

A COMPUTER-AIDED TOOL FOR THE SIMULATION AND OPTIMIZATION OF THE COMBINED HDS-FCC PROCESSES

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A computer-aided tool for the simulation, optimization and analysis of the combined operation of the hydrodesulphurization (HDS) and fluid catalytic cracking (FCC) processes in an oil refinery is presented. The optimization of these processes is an important yet difficult engineering task, because of the complexity in the integration of the two units, the large number of interacting variables, the product quality specifications and the financial benefits associated. The proposed tool is developed in a user-friendly Visual Basic environment and operates in two different modes: the modelling-prediction mode and the optimization-sensitivity analysis mode. The modelling of the processes is based on 'short form' models, which were created following statistical and neural network approaches. This kind of model usually has short computing time requirements, which is critical for the optimization mode. The optimization algorithm is based on a financial objective function with a flexible form, which gives the user the option to explore a variety of scenarios. Industrial runs have verified the modelling accuracy of the tool. The optimization scenarios examined include the contemporary needs of modern refineries for LPG and gasoline maximization, subject to strict quality specifications. The demonstration of this tool aims to give an insight into the system dependencies and add knowledge on the possibility of a more profitable operation of such a complex process.

Keywords: computer-aided tools; process modelling; simulation; optimization; fluid catalytic cracking; hydrodesulphurization.

INTRODUCTION

Computer-aided tools are nowadays a significant part of the engineering practice. They are advanced computer programs mainly used as decision support systems (DSS), assisting decision-makers in obtaining optimal solutions in complicated problems, where it is not possible or desirable to have a completely automated system to perform the entire decision process. The overall architecture of these tools depends on the type of the problem and, more importantly, on the phase where the tool assists the decision of the experts. While the type of the problems that computer-aided tools deal with is varying, one can generally distinguish two main phases of their implementation in problem solving: the design-decisions phase, in which the computer-aided tool helps the expert to build different scenarios during the design stage of the process (Kheawhom and Hirao, 2002; Draman *et al.*, 2002) and the operational-decisions phase,

during which the expert creates and examines various optimization scenarios for the operational variables of a given process design (Sundararajan *et al.*, 1998).

One decisive criterion for the implementation of these tools is their user-friendliness. Typical production engineers or managers, who are generally the users of such tools, do not have sufficient mathematical and programming expertise to formulate, for instance, complex objective functions and constraints, which is a necessary part of every optimization procedure. Therefore, the environment in which the user communicates with the system should be as comprehensible as possible and interact with the user only in the 'real system level', hiding at the same time the complicated mathematical aspects (Draman *et al.*, 2002).

In this work a computer-aided tool for the simulation, optimization and analysis of the combined HDS-FCC process is presented. The tool does not interfere with the design of the process, since it is based on the operational data of a specific commercial unit (Aspropyrgos Refinery of Hellenic Petroleum S.A, Athens). The simulation and optimization of the integrated operation of the HDS and the FCC processes pose great challenge for every petroleum refinery. The FCC unit is considered to be the workhorse of

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a modern refinery, producing around 40% of the total refinery gasoline and many other valuable products such as liquefied petroleum gas (LPG) and diesel (LCCO). Its complexity arises from the strong interactions between the operational variables of the reactor and the regenerator. Moreover, there is a large degree of uncertainty in the kinetics of the cracking reactions and catalyst deactivation by coke deposition in the riser reactor and the coke burning process in the regenerator (Christensen *et al.*, 1999). While the FCC unit is responsible for the 40% of the total gasoline pool, its contribution to the total gasoline sulphur reaches almost 90%. Owing to the strict environmental regulations regarding fuel emissions, the hydro-treatment of the FCC feed is now required and this is mainly achieved in the HDS unit. Another effect of the hydro-treatment is the decrease of the nitrogen content in the FCC feed, which contributes significantly to lower NO_x emissions from the FCC regenerator. Furthermore, the hydro-treatment decreases the density of the FCC feed, which corresponds to an increase of its crackability and thus to an improvement of its quality. The main difficulties in the modelling of an HDS unit are that catalyst deactivation occurs with complex reaction kinetics, small changes in the unit operating conditions may result in large changes in product properties and the operational variables range is too short to create a reliable model based on industrial datasets.

The complex and non-linear interactions between the two processes constitute their simultaneous treatment quite serviceable, especially when the optimization of their combined operation is concerned. Furthermore, the simultaneous treatment raises the simplicity and the user-friendliness of the simulator interface, in which the user examines the two processes globally, in a manner reflecting the commercial reality. For that reason petroleum companies have two options to deal with their cracking processes. One is to buy a commercial simulator like ASPEN, PRO II, PACE, KBC Model etc., and the other is to develop a black box model to simulate their specific refinery processes. Each method has its advantages and disadvantages. The commercial simulators are mainly based on fundamental mass and energy balances and sometimes on empirical equations, which are adapted and validated for the special case of the FCC and HDS units. However, due to the complexity of these processes, the usual trade-off phenomenon between generalization and specialization appears. This means that these tools may be by default appropriate for a variety of FCC units (generalization), providing at the same time a number of options, so that the user can bring the simulator closer to a specific process setup. On the other hand, if one is interested in satisfying all the idiosyncrasies of a specific commercial unit (specialization), he can adopt the black box modelling approach. This approach follows the reverse logical path compared with the aforementioned simulators: a model is built based on the needs of the specific process setup and the conclusions drawn from the analysis of this model are less accurate for non-similar setups. Such approaches become more and more popular, as the development of powerful black box models like neural networks becomes significantly easier. Moreover, approaches like the one presented here are much less expensive for the industry, compared with the very expensive commercial simulators mentioned.

Consequently, the simulation of the combined operation of the HDS and the FCC units is now the key for a profitable

operation of a modern refinery, as far as the production of 'clean fuels' is concerned. Their serial operation, their complexity and their economic importance make a specialized computer-aided tool necessary for this challenging research subject.

PROCESS DESCRIPTION

In the present study the commercial data of Aspropyrgos Refinery of Hellenic Petroleum S.A., the largest and most complex oil refinery in Greece, were used to develop predictive models for the integration of the two units and examine the economic benefits of their optimization. The industrial system examined consisted of a two-stage FCC feed hydro-treater and a typical riser-type fluid catalytic cracking unit. The connection of the two units is serial in the sense that the liquid product of the HDS is a significant part of the FCC feed. The HDS feed is usually vacuum gas-oil (VGO) or straight run gas-oil of high sulphur content, while the FCC feed is the desulphurized HDS product supplemented with high sulphur VGO, in a ratio proportional to the refinery needs.

As shown in Figure 1, in the commercial HDS unit under consideration, the total hydrogen feed, which consists of the recycled hydrogen and the hydrogen make-up, is split into three parts: the main feed of the first reactor, the first quench at the middle of the first reactor and the second quench at the entry of the second reactor. The purpose of the two quenches is to reduce the reactor temperature as well as the partial pressure of the H₂S produced. In the HDS process the high-sulphur vacuum gas-oil contacts the hydrogen in the presence of catalyst and hydrogenation reactions occur. The main reactions are the desulphurization, the denitrogenation and the saturation of aromatics and double hydrocarbon bonds. The process is carried out in a trickle bed reactor in two stages. In the first-stage the cobalt-molybdenum (CoMo) catalyst provides the sulphur removal and in the second stage the nickel-molybdenum (NiMo) catalyst promotes mainly the saturation reactions. The hydrogen recycling rate, the unit pressure and temperature, as well as the feed and catalyst quality, are the most important parameters that affect the process.

The commercial FCC unit operates in a fully circulating mode and consists of the riser, the stripper and the

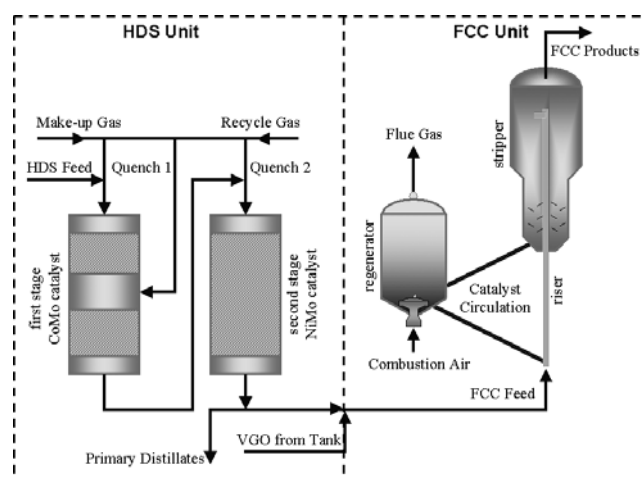


Figure 1. Schematic diagram of the commercial HDS-FCC system studied.

regenerator. At the reactor bottom the gas-oil contacts the hot catalyst that flows from the regenerator and evaporates. The heat consumed by the endothermic cracking reactions is regained from the burning reactions in the regenerator. In the FCC process the high molecular weighted feed is cracked to lighter hydrocarbons (diesel, gasoline, LPG and sour gas). The reactor temperature, the catalyst-to-oil ratio, the catalyst type and the feed quality are the most important parameters that affect the process.

