		-14635.8		
Isomerisation	-1015.2	-4,232.674	-1328983.0	-39042.4			12135.1	10116.5	
Reforming	-187453.9	-9,434.483	-7609842.0	-39837.2	-9360.2		61135.0	-158263.5	
Visbreak	-451137.3	-20,947.930	-28162510.0		50047.4		-22809.2	-41410.9	
Th. Crack.	-46619.5	-2,878.604	-1266991.0		6512.3		9071.7	10541.4	
Mild Hydr	-79445.3	-20,015.350	-3245733.0				-17851.5		
Sulphur		-5,235.557	-9812244.0		4331.3		-49713.8	-34423.7	-9703155.0
MH Rec									
TC Rec									
F. Gases	2337333.0								
H20 R		-39,290.490	74133000.0						
OC Forni									
ST DG						-298646.4	298646.4		
Hot Oil	-403619.3	-2,793.055		327055.6					
Boilers	-543850.3					767824.8	-13283.4	-129839.2	
Turbines		47,349.480				-469178.3		469178.3	
MS TH									
H2 Rec.									
VN ref+hot oil	108466.7								
Crude Pipeline		-25,000.000					-100000.0	-100000.0	
Bit. Delivery				-61060.5			-183181.4		
Utilities purchase		136,162.000							9703155.0
Utilities sale					-116207.0				
Tank Farm									
Total	0.0	0.0		0.0	0.0		0.0	0.0	
		1	- 1				1	1	
<u> </u>	Add Duplicate	e Dejete	Export	Import		_	Preview	<u>E</u> xit	Apply

Figure 6 – Plant Utility Production/Consumption Balance

Imports Characterisation

Imports are available in SIMRAF to model the intermediate streams fed to the refinery and not produced by crude oil processing: these can be of three types; depending on the type the Specific CO_2 emission is estimated as follows:

- *Light Ends*: mixtures of low-boiling pure components for which the Specific CO₂ emission is automatically calculated from the pure component % mix.
- *Light Streams and Heavy Streams*: streams boiling respectively in gasoline and distillates/fuel oil ranges for which the Specific CO₂ emission has to be entered.

Finished Product Characterisation

It is necessary to estimate also the Specific Emission associated to the Finished Products that can be used for internal consumption: in this case it is possible to define a fixed value (following the same approach adopted in case of Imports) or to estimate the real Specific Emission through a recursive process (the optimal recipe of a given product is not known in advance); anyhow this last method resulted to be excessively sophisticated: product composition is affected by many variables and for a given processing scheme the Specific Emission of internal combustibles does not change enough to justify a recursive calculation.

Managing Emissions

Once the Specific Emission of each stream involved in the simulation is defined, it is necessary to activate Emission Management: this is firstly done defining an Emission Object that is to be associated to the Specific Emission Property previously defined: in this way the system knows which Property is to be used to calculate the Emissions.

 CO_2 Emission Object is currently predefined in the system while other Emission Objects must be added: Figure 7 shows the definition of an Emission Object useful for SO2 Emission control.



Figure 7 – Defining Emission Objects

To set Emission constraints it is necessary to define a specific bound in the model and to associate it to the Emission Object: it is possible to associate more bounds to the same emission and/or more emissions to the same bound; moreover it is possible to set a coefficient specifying how the contribution of a given emission to a specific bound is to be accounted.

For Example, in the case showed in Figure 8 three different bounds have been defined: one for CO_2 and SO_2 Emissions respectively (CO2M and SO2M) and one to evaluate the combined effect of the two (GRHE). In this last case, the SO_2 Emission will be accounted four times.

For each Bound and for each period defined in the model it is be possible to define the Minimum and Maximum Capacity Constraints that the Model is forced to respect (Tab Capacities in Figure 8).

DEMO EMISSION 01 Settings Tim Periode	Definition Capacities	=>1 - HYDROCC	DNVERSION SCHEME=>E	ounds=>Emissions		
	Name Description Type Unit Type CO2E (CO2 Emissions) SO2E (SO2 Emission)	CO2M S Max CO2 M Emissions E Weight V YES N NO Y	02M GRHE fax S02 Green House I missions Emissions /eight Weight IO YES ES	Effect		
Granger Forders Gran	R Add	Duplica	te Dejete	Export Import	<u>Preview</u>	it <u>Apply</u>
 	Definition Capacities	=>1 - HYDROCC	INVERSION SCHEME=>E	ounds=>Emissions		
 ☐ Connections ☐ Products ☐ Spectromics 	Name Signature CO2M 1 - 30 M SO2M 1 - 30 M GRHE 1 - 30 M	Start Period ar/22 Feb 2010 ar/22 Feb 2010 ar/22 Feb 2010	End Period 1 - 30 Mar/22 Feb 2010 1 - 30 Mar/22 Feb 2010 1 - 30 Mar/22 Feb 2010	Min Qty ton	Max Qty 600000.0 ton 5544.0 ton 630000.0 ton	
Emissions	? A <u>d</u> d	Duplica	te Dejete	Export Import	Preview <u>E</u> x	it <u>Apply</u>