PROCESS MODELS

The simulator of the HDS-FCC combined operation consists of two sub-models. They have been developed focusing on each process separately and then connected in a way representing the reality of the commercial unit. In this way, problems of complexity and inflexibility of the overall multivariable system have been solved. These sub-models are also used during the optimization phase, which involves the consideration of many operational variables and may have to fulfill a variety of constraints. Consequently, fast and flexible models are needed, so that the optimization procedure requires short computational time to converge. Short-form models fulfill this need. The term 'short-form models' is used to describe models which relate input and output variables through a concrete functional relationship of algebraic form. Such models may be developed with regression analysis or more sophisticated techniques like neural networks, which belong to the class of 'black box' modelling tools (Qi *et al.*, 1999). However, the main disadvantage of the black box modelling approach is that its empirical nature and its lack of fundamentality constitute the final models applicable with safety only for the specific process setup and within the range of the original training dataset, based on which they were developed. Thus, one has to weigh the pros and cons of the black box modelling approach, being aware of the limitations regarding extrapolation abilities on the one hand and the high accuracy and simplicity in the development and use of such models on the other.

Furthermore, if black box models are designated to be used for optimization purposes, a more precise analysis of the interdependencies between the process variables is required. If such dependencies are present in the set of the input variables of the model, they may not affect its predictions regarding realizable experimental situations, but they play an important role in the determination of the process-manipulated variables during optimization scenarios. The latter must be constructed according to the process freedom degrees and of course the experimental experience. However, the detailed analytical solution is typically unavailable in processes, where black box models are necessary. In such cases the main mass and energy balances of the entire system can be written including all the system variables in a generalized theoretical pattern. Based on this pattern the corresponding system can be analysed and the degrees of freedom and the manipulated variables can be determined. Such an attempt of analysing the closed system of the FCC unit follows.

The effects of the stripper, the cyclones and the lift lines on the total unit performance are neglected, since their operation is rather constant in the commercial unit and has a much lower impact on the final product compared to this of the riser and the regenerator. Considering that the feed rate (F_{VGO}), the catalyst circulation rate (CCR), the riser pressure (P_R), the

riser temperature (T_{RX}), the coke on regenerated catalyst (C_{REG}) and the feed and catalyst properties [$P(\text{feed})$, $P(\text{catalyst})$], all influence in a lower or higher extent the catalytic reactions, the mass balances [equations (2)–(6)] for each of the five products (gasoline, coke, LPG, LCCO, sour gas) can be written. Furthermore, the unconverted feed, namely the slurry, can be calculated from the total mass balance of the riser reactor as shown in equation (1). In equation (7) a generalized heat balance of the total riser height is presented. The functions g and c in equation (7) express the enthalpy change of the FCC feed and catalyst, which enter the riser at rates F_{VGO} and CCR and temperatures T_{PR} and T_{REG} , respectively, and exit from the riser top at temperature T_{RX} . The enthalpy of feed vaporization ΔH_{vap} [equation (8)] is mainly a function of the feed properties, the feed and catalyst circulation rates and the catalyst-feed mix temperature. Finally, the heat consumption by the endothermic cracking reactions ΔH_{crack} is a function of the feed rate, the product yields, the reaction temperature and the feed properties as expressed in equation (9).

$$F_{VGO} - F_{VGO} \sum y_i = 0 \quad (1)$$

$$y_i = f_i[F_{VGO}, CCR, P_R, T_{RX}, C_{REG}, P(\text{feed}), P(\text{catalyst}), F_{CAT}] \quad (2)–(6)$$

$$F_{VGO} \cdot g[T_{PR}, T_{RX}, P(\text{feed})] + CCR \cdot c[T_{REG}, T_{RX}, P(\text{catalyst})] + \Delta H_{vap} + \Delta H_{crack} = 0 \quad (7)$$

$$\Delta H_{vap} = F_{VGO} \cdot h[F_{VGO}, CCR, T_{PR}, T_{REG}, T_{RX}, P(\text{feed})] \quad (8)$$

$$\Delta H_{crack} = F_{VGO} \cdot h[y_i, T_{RX}, P(\text{feed})] \quad (9)$$

where i = gasoline, coke, LCCO, sour gas, LPG.

It should be noted that the catalyst addition rate F_{CAT} , although an operational variable, was categorized as a catalyst property since it does not affect any other variable of the process except the catalyst quality. However, the high cost of the catalyst supply makes the catalyst addition rate an important parameter for the financial objective function.

Under the same pattern the mass and energy balances are written for the regenerator in equations (10)–(13). The flue gases, namely the carbon dioxide and monoxide, the oxides of sulphur and nitrogen and the combustion air surplus, are lumped for simplicity into the variable F_{GAS} as shown in equation (11). Equation (10) presents the total mass balance for the coke and gas in the regenerator, while equation (12) expresses the heat balance where ΔH_{comb} is the energy gain due to the combustion of coke [equation (13)].

$$y_{Coke} F_{VGO} + F_{AIR} - F_{GAS} - C_{REG} = 0 \quad (10)$$

$$F_{GAS} = f(y_{Coke}, F_{VGO}, F_{AIR}, CCR, T_{REG}, P(\text{air})) \quad (11)$$

$$c[CCR, T_{RX}, T_{REG}, P(\text{catalyst})] + u[F_{AIR}, T_{AIR}, T_{REG}, P(\text{air})] + \Delta H_{comb} = 0 \quad (12)$$

$$\Delta H_{comb} = q[y_{Coke}, F_{VGO}, F_{AIR}, CCR, T_{REG}, P(\text{air})] \quad (13)$$

In commercial applications the combustion air enters the regenerator at ambient conditions, thus the air properties [$P(\text{air})$] and the air preheat temperature T_{AIR} can be considered constant. After all the above assumptions, the number

of equations that theoretically can describe the closed FCC unit is 13, while the operational variables (unknowns) used are 20. The seven free variables that are typically used for unit manipulation in the real process level are the feed rate, the feed preheat temperature, the riser exit temperature, the riser pressure, the regenerator air feed and of course the feed and catalyst quality, which in our case were expressed with $P(\text{feed})$ and $P(\text{catalyst})$ respectively.

HDS Model

The HDS model consists of four short-form equations for the prediction of the HDS product properties, namely the estimation of % wt sulphur content, % wt nitrogen content, the refractive index and the specific gravity of the hydro-treated feed. The general form of the equations is presented in equation (14). Each equation contains 13 constant factors and seven variables and is described in detail in Bellos *et al.* (2001):

$$p = \frac{K_1 e^{K_2 T_{\text{HDS}}} P_{\text{HDS}}^{K_3} F_{\text{VGO,HDS}}^{K_6} (1 + K_{10} Q_{\text{H,q1}}^{K_{11}}) \times (1 + K_{12} Q_{\text{H,q2}}^{K_{13}})}{(1 + K_8 Q_{\text{H,M}}^{K_4})(1 + K_9 Q_{\text{H,R}}^{K_5})} + K_7 \quad (14)$$

In equation (14) T_{HDS} is the HDS temperature, P_{HDS} the unit pressure, $F_{\text{VGO,HDS}}$ the feed rate, $Q_{\text{H,M}}$ the hydrogen make-up, $Q_{\text{H,R}}$ the recycled hydrogen rate, $Q_{\text{H,q1}}$ and $Q_{\text{H,q2}}$ are the first and second quench rates and p is the corresponding property estimated. Moreover, the mean average boiling point of the hydrotreated feed was estimated from the specific gravity and the refractive index [as they are calculated from equation (14)], based on an empirical correlation presented in the literature (Riazi and Daubert, 1986).

For the development of the short-form models of equation (14) the meta-modelling approach was adopted. At first experiments were performed in a pilot plant, operating in the National University of Athens at conditions similar to those of the commercial unit. Based on the pilot data a kinetic model was developed, which includes the mass and energy balances considering the two stages of the HDS process as an ideal plug flow reactor. Then, short-form models [equation (14)] were developed to simulate the performance of the kinetic model and thus the operation of the commercial unit. The main reason for choosing short-form models was the computational load. Namely, the response time of the short-form models was 1/2000 compared with that of the detailed kinetic model. This would correspond to a major increase in the time consumption of the optimization process, in which the HDS models were called several times, if the kinetic model was used. For the development of the short-form models, 8640 repeated runs of the kinetic model were performed to estimate the values of the total 52 parameters of equation (14). The achieved absolute values of the relative error had a mean of 2.21% for the sulphur content, 1.70% for the nitrogen content, 0.086% for the specific gravity and 0.027% for the refractive index of the hydrotreated feed. The short-form models were developed with the properties of only one feed and one catalyst, namely those used in the commercial unit, with properties $S = 2.12\%$ wt, $BN = 0.06\%$ wt, $SG = 0.922$, $RI = 1.4937$. Whenever the feed or catalyst quality change,

the short-form models need to be recalibrated in order to estimate new K values for equation (14). The ranges in which the HDS short-form models were developed are presented in Table 1.

FCC Model

The overall FCC model consists of short-form models, which predict the output variables of the FCC process presented in Table 2. These variables refer to the distribution of the main products of the process, their analysis in some chemical compounds of interest and their quality characteristics (gasoline octane number and sulphur content). As shown in Table 2, most of the output variables were predicted by a neural network (NN), and the rest by parametric models based on regression analysis (PR). The latter modelling approach was used for those output variables for which the quantity of available data was inadequate to train a neural network. The parametric models presented in the following paragraphs were created using the statistical package SPSS (SPSS Inc.), while the artificial neural networks were created using the Neurosolutions (NeuroDimension Inc.) software package.

Table 3 shows the input variables that were used for the training of the neural network. These variables were selected in cooperation with the process engineers of the commercial unit according to the generalized degrees of freedom analysis described above. The available database of the commercial unit covered a period of two years. The data screening for outliers detection has been based on typical statistical techniques and valuable information from the process engineers indicating startup and shutdown periods. This procedure has resulted in 350 data series and determined the ranges of the input variables presented in Table 3.

The neural network was a multi-layer perception (MLP) consisting of three layers: an input layer with as many nodes as the input variables (15), a hidden layer with number of nodes varying from 1 to 5 and an output layer with as many nodes as the output variables (16). The most common training algorithm was used, that is the error back propagation (EBP). In order to avoid over-fitting and over-training phenomena, a version of the 'cross validation-winner model algorithm' described in the literature (Michalopoulos *et al.*, 2001) was used for the selection of the appropriate number of nodes in the hidden layer of the neural models. The 350 data series were randomly split into training and validation

Table 1. Ranges and optimization usage of the HDS sub-model variables (Par = optimization parameter; Var = optimization variable).

Input variables	Notation	Training range	Usage
HDS temperature (°C)	T_{HDS}	335–355	Par
HDS pressure (bar)	P_{HDS}	74–86	Par
HDS hydrogen make-up ($\text{kN m}^3 \text{h}^{-1}$)	$Q_{\text{H,M}}$	15–30	Var
Recycle hydrogen rate ($\text{kN m}^3 \text{h}^{-1}$)	$Q_{\text{H,R}}$	79–94	Par
HDS VGO feed rate (th^{-1})	F_{HDS}	175–225	Var
First quench rate ($\text{kN m}^3 \text{h}^{-1}$)	$Q_{\text{H,q1}}$	4–12	Par
Second quench rate ($\text{kN m}^3 \text{h}^{-1}$)	$Q_{\text{H,q2}}$	7–11	Par

Table 2. Output variables, model type and mean absolute relative error (MARE) of the FCC sub-models (NN = neural network; PR = parametric regression).

Output variables	Notation	Training range	Model type	MARE
Sour gas (% wt)	y_{SourGas}	4.3–6.1	NN	3.4
LPG (% wt)	y_{LPG}	13.5–16.5	NN	1.7
Gasoline (% wt)	y_{Gasoline}	45.0–53.0	NN	1.4
LCCO (% wt)	y_{LCCO}	13.9–22.0	NN	4.5
Slurry (% wt)	y_{Slurry}	5.8–11.2	NN	5.3
Coke (% wt)	y_{Coke}	3.5–4.1	NN	0.9
Aromatics in gasoline (% wt)	$W_{\text{Aromatics}}$	22.1–28.3	PR	7.1
Olefins in gasoline (% wt)	W_{Olefines}	22.3–33.0	PPR	6.1
Paraffins in gasoline (% wt)	$W_{\text{Paraffins}}$	20.1–30.8	PR	6.1
Naphthens in gasoline (% wt)	$W_{\text{Naphthens}}$	10.6–14.4	PR	5.9
Propane in LPG (% wt)	W_{Propane}	7.3–13.6	NN	6.9
Propylene in LPG (% wt)	$W_{\text{Propylene}}$	22.8–46.0	NN	7.5
Butane in LPG (% wt)	W_{Butane}	3.3–6.3	NN	7.2
<i>i</i> -Butane in LPG (% wt)	$W_{i\text{-Butane}}$	13.5–21.3	NN	4.5
Butenes in LPG (% wt)	W_{Butenes}	23.0–45.8	NN	7.2
LCN in gasoline (% wt)	W_{LCN}	80.0–88.5	NN	1.1
RON of LCN	RON_{LCN}	92.1–94.1	NN	0.2
RON of HCN	RON_{HCN}	85.7–93.0	NN	0.6
Sulphur in LCN (% wt)	S_{LCN}	0.004–0.085	NN	18.1
Sulphur in HCN (% wt)	S_{HCN}	0.050–0.637	NN	26.1
Sulphur in LCCO (% wt)	S_{LCCO}	0.47–2.83	NN	7.7

sets consisting of 225 and 125 data series, respectively. The first set was used for the neural network training procedure, and the second for monitoring the generalization abilities of the neural network according to the algorithm mentioned above. One of the end criteria for this algorithm was the number of nodes in the hidden layer, which as mentioned was set at a maximum value of 5, in order to keep the ‘data to network weights’ ratio as high as possible. The other important training parameter of the algorithm, namely the number of training epochs, had an upper limit equal to 10,000, which is a logical choice considering the convergence speed of the EBP algorithm. According to this procedure, the ‘winner’ neural model consisted of three nodes in the hidden layer.

The performance of the FCC model in terms of normalized mean square error (NMSE) for each output variable is presented in Figure 2, where it can be seen that the

over-fitting phenomenon has been avoided. Table 2 presents the model performance according to the mean of the absolute values of the relative error (MARE). The model performance deteriorates only for the prediction of sulphur in gasoline fractions, while for the rest of the variable MARE lies between 1 and 8%, which is considered satisfactory. The error in the prediction of the gasoline sulphur can be attributed to the combination of higher experimental error and low values. Figure 3 presents the performance of the neural model for two of the most important output variables, the yields of gasoline and LPG, and demonstrates a typical example of the prediction accuracy of the model. The performance is evaluated over all 350 available data series, the last part of which depicts the validation set. It is obvious that the neural model is able to follow the trend satisfactorily, which is of great importance for the needs of the optimization case studies.

Table 3. Ranges and optimization usage of the input variables of the FCC neural sub-models. Column Orientation denotes the unit to which the variable refer (*HDS* = output variable of the HDS unit, *Tank* = input variable of the VGO from Tank, *FCC* = input variable of the FCC unit. Column Usage denotes the use of each variable in the optimization procedure (Par = Optimization Parameter, Var = Optimization Variable).

Input variables	Notation	Training range	Orientation	Usage
Feed specific gravity	SG	0.896–0.921	HDS-Tank	Par
Refractive index (at 20 °C)	RI	1.482–1.495	HDS-Tank	Par
Sulphur in feed (% wt)	S	0.30–1.85	HDS-Tank	Par
Basic nitrogen in feed (wppm)	BN	158–421	HDS-Tank	Par
Mean average boiling point (°C)	$MeABP$	438–472	HDS-Tank	Par
FCC VGO feed rate (th ⁻¹)	F_{VGO}	236–284	HDS-Tank	Var
FCC feed preheat (°C)	T_{PR}	360–396	FCC	Var
FCC riser top temperature (°C)	T_{RX}	519–526	FCC	Var
FCC riser pressure (kg cm ⁻²)	P_{R}	2.1–2.4	FCC	Par
FCC regenerator air feed (kNm ³ h ⁻¹)	Q_{AIR}	99–115	FCC	Par
FCC catalyst addition rate (Mt day ⁻¹)	F_{CAT}	0.0–4.9	FCC	Par
Catalyst micro activity	MAT	66.0–75.3	FCC	Par
Catalyst average particle size (µm)	APS	74–84	FCC	Par
Catalyst total surface area (m ² g ⁻¹)	SA	129–171	FCC	Par
Catalyst average bulk density (g m ⁻³)	ABD	0.86–0.94	FCC	Par

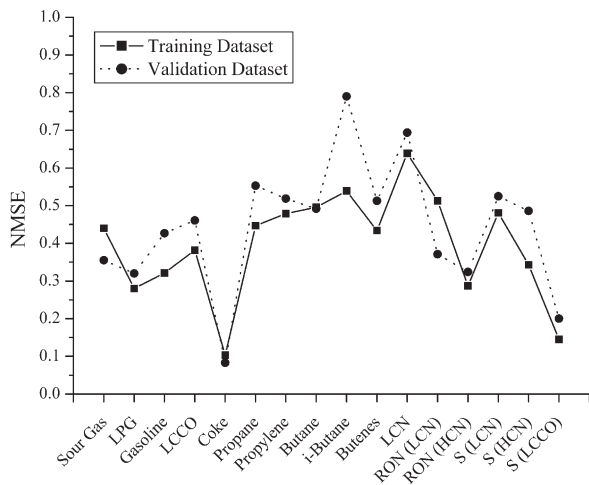


Figure 2. Performance of the neural network in terms of NMSE for all the output variables.

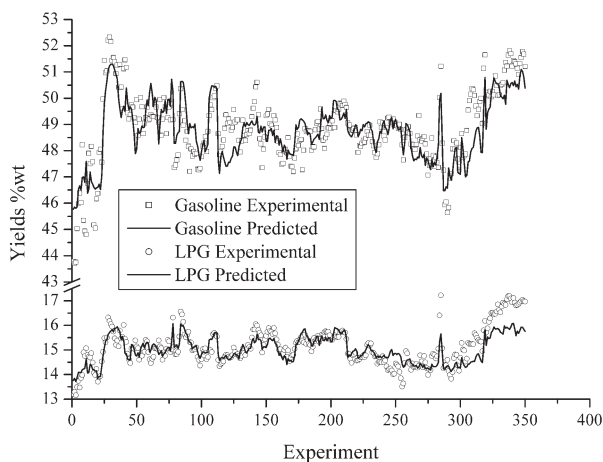


Figure 3. Performance of the neural network (gasoline and LPG yields).