Figure 8 – Defining Emission Constraints

Emissions Economics

As well as for any other object directly purchased or sold (crude oils, imported streams, products, Hydrogen and utilities, investments), specific tables dedicated to Emissions Economics have been inserted to specify also the Emissions Trading prices and limiting quantities (Figure 9).

Items' purchase/sale prices and volumes are set for each period defined in the simulation; importing facilities permitting to automate the updating of economic data are available. Depending on Emissions cost and operating requirements the model will be able to choose whether to buy, sell EUA (in case of Cap and Trade Modelling), modify optimal operative asset or both; two records (Purchase, Sell) are available for each Emission Object for each period. Utility economics also affect Emissions Management since their price and availability influence the choice between internal production and importing.

_ A						
	Name	Period	Purchase/Sell	Price	Min Qty	Max Qty
	COOF (COOF 1 1 1	1 - 30 Mar/22 Feb 2010	P	20.0 \$/ton	ton/day	500 ton/day
III Periods	CUZE (CUZ Emissions)	1 - 30 Mar/22 Feb 2010	S	0.0 \$/ton	ton/day	100 ton/day
😑 🔛 1 - HYDROCONVERSION SCHEME		1 - 30 Mar/22 Feb 2010	P	200.0 \$/ton	ton/day	0 ton/day
	SO2E (SO2 Emission)	1 - 30 Mar/22 Feb 2010	S	50.0 \$/ton	ton/day	0 ton/day
🕀 🙀 Set-Up Data		1 001/01/22100/2010	•	00.0 \$1.011	torn day	o torn day
🕂 🐰 Raw Materials	Name	Period	Purchase/Sell	Price	Min Qtu	Max Dtu
		1 - 30 Mar/22 Feb 2010	P	\$/MKcal	MKcal/day	MKcal/day
	FUEL (Heat from Fuels)	1 · 30 Mar/22 Feb 2010	S	\$/MKcal	MKcal/day	MKcal/day
	ELEN (Electric Energy)	1 - 30 Mar/22 Feb 2010	P	80.0 \$/MWh	KWh/day	6000000 KWh/day
Lonnections	EEEN (Electric Energy)	1 · 30 Mar/22 Feb 2010	S	50.0 \$/MWh	KWh/day	0 KWh/day
庄 Products	H20B (Befineru H20)	1 · 30 Mar/22 Feb 2010	P	\$/m3	m3/day	m3/day
🖃 🥪 Economics	Theory (Housing)	1 · 30 Mar/22 Feb 2010	S	\$/m3	m3/day	m3/day
	HOLL (Hot Dil)	1 · 30 Mar/22 Feb 2010	P	\$/MKcal	MKcal/day	MKcal/day
All Innerto Directions		1 · 30 Mar/22 Feb 2010	S	\$/MKcal	MKcal/day	MKcal/day
S imports Fulchase	TELE (Tele Heating)	1 · 30 Mar/22 Feb 2010	P	\$/MKcal	MKcal/day	MKcal/day
	- L L L (+ 610 + 100 d m (g))	1 · 30 Mar/22 Feb 2010	S	1.9 \$/MKcal	MKcal/day	215000.0 MKcal/day
	HPST (HP Steam)	1 · 30 Mar/22 Feb 2010	P	50.0 \$/ton	ton/day	ton/day
	in or (in origin)	1 · 30 Mar/22 Feb 2010	S	\$/ton	ton/day	ton/day
	MPST (MP Steam)	1 · 30 Mar/22 Feb 2010	P	41.0 \$/ton	ton/day	480 ton/day
CINISSIONS	in or phi otodinj	1 · 30 Mar/22 Feb 2010	S	\$/ton	ton/day	ton/day
- S Exchanges	LPST (LP Steam)	1 · 30 Mar/22 Feb 2010	P	\$/ton	ton/day	ton/day
	a or (a orodin)	1 · 30 Mar/22 Feb 2010	S	\$/ton	ton/day	ton/day
H- Rounds	OXIG (Ovigen)	1 · 30 Mar/22 Feb 2010	P	0.1 \$/m3	m3/day	1.6E+07 m3/day
	or not (onigon)	1 · 30 Mar/22 Feb 2010	S	\$/m3	m3/day	m3/day
Lug						

Figure 9 – Emissions Economics

Matrix Generation And Optimisation

Once intermediate streams quality and yields have been calculated, it is possible to run Matrix Generation and Optimisation Processes: no specific mathematical skills are requested to the User since the system manages this phase autonomously; Emissions has been Modelled adopting the same approach.