The general form of the parametric models is presented in equation (15):

$$i\text{-component (\%wt)} = f(\text{feed properties}) \times g(\text{operating conditions}) \cdot CI \quad (15)$$

where the i -component is one of the four gasoline components presented in Table 2. The mathematical function for the feed properties effect was selected to be linear and includes the physical properties which mostly affect the gasoline composition and can be measured on a daily basis in the refinery laboratory (specific gravity, % wt sulphur content, % wt basic nitrogen content, mean average boiling point and refractive index as presented in Table 3). The operating conditions function was also selected to be linear and incorporated the riser temperature, the catalyst-to-oil ratio and the weight hourly space velocity, which are known to adequately describe the FCC process in steady-state conditions (Wollaston *et al.*, 1975; Arbel *et al.*, 1995; Bollas *et al.*, 2003). Linear models were found to adequately predict the gasoline composition (Lappas *et al.*, 1999) and they were chosen for the simplicity in their development and use. The use of the catalyst-to-oil ratio and the weight hourly space velocity in equation (15) requires the prediction of the CCR based on the variables presented in Table 3. This is achieved with a neural network following the same procedure as described in the previous paragraph. The accuracy levels of this neural model were very high, reaching $MARE = 0.9\%$, confirming that CCR is actually a dependent variable. Finally the catalyst effect was incorporated through a catalyst index, CI , which is a multiplier to the product of operating and feed effect functions. The reason for using a simple multiplier to characterize the catalyst effect on the cracking reaction is that the development of a predictive catalyst function appears quite complex. Generally, the concept of describing catalyst activity and selectivity with a catalyst index is a common industrial strategy, in order to validate catalyst performance in commercial units.

Combined Model Interconnections

The integration of the models included in the tool was made in a sequential form as shown in Figure 4. This means

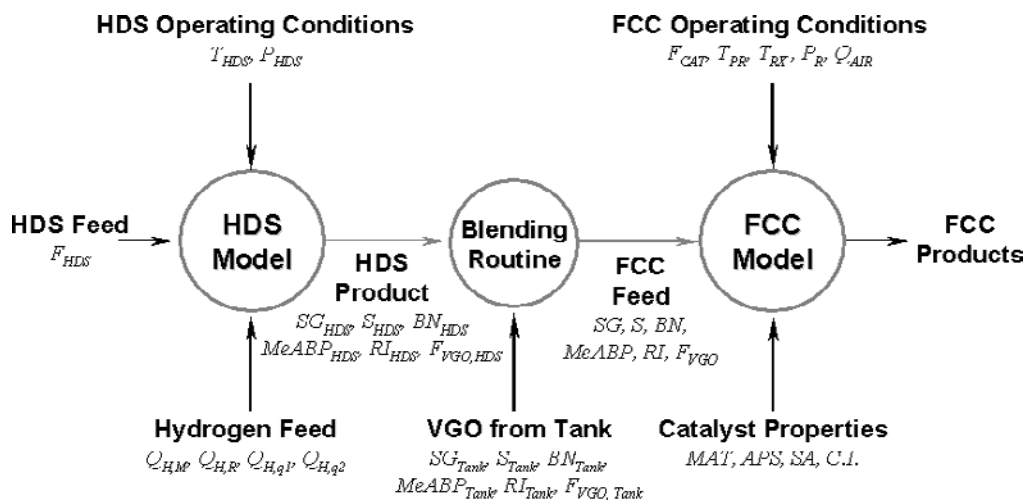


Figure 4. HDS-FCC sub-models integration.

that the predictions of the short-form models applied for the simulation of the HDS unit are entered as input variables to the blending routine, where the properties of the VGO from tank and the HDS liquid product are mixed. For the estimation of the properties of the blended FCC feed the weighted average of the respective properties of the HDS product and the VGO from tank was used. This average can be very accurate, as the blended hydrocarbon mixtures are of similar molecular weights and structures (American Petroleum Institute, 1992). Furthermore, a typical 25% of the HDS product is considered primary distillates and subtracted from the liquid product that is blended with the VGO from tank. This value can be altered according to the specific HDS operation.

OPTIMIZATION APPROACH

Objective Function

The financial objective function is based on the mass balances of the two units, while the energy consumption costs are considered negligible. The cost of preheating the FCC feed is neglected, since it is considered that hot streams of other processes could be used for that reason. This assumption is correct for the commercial unit examined. Furthermore, the cost of preheating the feed is rather small compared with all other costs of the total process (hydrogen consumption, feed and catalyst supply, etc.). Thus, the financial objective takes the form of equation (16):

$$\begin{aligned} Z &= (\text{price of products}) - (\text{cost of raw material}) \\ &= Z_i - Z_o \end{aligned} \quad (16)$$

The term 'cost of raw material' of equation (16) is calculated by the following equation:

$$\begin{aligned} Z_o &= F_{\text{VGO,HDS}} \cdot I_{\text{VGO,HDS}} + F_{\text{VGO,TANK}} \cdot I_{\text{VGO,TANK}} \\ &\quad + F_H \cdot I_H + F_{\text{CAT}} \cdot I_{\text{CAT}} \end{aligned} \quad (17)$$

where $F_{\text{VGO,HDS}}$, $F_{\text{VGO,TANK}}$, F_H and F_{CAT} are the feed rates (t h^{-1}) of the VGO into the HDS and from the tank into the FCC, of the hydrogen used in the HDS and of FCC catalyst make-up respectively, while $I_{\text{VGO,HDS}}$, $I_{\text{VGO,TANK}}$, I_H and I_{CAT} are the respective costs per mass of the 'raw material' ($\text{\$ t}^{-1}$).

The term 'price of products' in equation (16) refers to the value of the FCC products (sour gas, LPG, gasoline, LCCO and slurry). In the following equations, where the various components of this term are expressed, F_{VGO} denotes the total feed rate into the FCC (t h^{-1}), y_i the yield of the FCC concerning the i -product and I_i its respective monetary value per mass. More specifically the price of sour gas is calculated by the following equation:

$$Z_{i,\text{SourGas}} = F_{\text{VGO}} \cdot y_{\text{SourGas}} \cdot I_{\text{SourGas}} \quad (18)$$

while the price of LPG depends on the distribution of the chemical compounds, of which it consists, namely propane,

propylene, butane, iso-butane and butenes. It is given by the following functional form:

$$\begin{aligned} Z_{i,\text{LPG}} &= F_{\text{VGO}} \cdot y_{\text{LPG}} \cdot (W_{\text{Propane}} \cdot I_{\text{Propane}} \\ &\quad + W_{\text{Propylene}} \cdot L_{\text{Propylene}} + W_{\text{Butane}} \cdot I_{\text{Butane}} \\ &\quad + W_{i-\text{Butane}} \cdot I_{i-\text{Butane}} + W_{\text{Butenes}} + I_{\text{Butenes}}) \end{aligned} \quad (19)$$

where W_j is the weight fraction of the j -component of LPG. The gasoline price depends on its distribution of light cut naphtha (LCN) and heavy cut naphtha (HCN), as well as its octane number (RON) and sulphur content (S). This is expressed in the following equation:

$$\begin{aligned} Z_{i,\text{Gasoline}} &= F_{\text{VGO}} \cdot y_{\text{Gasoline}} \{ W_{\text{LCN}} \cdot I_{\text{LCN}} \cdot [1 + \delta_{\text{LCN},\text{RON}} \\ &\quad \times (RON_{\text{LCN}} - RON_{\text{LCN}}^*) + \delta_{\text{LCN},\text{S}} \\ &\quad \times (S_{\text{LCN}} - S_{\text{LCN}}^*)] + W_{\text{HCN}} \cdot I_{\text{HCN}} \\ &\quad \times [1 + \delta_{\text{HCN},\text{RON}} \cdot (RON_{\text{HCN}} - RON_{\text{HCN}}^*) \\ &\quad + \delta_{\text{HCN},\text{S}} \cdot (S_{\text{HCN}} - S_{\text{HCN}}^*)] \} \end{aligned} \quad (20)$$

where the influence of RON and S is expressed by their differences from the reference values RON_i^* , S_i^* of the LCN and HCN fractions, multiplied by a respective factor, δ , which refers to the importance of this difference. The reference values RON_i^* , S_i^* are the values of RON and S corresponding to the standard prices (I_i) of the two fractions.

The price of LCCO depends on its quality expressed by the sulphur content in a similar way to gasoline:

$$\begin{aligned} Z_{i,\text{LCCO}} &= F_{\text{VGO}} \cdot y_{\text{LCCO}} \cdot I_{\text{LCCO}} \cdot [1 \\ &\quad + \delta_{\text{LCCO},\text{S}} \cdot (S_{\text{LCCO}} - S_{\text{LCCO}}^*)] \end{aligned} \quad (21)$$

while the case of slurry is handled like sour gas:

$$Z_{i,\text{Slurry}} = F_{\text{VGO}} \cdot y_{\text{Slurry}} \cdot I_{\text{Slurry}} \quad (22)$$

Optimization Variables and Constraints

Above, the manipulated variables of the FCC unit were determined based on a generalized degrees of freedom analysis. The free input variables of the FCC unit shown in Table 3 were categorized as optimization variables or parameters according to their possibility of receiving any random value and the extent of their effect on the FCC yields and quality. Thus, the properties of the VGO from the tank and the FCC catalyst were categorized as optimization parameters, as the feeds and catalysts available to the refinery determine them. Furthermore, the FCC unit pressure (P_R) and the regenerator combustion air (Q_{AIR}) were categorized as parameters, since they do not affect significantly and directly the process outcome. Finally, the most important variables for the HDS unit operation, namely the HDS feed rate (F_{HDS}) and the hydrogen make-up ($Q_{\text{H,M}}$), were chosen as the optimization variables for that unit.

The discrimination of the optimization variables (marked Var) and the optimization parameters (marked Par) is presented in Tables 1 and 3. The ranges in these tables, as well as in Table 2, serve as the default constraints for the optimization procedure. Starting from this point the user has the choice of defining smaller ranges or even specific values for any of the two classes of constraints (input and output), which increases the flexibility of the tool and makes the

examination of a vast number of case studies possible. As mentioned, the FCC unit produces around 40% of the total refinery gasoline. Consequently, the operating limits of the FCC unit usually determine those of the combined HDS-FCC units and generally the operation of the total refinery. However, if the operation of the complete refinery restricts the operating limits of the HDS-FCC process, then the user can alter the constraints of the variables accordingly.

Optimization Algorithm

The optimization procedure uses the optimization algorithms provided in the edition Small-Scale NLP/NILP DLL V3.5 of the software package SOLVER (Frontline Systems Co.), which was incorporated in the tool. Its ability to handle non-linear optimization problems including up to 400 variables and 200 constraints makes it a powerful tool for complex multivariate optimization.

Three algorithms were included in the software package: a quasi-Newton, a conjugate gradient and a genetic algorithm. The two first methods belong to the same class, namely the class of methods based on derivative (first or second order) calculation of the objective function. The quasi-Newton method approximates the Hessian matrix, based on a function of the gradient of the objective function (Press *et al.*, 1986; Dennis and Schnabel, 1983). The conjugate gradient algorithm is analogous to Newton's method in the sense that it also uses the derivatives of the objective function but in a manner that avoids extensive computation. More specifically, it is well known that, although the objective function decreases more rapidly along the steepest descent direction (negative of the gradient of the objective function), this does not necessarily produce the fastest convergence. In the conjugate gradient algorithms a search is performed along conjugate directions, which produces generally faster convergence (Fletcher and Reeves, 1964).

The combination of these fast optimization algorithms with the short-form modelling approach makes the tool respond almost instantly. However, when the optimization scenario is a multisolution problem, these two algorithms may get stuck in local maxima. Therefore, the option of a genetic algorithm based on a completely different philosophy has been included in the tool. Genetic algorithms are founded on the basic tenets of natural selection and evolution (Goldberg, 1989), which in terms of optimization means that the variable values are changed randomly or heuristically in order to minimize the objective function and not according to its derivatives. Falling into the category of stochastic optimization techniques, they share their advantage of small possibility of getting stuck into a local minimum. However, if some of their parameters are not properly handled, processing speed and data storage costs may become large, which negatively affects its convergence speed (Fogel, 1994).

Once more it must be pointed out that the short-form modelling approach contributes to the direction of convergence speed by not overloading the computational task and therefore helping these algorithms to achieve their task in acceptable time. After all, it is among the user's options in the integrated tool to select the algorithm that best suits the optimization procedure. However, the parameters of the algorithms are not adjustable. Their values have been selected and kept constant during the development of the

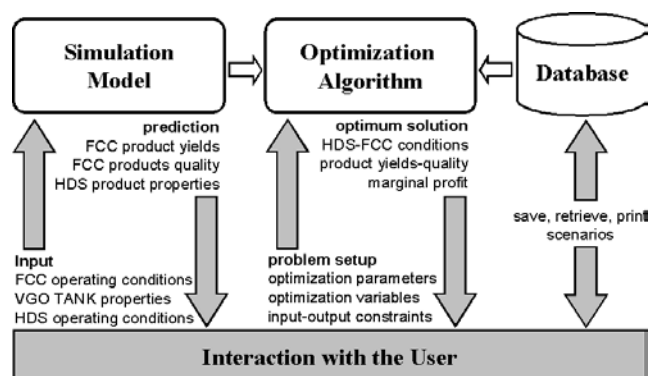


Figure 5. The structure of the HDS-FCC tool.

tool, taking into account the precision limits of the prediction models. The interaction of the user with such details of the algorithms would make the tool cumbersome for the non-expert user.

OPERATIONAL ASPECTS

The overall structure of the developed DSS tool is presented in Figure 5. It consists of three main components, which strongly interact with each other and most importantly with the user:

- (1) The process models, which simulate the operation of the HDS and the FCC units, as well as the interconnection between them in steady-state conditions.
- (2) The database, where each steady-state run can be stored to be available for later usage.
- (3) The optimization algorithm, which is based on a financial objective function that takes into account the marginal profit of the combined operation, based on a financial database provided.

The system was implemented within the computational environment of Microsoft Visual Basic and can be used in any standard personal computer running Microsoft Windows operating system. The interface of the tool includes two basic modes: (1) the simulation mode, where the input variables of the system are entered and the predictions of the integrated model are calculated; and (2) the optimization mode, where the integrated model runs backwards to estimate the optimum values for some of the input variables for a 'desired solution', or forward to perform sensitivity analysis and reveal in a diagrammatic form the input parameters effect on the most important output variables.

The environment of the simulation mode is presented in Figure 6. The integrated model predictions include the FCC product yields, namely the yields of gasoline, coke, LPG, LCCO, sour gas and slurry as well as the HDS liquid product properties. Furthermore, the prediction of the products quality includes the composition of gasoline, LPG, the % wt sulphur in LCN, HCN and LCCO, the percentage of LCN in gasoline and the RON of LCN and HCN. The 'catalyst index' mentioned above is calculated with a regression routine included, where the data of at least one experimental run are required to calculate the index for the catalyst characterization.

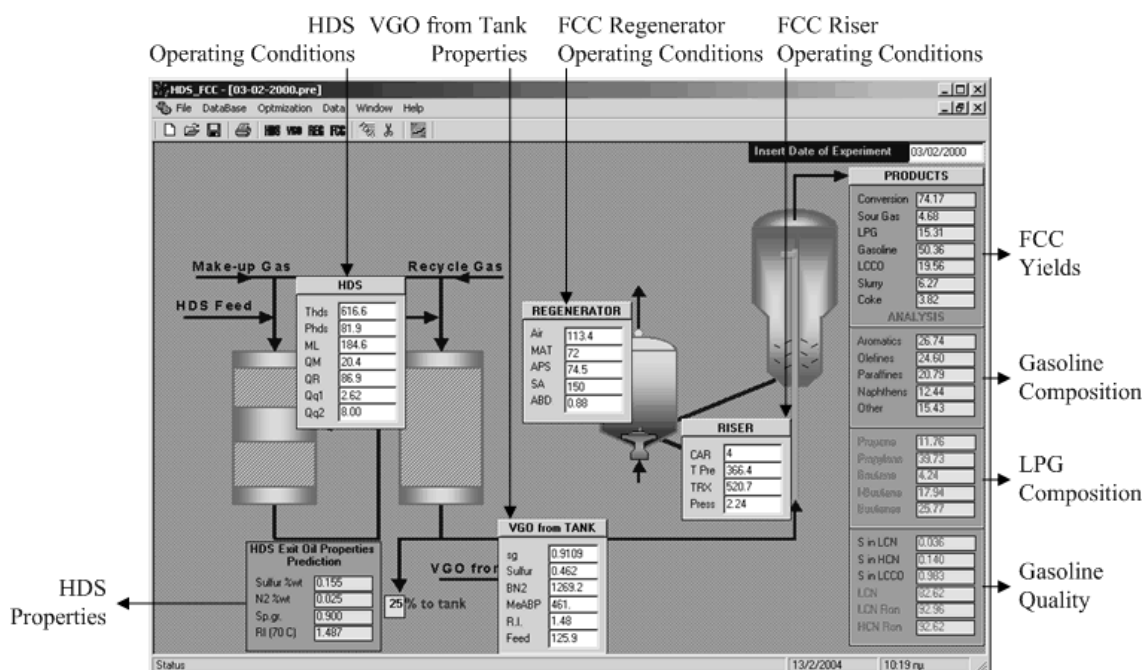


Figure 6. The interface of the HDS-FCC simulator: prediction mode.

The second mode of the tool performs the optimization of the integrated HDS-FCC system in the environment presented in Figure 7. The model input variables are split into optimization variables, which are expected to deliver the optimum solution for the integrated system, and optimization parameters, which are kept constant, equal to a value selected *a priori*. The optimization solution can be requested for a subset of the optimization variables, while all other variables are categorized as optimization parameters and retain a constant value. Moreover, constraints can be entered for the input and output variables range, in order to

achieve a more realistic solution for the corresponding system. The market prices of the process products and raw materials are requested for the financial optimization of the system.