The LP Matrix Generator has been modified in order to add a coefficient for each type of Emission, for each plant operation of each feed, on the Balances linked to the Emission Bounds that have been specified; this for each processing period represented in the Model.

To the same Bound Balances Coefficients have been included permitting to model the Emission Trading Activities whose unitary costs are included in the Economic Function.

Reports

SIMRAF provides complete reporting and solution analysis tools. All Reports can be easily exported to MS Excel format. The refinery's economic balance: for each sale and purchase the Marginal Value is calculated. Information about Plants, Utilities, Logistics and Processing, including incentives in exceeding operational constraints. Quality and composition for every finished product.

Various tables have been modified or added to report the results connected to emissions management; below are some examples:

ECONOMIC BALANCE

Available for each refinery/period defined in the simulation, this report extracts from the solution the best Economic Balance obtainable given all the constraints.

Marginal values quantify the specific incremental advantage (e.g. US\$/ton) achievable relaxing the limiting constraint. This report includes either imported materials and Utilities and Emission Trading results (Figure 10).

- CRUDE OILS - IMPORTS - PRODUCTS	PROCESSED QTY ton	SOLD QTY ton	PRICE \$/ton	TOTAL \$	INCR.VALUE \$/ton
Natural Gas	50000.0		377.0	-18850000.0	85.8
MTBE	41164.4		574.5	-23647310.0	
Bio Diesel	20000.0		308.3	-6165400.0	148.0
Carica MHC			397.0		-397.0
Imported H2 - purchase	9950.1		1300.0	-12935070.0	
L.P.G. (01)		10000.0	385.0	3850000.0	
Propane (01)		27694.9	385.0	10662550.0	
Butane (01)		63387.8	385.0	24404310.0	
Unl.95 (Retail)		148416.7	547.4	81240000.0	61.0
Unl.95 (Export)			454.7		-31.6
Unl.95 (Oil Companies)		386789.9	486.3	188108800.0	
Unl.95 (Domestic)		111312.5	492.0	54765000.0	5.7
H.Naph. (Domestic)		169733.9	400.1	67910530.0	
VN forni (01)			0.0		-400.1
Jet A1 (01)		100000.0	570.0	57000000.0	21.0
GO ULSD (Export)			447.9		-30.3
GO ULSD (Oil Comp.)		323715.6	478.2	154805300.0	
GO ULSD (Domestic)		1261569.0	491.5	620100000.0	13.3
GO ULSD (Retail)		231287.7	541.5	125235000.0	63.3
GO Alpino (01)		18077.6	517.4	9352702.0	
GO Riscald. (Export)			420.2		-53.6
GO Riscald. (Domestic)		367155.9	478.5	175692000.0	4.7
Bunker (01)		415418.0	196.7	81712730.0	
LSFO 1% (01)			251.7		-79.3
Bit70100 (Road)		410000.0	209.9	86059000.0	0.9
Bit. Ind. (01)		410000.0	209.9	86059000.0	2.9
Bit.5070 (Road)		401209.2	209.9	84213810.0	
OC forni (01)			0.0		-241.2
Sulphur (01)		36677.7	50.0	1833887.0	
Gross Total	5121115.0	4892447.0		307886900.0	
Operative Costs				-19149200.0	
Electric Energy purchase [MWh]	135,727.000		-80.0	-10858160.0	
Tele Heating sale [MKcal]		127126.6	1.9	244083.0	
Oxigen purchase [m3]	9703166.0		-0.1	-703479.5	
CO2 Emissions purchase [ton]	83226.1		-20.0	-1664521.0	
Total Result				275755600.0	

Figure 10 – Economic Balance Report

USE OF FUELS

This report details the production of the heat required by the processing; available Fuels are listed as well as the amounts burned according to the optimal solution (Figure 11).

The last column of the table reports the incremental value that in this case indicates how much the economical result would be reduced by burning an additional ton of the corresponding Fuel: its value is influenced by various variables including EUA cost.

- FUEL UTILITY	HEATING SYSTEMS	FUELS ton	HEATING VALUE MKcal/ton	TOTAL HEAT MKcal	INCR.VALUE \$/ton
	F. Gases Ammonia		5.0000		
FUEL (Heat from Fuels)	F. Gases Fuel Gas	109369.4	11.8830	1299636.0	
	F. Gases Natural Gas	50000.0	11.8500	592500.0	
	F. Gases Reforming H2		28.0000		229.6
 FUEL (Heat from Fuels) 	F. Gases Imported H2		28.0000		229.6
	F. Gases H2 a Fuel Gas	5195.5	28.0000	145473.4	
	F. Gases OC forni	30785.1	9.7360	299723.4	
	OC Forni OC forni		9.5000		9.0
	VN ref+hot oil VN forni	10330.2	10.5000	108466.7	
	Total	205680.1		2445800.0	

Figure 11 – Use of Fuels Report

Emissions

This report details the contribution provided by each refinery unit (either process or utility) to refinery emissions balances. For each balance (Emission Bound) specified in the simulation the contribution of emission trading (emission purchases, sales) is also reported (Figure 12)

-	Max CO2	Green House Effect	Max SO2
UNIT	- ton	- ton	- ton
Crude Oil Unit	46936.1	49229.9	573.5
Nafta Splitter	2900.9	2900.9	0.0
DeisoC5	789.4	789.4	0.0
NaftaHydr	2905.6	2912.1	1.6
KeroHydr	1725.4	1738.9	3.4
HP GoHydr	1587.1	1652.0	16.2
LP GoHydr	2680.6	2767.5	21.7
Isomerisation	316.0	316.0	0.0
Reforming	1266.8	1266.8	0.0
Visbreak	6976.3	7542.1	141.4
Th. Crack.	503.7	503.9	0.0
Mild Hydr	3068.6	3235.2	41.6
Sulphur		11564.6	2891.1
MH Rec		0.0	0.0
TC Rec		0.1	0.0
F. Gases	464181.1	464181.1	
H20 R			
OC Forni	96966.4	104354.3	1847.0
ST DG			
Hot Oil			
Boilers			
Turbines			
MS TH			
H2 Rec.	18297.2	18297.2	
VN ref+hot oil	32126.7	32152.0	6.3
Emissions purchases	-83227.9	-83227.9	
Emissions sales			
Total	600000.1	622176.0	5544.0

Figure 12 – Emissions Report

CASE STUDY

To explore some of the variables that can be affected by the emission limits and the EUA market price, we have built a model of a modern refinery of 5 million tons per year with a refining scheme including Crude Unit, Light distillate fractionation, Kerosene Hydrofining, Two Gasoil Hydrofining, Isomerisation, Reforming, Visbreaking, Thermal Cracking, Mild Hydrocracking, Hydrogen Recovery Unit.

From the stand point of utilities, are considered:

- Heat Production System with refinery and imported gases, Virgin Naphtha and 1 % Sulphur Fuel Oil,
- Heat Production System fed by 2% Fuel Oil,
- High Pressure Steam Production with Boilers,
- Electric Energy and Low Pressure Steam production through turbines,
- Medium Pressure Steam and Low temperature Heat production from heat exchange in process units,
- Hot Oil production,
- Cooling Water System.

The Model foresees the possibility to import limited quantities of:

- Natural Gas (max 60.000 Tons/year)
- Hydrogen (max 16.500 Tons/year)
- Electric Energy (max 250 MWh/h)

• Medium Pressure Steam from a Cogeneration Plant max 20 Tons/hour

The Model foresees the possibility to export limited quantities of Low level Heat for house heating (max 9 MMKcal/h) and to trade up to a max of 165.000 EUA/year.

In the Model three Emission Bounds have been specified:

- Sulphur Dioxide Emission due to the sulphur content of the burned fuel oils and flared gases (quantity calculate as correspondent to the process plant losses), and due to the Sulphur Dioxide emitted by the Sulphur Plant exhausted gases burning. This emission is controlled by many years to avoid Acid Rains and the corresponding maximum emission allowed is 700 kg per hour, equal to 5544 tons per year.
- Carbon Dioxide Emission that for this refinery a EUA Cap value has been considered of 600.000 EUA
- Green House Gases Global Emission has been added to this model, considering that the SO2 Green House Effect of four times the CO₂ Green House Effect, the "CO₂ +4 SO₂" formula, with the limit of 630.000 Units per year.