Finally, the trends of some product yields and their properties vs the most important system input variables are presented (Figure 8). That was made with sensitivity analysis runs of the integrated system and provides an estimation of what should be expected when the values of the selected input variables are changed. The process variables that were chosen *a priori* for this demonstration of

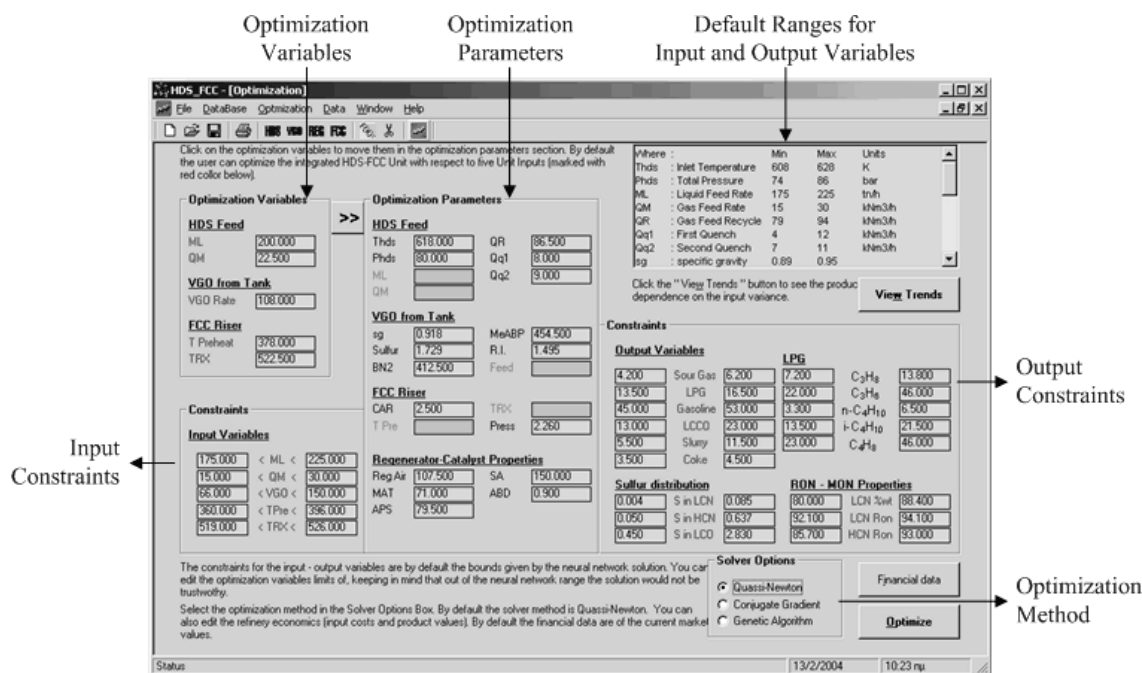


Figure 7. The interface of the HDS-FCC simulator: optimization mode.

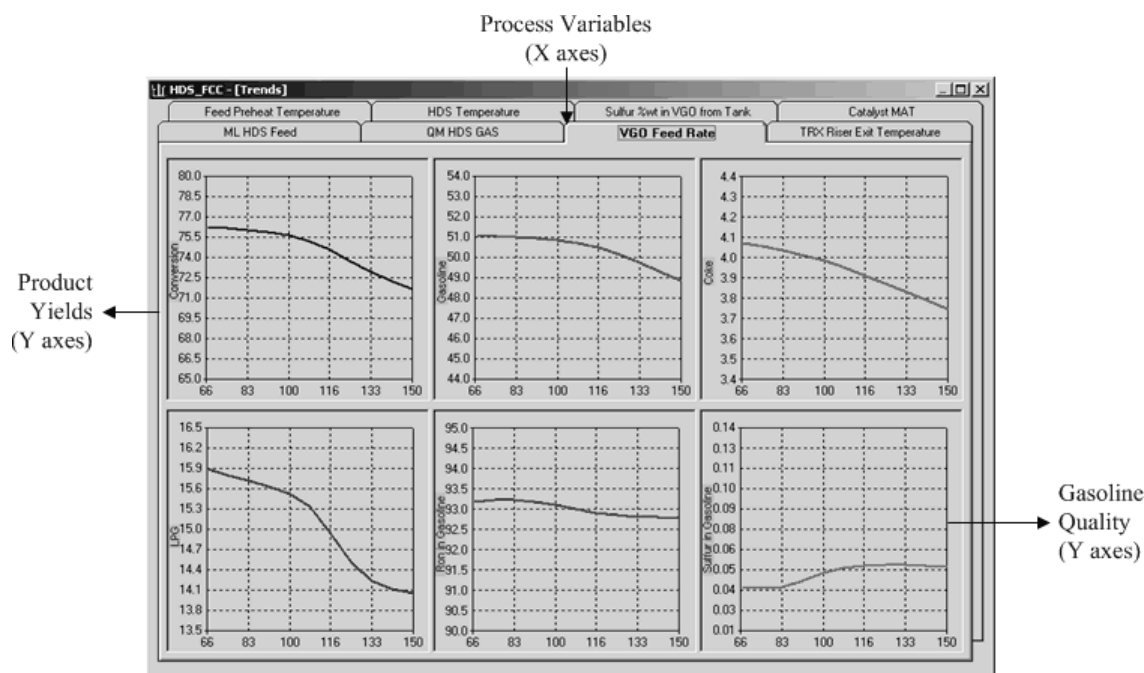


Figure 8. The interface of the HDS-FCC simulator: sensitivity analysis runs. Effect of the VGO feed rate on some FCC product yields and quality.

segregate influences were the HDS feed rate, the HDS hydrogen make-up, the HDS temperature, the VGO from tank rate and its sulphur content, the FCC feed preheat temperature, the FCC riser exit temperature and the catalyst MAT activity. This analysis provides a sense of how these variables of the integrated HDS-FCC system affect its operation and the final product yields and quality.

CASE STUDIES

Prediction Mode

The predictive accuracy of the tool was evaluated with three commercial tests, which were not included in the training

Table 4. The values of the input variables in the industrial runs used for the evaluation of the tool prediction mode.

Input variables	Test 1	Test 2	Test 3
Feed specific gravity	0.910	0.905	0.912
Refractive index (at 20 °C)	1.490	1.486	1.488
Sulphur in feed (% wt)	0.99	0.30	1.10
Basic nitrogen in feed (wppm)	219	730	178
Mean average boiling point (°C)	453	461	444
FCC VGO feed rate (t h ⁻¹)	259	267	280
FCC feed preheat (°C)	365	366	373
FCC riser top temperature (°C)	520	521	520
FCC riser pressure (kg cm ⁻²)	2.17	2.24	2.39
FCC regenerator temperature (°C)	732	732	730
FCC catalyst addition rate (Mt day ⁻¹)	4.2	4.0	3.6
Catalyst micro activity	68	72	71
Catalyst average particle size (µm)	79	75	84
Catalyst total surface area (m ² g ⁻¹)	153	150	157
Catalyst average bulk density (g m ⁻³)	0.89	0.90	0.88

procedure of the models. Table 4 presents the values of the input variables of the models in these three runs. The first commercial test was a routine run of the industrial unit, in which all input variables laid within their training range and most of them near their mean values. In the second commercial test some of the variables had marginal values regarding their training range [namely the % wt sulphur content (*S*) and the average catalyst particle size (APS)], while another one (the % wt basic nitrogen content, BN) was out of its respective training range. In the third commercial test even more input variables had marginal values. Table 5 presents the values of the output variables, as these were measured in the commercial tests and predicted by the tool implementation. The comparison shows that in all cases the tool performed within the accuracy determined during the model's development and analysis. Focusing on the gasoline quality, which is of great importance for the refinery, the prediction of *RON* and sulphur content lies within the accuracy demanded, which encourages the user to trust the results of the optimization scenarios based on gasoline quality requirements.

Optimization Mode

The scenarios presented here demonstrate the capabilities of the optimization mode of the presented computer-aided tool. They are mainly focused on realistic situations which depict the contemporary needs regarding the products of the FCC unit. The maximization of the refinery marginal profit, using constraints on the gasoline yield and quality, constitutes such scenarios. The values of the product prices and raw material costs, which are necessary for the financial objective function, are presented in Table 6. These are the default values that Aspropyrgos Refinery of Hellenic Petroleum provided and the tool takes into account, unless the user provides other financial data.

Table 5. HDS–FCC tool validation in the prediction mode (CT = commercial test; MP = models prediction; RE = absolute relative error %).

Output variables	Test 1			Test 2			Test 3		
	CT	MP	RE	CT	MP	RE	CT	MP	RE
Conversion (% wt)	72.1	72.4	0.5	72.8	75.2	3.3	70.9	72.0	1.4
Sour gas (% wt)	4.4	4.7	7.1	4.6	4.9	5.9	5.1	5.0	1.5
LPG (% wt)	15.1	14.9	1.3	15.0	15.5	3.3	14.7	14.9	1.5
Gasoline (% wt)	48.6	48.8	0.5	49.3	50.8	3.2	47.3	48.2	1.9
LCCO (% wt)	20.0	18.9	5.4	19.6	16.8	14.3	20.3	19.2	5.6
Slurry (% wt)	7.9	8.7	9.4	7.6	8.0	5.3	8.7	8.9	1.4
Coke (% wt)	4.0	4.0	0.9	4.0	4.0	1.8	3.9	3.9	0.3
Aromatics in gasoline (% wt)	26.0	22.5	13.5	24.5	26.8	9.4	24.6	22.2	9.8
Olefins in gasoline (% wt)	31.0	32.2	3.9	29.0	25.1	13.4	32.0	30.7	4.1
Paraffins in gasoline (% wt)	23.2	24.9	7.3	27.0	21.7	19.6	24.5	24.8	1.2
Naphthens in gasoline (% wt)	13.3	12.3	7.5	12.1	12.7	5.0	13.2	12.0	9.1
Propane in LPG (% wt)	8.8	9.1	3.0	10.3	9.8	4.7	9.9	10.3	4.0
Propylene in LPG (% wt)	30.2	30.6	1.4	36.2	34.5	4.8	31.8	33.5	5.4
Butane in LPG (% wt)	5.3	5.4	1.8	4.6	4.8	4.1	5.2	5.1	1.8
<i>i</i> -Butane in LPG (% wt)	17.9	17.6	1.8	17.7	17.0	3.6	17.9	17.3	3.3
Butenes in LPG (% wt)	37.1	36.9	0.5	30.8	33.6	9.4	34.9	33.4	4.4
LCN in gasoline (% wt)	86.9	84.7	2.5	84.4	85.1	0.8	84.5	84.6	0.1
RON of LCN	92.6	92.9	0.3	93.1	93.2	0.1	93.5	93.1	0.5
RON of HCN	89.1	89.9	0.9	91.1	90.0	1.2	91.8	91.7	0.1
Sulphur in LCN (% wt)	0.04	0.04	27.3	0.02	0.03	31.8	0.07	0.06	20.9
Sulphur in HCN (% wt)	0.32	0.30	5.3	N/A	0.25	N/A	0.22	0.27	21.5
Sulphur in LCCO (% wt)	1.59	1.74	9.3	0.63	1.12	77.8	1.78	1.77	0.4

Gasoline Maximization (Base Case)

This scenario considers a variety of conditions, under which the maximization of the gasoline yield can be achieved. In the base case the optimization algorithm was asked to achieve the most profitable solution for the operation of the combined HDS–FCC units, by changing all the optimization variables of Tables 1 and 3, while keeping the optimization parameters constant at their mean values. This scenario was repeated three times with the three optimization methods (quasi-Newton, conjugate gradient and genetic algorithm), in order to explore the accuracy of each method. As shown in Table 7, all three algorithms delivered the same solution, with the gasoline yield reaching 50.3% wt. However, only the genetic algorithm was systematically converging to the global solution, while the other two methods occasionally stuck in local maxima. For that reason all the optimization scenarios presented were performed with the genetic algorithm.

Table 6. Product and raw material prices (default values). (Reference: personal communication with Aspropyrgos Refinery of Hellenic Petroleum S.A., 2001.)

<i>Product prices (\$ t⁻¹)</i>	
Sour gas	156
LCCO	200
Slurry	132
LCN	296
HCN	243
Propane	313
Propylene	313
<i>n</i> -Butane	313
<i>i</i> -Butane	313
Butene	313
<i>Material costs (\$ t⁻¹)</i>	
HDS-feed	156
VGO from tank	186
Hydrogen in HDS	300
FCC catalyst	1710

Starting from the base case scenario we tried to explore the effect of maximizing the yield of gasoline on the total profit. This was done by sequentially increasing the constraint of gasoline yield from the value of the base case scenario until no feasible solution could be reached. As shown in Table 7, the maximization of the gasoline yield was mainly achieved by increasing the ratio of HDS feed to VGO from tank rates, which corresponded to better FCC feed quality. At gasoline yield of 51.0% wt the HDS feed rate reached its maximum value and after that no feasible solution could be achieved, which means that, with the optimization parameters receiving their average values, the maximum gasoline yield that can be produced is around 51% wt.

Constraints on Gasoline Yield

The scenarios of this category examine some cases of profitable operation of the combined HDS–FCC units using constraints to the gasoline yield over 50% wt and varying variables concerning the catalyst and the unit operation. Starting from the base case of Table 7, we observed the influence of an optimization parameter concerning the catalyst, namely the MAT activity index. For this reason the base case optimization scenario was repeatedly performed, varying the MAT value to cover all its respective range, as shown in Table 8. What was interesting was that, along with the expected increase in the product yields (conversion, gasoline yield and LPG yield), a relation of the sulphur content in LCN and the total gasoline sulphur with MAT was obvious. That means that among the many solutions the system can reach in order to produce gasoline yields over 50% wt, there are some that favour better product quality; for instance more active catalyst (greater MAT) leads the system to the production of light products with lower sulphur content. Another important remark is that greater MAT values allow the system to operate at higher VGO tank rates, implying that better catalyst quality can crack more feed of worse quality, which is in agreement

Table 7. HDS–FCC tool optimization mode: base case scenario. Effect of optimization method (QN = quasi-Newton; CG = conjugate gradient; GA = genetic algorithm) and gasoline constraints for gasoline maximization (units are as defined in Tables 1–3).

	Base case			Gasoline constraints			
	QN	CG	GA	>50.4	>50.7	>51.0	>51.3
HDS VGO feed rate (th ⁻¹)	175.0	175.0	175.0	175.0	199.0	220.0	
HDS hydrogen make-up (kNm ³ h ⁻¹)	15.0	15.0	15.0	15.0	15.0	15.0	
VGO tank feed rate (th ⁻¹)	124.9	124.9	125.0	125.0	107.7	79.0	
FCC feed preheat (°C)	362.1	362.0	362.2	360.2	360.0	360.0	
FCC riser top temperature (°C)	521.4	521.4	521.4	521.7	522.3	526.0	
Conversion (% wt)	74.6	74.6	74.6	74.6	75.0	75.5	No feasible solution
LPG (% wt)	15.3	15.3	15.3	15.3	15.3	15.5	
Gasoline (% wt)	50.3	50.3	50.3	50.4	50.7	51.0	
Coke (% wt)	17.1	17.1	17.1	17.2	17.2	17.1	
Sulphur in LCN (% wt)	0.035	0.035	0.035	0.035	0.032	0.028	
Sulphur in HCN (% wt)	0.281	0.281	0.281	0.284	0.273	0.241	
Sulphur in gasoline (% wt)	0.072	0.072	0.072	0.072	0.068	0.061	
LCN in gasoline (% wt)	85.2	85.2	85.2	85.1	84.8	84.7	
RON of LCN	93.2	93.2	93.2	93.2	93.2	93.2	
RON of HCN	90.1	90.1	90.1	90.1	90.0	90.1	
RON of naphtha	92.7	92.7	92.7	92.7	92.7	92.7	
Total margin	5064	5064	5064	5057	4766	4229	

with the respective FCC theory and the experimental experience. At this point it should be pointed out that the increase in the MAT property of the catalyst generally corresponds to an additional expense for the refinery, which was not included in this scenario.

As stated above, the flexibility of the tool provides the option of setting an optimization variable as optimization parameter and in this way testing a variety of optimization scenarios for different constant values of this parameter. We have exploited this ability of the tool for the case of the feed preheat temperature. Moreover, we have kept constant the MAT parameter at its lowest value (MAT = 66), which refers to a catalyst of worse quality. The results have shown that the gasoline constraint can still be satisfied under these conditions (Table 9). In the real process an increase in the feed preheat temperature should lead to an immediate decrease in the catalyst circulation rate (for constant T_{RX} temperature), as the mass and heat balances of the closed loop FCC system impose. This is evident in Table 9 for the

scenarios in which the riser temperature remains relatively constant (T_{PR} 360–370 and T_{PR} 380–390K). Moreover, it is observed that as the feed preheat temperature increases, the T_{RX} also increases, while the VGO from tank decreases. At T_{PR} 380°C the T_{RX} reaches its maximum value and probably the relation of these two temperatures allows the catalyst circulation rate to reach a maximum and the total system to reach the most profitable solution of this scenario. From this point on the rise of T_{PR} leads to less profitable solutions and at T_{PR} 396°C the gasoline constraint cannot be satisfied.

Constraints to Gasoline Quality

The scenarios of this category examine some cases of profit maximization under strict specifications for the gasoline RON. The constraints for RON were set for those FCC products (LCN, HCN), which compose the gasoline fraction. More specifically, specifications were set for RON_{LCN} and RON_{HCN} to be greater than 93.4 and 92.0 respectively.

Table 8. HDS–FCC tool optimization mode: MAT activity effect (gasoline constraints to 50% wt). (Units are as defined in Tables 1–3.)

Catalyst micro activity	66	68	71	73	75
HDS VGO feed rate (th ⁻¹)	175.0	175.0	175.0	175.0	175.0
HDS hydrogen make-up (kNm ³ h ⁻¹)	15.0	15.0	15.0	15.0	15.0
VGO tank feed rate (th ⁻¹)	120.7	122.9	125.0	125.7	125.9
FCC feed preheat (°C)	360.0	360.0	362.2	363.1	363.5
FCC riser top temperature (°C)	520.6	520.8	521.4	522.0	522.7
Conversion (% wt)	74.3	74.4	74.6	74.7	74.8
LPG (% wt)	15.1	15.2	15.3	15.3	15.3
Gasoline (% wt)	50.3	50.3	50.3	50.4	50.5
Coke (% wt)	4.0	4.0	4.0	4.0	4.0
Sulphur in LCN (% wt)	0.037	0.036	0.035	0.034	0.033
Sulphur in HCN (% wt)	0.277	0.279	0.281	0.280	0.276
Sulphur in gasoline (% wt)	0.073	0.073	0.072	0.071	0.069
LCN in gasoline (% wt)	85.1	85.2	85.2	85.1	85.0
RON of LCN	93.2	93.2	93.2	93.2	93.2
RON of HCN	90.5	90.4	90.1	90.0	90.0
RON of naphtha	92.8	92.8	92.7	92.7	92.7
Total margin	4840	4948	5064	5114	5150

Table 9. HDS–FCC tool optimization mode: feed preheat temperature effect (gasoline constraints to 50% wt). (Units are as defined in Tables 1–3).