Two crude oils with different sulphur content and distillation curve has been given as available for the refinery, with the production of LPG, Gasoline, Naphtha, Kerosene, Gasoil, LSFO, HSFO, three grades of Bitumen and Sulphur: the prices of crude oils and of product are consistent to an European internal market.

EUA COST SENSITIVITY STUDY

The refinery model of the Case Study has been optimised with the only modification of the EUA Market price, starting from Zero USD/EUA up to 80 USD/EUA. For higher prices the optimal utility production/consumption asset does not change anymore. The higher price limit considered within this study is equal to 130 USD/EUA, corresponding to the fine that now in Europe has to be paid in case of exceeding the Emission, if no EUA will be available to be purchased.

Table 2 reports the economic result of each optimisation and the correspondent value of various elements that can be affected by the EUA market price change.

The same results are plotted in Figure 13: since the results depend on the market scenario that is considered to carry out the study, values have been plotted against the ratio between EUA and Crude Oil Price.

			PURCHASE					CONSUMPTION			
	Price	USD		377	80	41	1,300				
EUA	EUA /	Economic	EUA	Natural	Electric	MP Steam	Hydrogen	Hydrogen	Fuel Oil	Virgin	Total
Absolute	Crude	Gross		Gas	Energy					Naphtha	
Price	Oil Price	Result									
USD		MMUSD/Y	EUA/Y	TONS/Y	MWH/Y	TONS/Y	TONS/Y	TONS/Y	TONS/Y	TONS/Y	TONS/Y
0	0	277.443	91,015	50,000	136,162	0	8,784	0	30,778	11,029	206,372
5	0.02	277.004	83,262	50,000	135,746	0	9,951	0	30,784	10,529	203,820
10	0.03	276.588	83,262	50,000	135,746	0	9,951	0	30,784	10,529	203,821
15	0.05	276.172	83,262	50,000	135,746	0	9,951	0	30,784	10,529	203,821
20	0.06	275.755	83,228	50,000	135,727	0	9,950	0	30,783	10,533	203,810
30	0.10	274.977	51,425	50,000	135,723	0	13,864	3,914	30,889	0	197,294
40	0.13	274.463	51,425	50,000	135,723	0	13,864	3,914	30,889	0	197,294
50	0.16	273.950	51,318	50,000	135,652	0	13,868	3,913	30,889	0	197,255
60	0.19	273.459	32,993	43,796	135,648	0	16,500	6,542	30,889	0	193,665
70	0.23	273.194	0	32,592	138,847	152,499	16,500	6,542	30,889	0	182,461
80	0.26	273.194	0	32,592	138,847	152,499	16,500	6,542	30,889	0	182,461
Upper			165,000	50,000	160,000	158,400	16,500		60,000	39,600	
Bound					1						

Table 2 – EUA Price influence versus Consumption Key Variables

EMISSION UNIT ALLOWANCE MARKET PRICE SENSITIVITY



Figure 13 – EUA Market Price Sensitivity

CONCLUSIONS

From Table 2 it can be seen that if the refinery operates without CO_2 Emissions restrictions, and is only bounded to respect the SO₂ emission CAP of 700 kg/hour, the CO_2 emission will be 691.015 Tons/Y; the 91.015 EUA overcoming the 600.000 EUA CAP are purchased at a cost of 0 USD/EUA.

When the cost rises to 5 USD per EUA, the emission is immediately reduced of about 7.753 tons through the increase of purchase of Hydrogen from an external source and a decrease of Naphtha and Fuel Oil to furnaces.

A further reduction of 31.837 tons per year Emissions and of EUA purchases becomes profitable when the EUA price reaches 30 USD.

In this case it results profitable to acquire additional Hydrogen to be burned in furnaces, stop Virgin Naphtha burning and to reduce the fuel oil to furnaces.

Another emission reduction step of 18.325 tons per year becomes convenient when the EUA cost rises to 60 USD: in this case the Hydrogen import reaches its higher limit.

The last 32.592 tons per year of emission reduction, necessary to reach the CAP without EUA purchase, becomes convenient when the EUA cost reaches 70 USD: in this case the reduction is made possible by the acquisition of 152.499 tons per year (19.25 tons/hour) of Medium Pressure Steam from the same source of electric energy, that is from a energy producer through co-generation of electricity and steam.

From the Table it is possible to calculate also dimension of the economic impact of the Emission CAP and Trade: the Economic Gross Results difference between the EUA Zero Cost Case, and the EUA 70 UDS Cost Case, is of 4,249 Million Dollars per year.