	FCC feed preheat (°C)				396
	360	370	380	390	
	Catalyst circulation rate (m ³ h ⁻¹)				
	19.71	19.68	19.92	19.64	
HDS VGO feed rate (th ⁻¹)	175.0	175.0	175.0	204.0	
HDS hydrogen make-up (kN m ³ h ⁻¹)	15.0	15.0	15.0	15.0	
VGO tank feed rate (th ⁻¹)	120.7	119.7	142.4	90.9	
FCC riser top temperature (°C)	520.6	521.5	526.0	526.0	
Conversion (% wt)	74.3	74.2	74.5	74.9	No feasible solution
LPG (% wt)	15.1	15.2	14.9	15.6	
Gasoline (% wt)	50.3	50.1	50.3	50.0	
Coke (% wt)	4.0	4.0	3.9	3.9	
Sulphur in LCN (% wt)	0.037	0.039	0.038	0.036	
Sulphur in HCN (% wt)	0.277	0.283	0.332	0.224	
Sulphur in gasoline (% wt)	0.073	0.075	0.085	0.064	
LCN in gasoline (% wt)	85.1	85.3	83.8	85.1	
RON of LCN	93.2	93.2	93.4	93.4	
RON of HCN	90.5	90.5	90.0	90.6	
RON of naphtha	92.8	92.8	92.9	93.0	
Total margin	4840	4794	4914	4228	

The gasoline yield in the most profitable scenario is now based only in the financial data used in the objective function, which of course favour greater values of gasoline mass flow. This was done because the algorithm failed to meet the RON specifications and simultaneously achieve gasoline yields over 50% wt.

Another way to perform RON maximization without using hard constraints is to exploit the δ factors and the standard RON_i^* values, which were mentioned above. By default these parameters have zero value, which means that the objective function does not take into account the quality of the gasoline when converging to a solution. For the test presented here (Table 10), a δ factor equal to 10 and reference RON_i^* values equal to the minimum values observed in the experimental database during the develop-

ment of the models (92.1 for the RON_{LCN} and 85.7 for the RON_{HCN} fraction) were used. Such a large value for the δ factor is of course not realistic, yet it clearly demonstrates the possible use of this feature for a property optimization. What the optimizer has shown is that, even for the extreme case of $\delta = 10$, the RON values demanded could not be reached. That should be expected, as it is known that the gasoline RON is mostly affected by the feedstock properties (Magee *et al.*, 1978) and hydrotreated feeds with low aromatic content are not expected to deliver high RON values in the FCC gasoline. Thus, the effects of the refractive index (*RI*) and the specific gravity (*SG*) of the VGO from tank have been examined, as these two parameters compose a very good indicator of the aromaticity of a feedstock. What was observed (Table 10), was that, as the

Table 10. HDS–FCC tool optimization mode: constraints to gasoline RON scenario. (Units are as defined in Tables 1–4).

	Unconstrained case		RON constraints $\Delta RON = 0$			
	ΔRON		RI at SG = 0.89 (VGO tank)			
	0	10	1.48	1.49	1.5	1.51
HDS VGO feed rate (th ⁻¹)	175.0	208.8	175.0	175.0	175.0	175.0
HDS hydrogen make-up (kN m ³ h ⁻¹)	15.0	15.0	15.0	15.0	15.0	15.0
VGO tank feed rate (th ⁻¹)	125.0	150.0	80.0	78.9	77.6	76.2
FCC feed preheat (°C)	362.2	380.4	386.3	380.8	375.6	370.4
FCC riser top temperature (°C)	521.4	526.0	526.0	526.0	526.0	526.0
Conversion (% wt)	74.6	73.9	74.9	74.8	74.7	74.7
LPG (% wt)	15.3	14.7	16.1	16.0	16.0	16.0
Gasoline (% wt)	50.3	50.1	49.6	49.0	49.4	49.4
Coke (% wt)	4.0	3.9	4.0	4.0	4.0	4.0
Sulphur in LCN (% wt)	0.035	0.037	0.045	0.046	0.046	0.046
Sulphur in HCN (% wt)	0.281	0.352	0.208	0.210	0.212	0.214
Sulphur in gasoline (% wt)	0.072	0.089	0.067	0.068	0.068	0.069
LCN in gasoline (% wt)	85.2	83.7	86.5	86.6	86.6	86.6
RON of LCN	93.2	93.4	93.4	93.4	93.4	93.4
RON of HCN	90.1	89.4	92.0	92.0	92.0	92.0
RON of naphtha	92.7	92.8	93.2	93.2	93.2	93.2
Total margin	5064	7579	4026	3974	3919	3861

aromaticity of the feed was increased (high *RI* and low *SG*), the RON constraints were satisfied, but with a parallel decrease in the gasoline yield. That is what should be expected in this scenario, as high aromaticity favours high RONs, but also does not favour the crackability of the feed and thus the FCC unit conversion and gasoline yield (Magee *et al.*, 1980).

CONCLUSIONS

A computer-aided tool oriented to engineers/managers, who are involved in making decisions regarding the feed and catalyst properties as well as the operational aspects of the HDS–FCC integrated system, was presented. A comparison of the tool results with industrial measurements verified its prediction accuracy. It has also been demonstrated that the user can exploit such a tool to easily create the kind of scenarios that are more applicable regarding all the optimization aspects. Because of the complexity that arises from inherent difficulties in each process and the combination of the two processes, the everyday operational decisions that have to be made are not always straightforward. That was evident in almost all the optimization scenarios tested. The gasoline maximization, which is usually the goal-product of the FCC unit, was subjected to restrictions in its quality. The trend is for quality specifications to become stricter, which is one more factor for changes in the operation of the unit and therefore an additional argument for the necessity of such tools. The tool implementation provided a variety of options, as well as a financial evaluation of these different solutions. The trends revealed are consistent with the existing theory and experience, which also speaks for the overall behaviour and accuracy of the tool.

NOMENCLATURE

<i>APS</i>	catalyst average particle size, μm
<i>BN</i>	basic nitrogen in feed, wppm
<i>CCR</i>	FCC catalyst circulation rate, $\text{m}^3 \text{h}^{-1}$
<i>F_{AIR}</i>	FCC regenerator air feed mass flow, t h^{-1}
<i>F_{CAT}</i>	FCC catalyst addition rate, Mt day^{-1}
<i>F_{HDS}</i>	HDS VGO feed rate, t h^{-1}
<i>F_{VGO}</i>	FCC VGO feed rate, t h^{-1}
<i>MAT</i>	catalyst micro activity
<i>MeABP</i>	mean average boiling point, $^{\circ}\text{C}$
<i>P_{HDS}</i>	HDS pressure, bar
<i>P_R</i>	FCC riser pressure, kg cm^{-2}
<i>P_{RD}</i>	FCC riser pressure drop, kg cm^{-2}
<i>Q_{AIR}</i>	FCC regenerator air feed, $\text{kN m}^3 \text{h}^{-1}$
<i>Q_{H,M}</i>	HDS hydrogen make-up, $\text{kN m}^3 \text{h}^{-1}$
<i>Q_{H,q1}</i>	first quench rate, $\text{kN m}^3 \text{h}^{-1}$
<i>Q_{H,q2}</i>	second quench rate, $\text{kN m}^3 \text{h}^{-1}$
<i>Q_{H,R}</i>	recycle hydrogen rate, $\text{kN m}^3 \text{h}^{-1}$
<i>RI</i>	refractive index, at 20°C
<i>RON_{HCN}</i>	RON of HCN
<i>RON_{LCN}</i>	RON of LCN
<i>S</i>	sulphur in feed, % wt
<i>SA</i>	catalyst total surface area, $\text{m}^2 \text{g}^{-1}$
<i>SG</i>	feed specific gravity, at 15°C
<i>S_{HCN}</i>	sulphur in HCN, % wt
<i>S_{LCCO}</i>	sulphur in LCCO, % wt
<i>S_{LCN}</i>	sulphur in LCN, % wt
<i>T_{HDS}</i>	HDS temperature, $^{\circ}\text{C}$
<i>T_{PR}</i>	FCC feed preheat, $^{\circ}\text{C}$
<i>T_{RA}</i>	FCC riser average temperature, $^{\circ}\text{C}$
<i>T_{REG}</i>	FCC regenerator temperature, $^{\circ}\text{C}$
<i>T_{RX}</i>	FCC riser top temperature, $^{\circ}\text{C}$
<i>W_{Aromatics}</i>	aromatics in gasoline, % wt

<i>W_{Butane}</i>	butane in LPG, % wt
<i>W_{Butenes}</i>	butenes in LPG, % wt
<i>W_{i-Butane}</i>	<i>i</i> -butane in LPG, % wt
<i>W_{LCN}</i>	LCN in gasoline, % wt
<i>W_{Naphthens}</i>	naphthens in gasoline, % wt
<i>W_{Olefins}</i>	olefins in gasoline, % wt
<i>W_{Paraffins}</i>	paraffins in gasoline, % wt
<i>W_{Propane}</i>	propane in LPG, % wt
<i>W_{Propylene}</i>	propylene in LPG, % wt
<i>Y_{Coke}</i>	coke, % wt
<i>Y_{Gasoline}</i>	gasoline, % wt
<i>Y_{LCCO}</i>	LCCO, % wt
<i>Y_{LPG}</i>	LPG, % wt
<i>Y_{Slurry}</i>	slurry, % wt
<i>Y_{SourGas}</i>	sour gas, % wt

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The manuscript was received 10 July 2003 and accepted for publication after revision 8 April 2004.