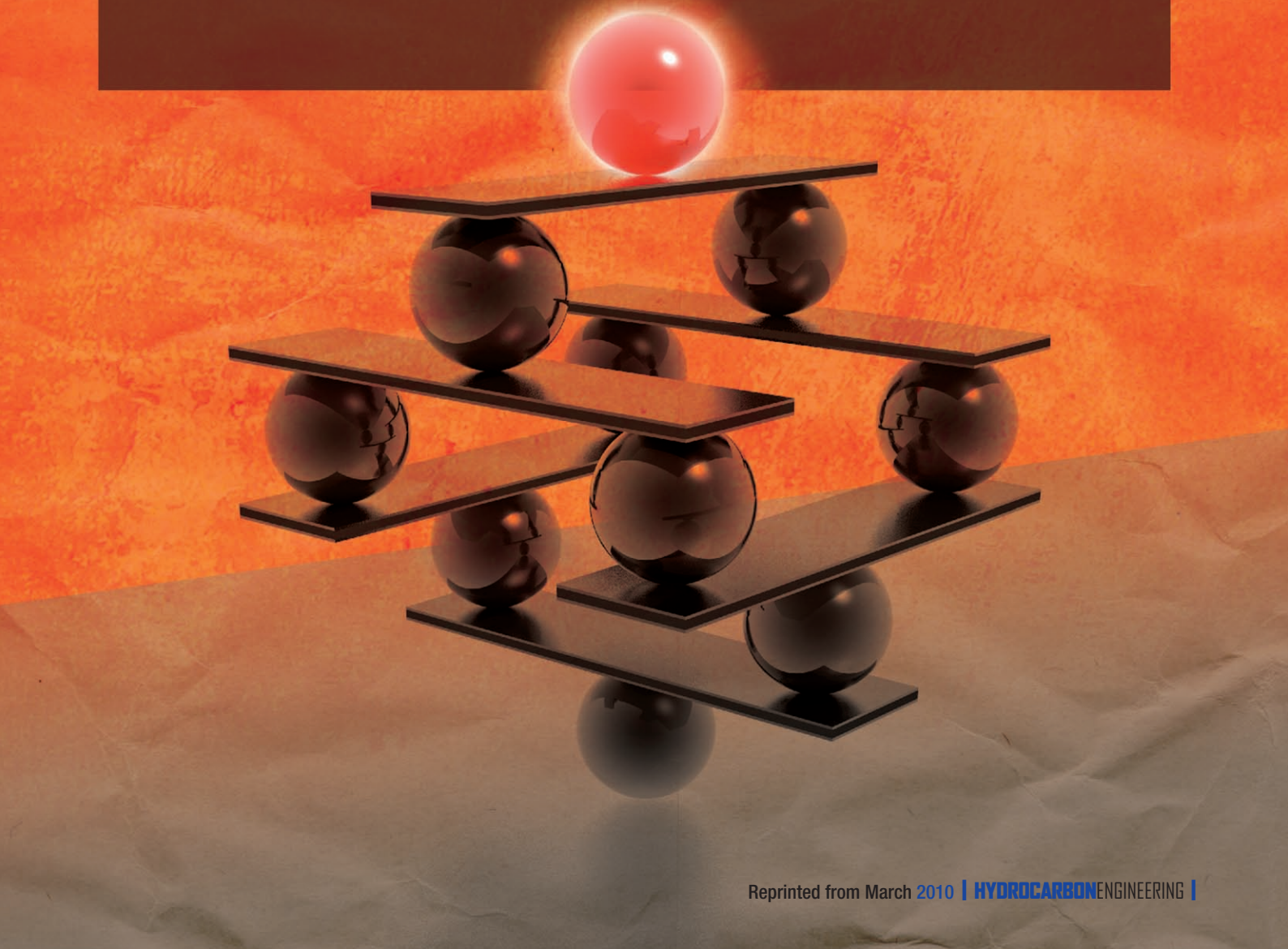
A UNIQUE APPROACH

D. Lambert, C. St Martin, M. Sanchez, B. Ribero, S. Beaucamp, TOPNIR™ Systems, France, explain FCC heavy feed characterisation for process control through Topnir analysis.

The goal of the fluid catalytic cracking (FCC) feed characterisation project, at a French refinery, is to facilitate offline and online optimisation of the FCC unit.

Previous situation

The current FCC unit application was optimised using conventional analytical measurements coming from the laboratory, and measured several days after their collection. The delay of the results does not allow optimisation of the FCC unit.



New situation after project completion

The Topnir FCC application is aimed at providing results to the FCC unit process control within 30 minutes in order to reduce turnaround in optimisation operation.

Project overview

The FCC feed characterisation system is composed of the NIR sampling performance excellence design (SPEED) system. The NIR SPEED system is an automatic lab system coupled to a spectrometer, which analyses spectra. The NIR SPEED system acquires automatically diluted spectra of the FCC feed and determines the spectrum of the pure feed product. This system optimises the laboratory workload by the automatic injection and dilution of samples, the management of the injection and the spectra acquisition.

From the spectra of FCC feeds, or from components of the FCC feeds such as residue, the Topnir model predicts a vector of chemical properties: Conradson carbon, aromatic content, distillation (7 points), total ammonia nitrogen (TAN), sulfur, basic nitrogen, density and viscosity at 100 °C.

Located in the central laboratory of the refinery, the NIR SPEED systems automatic lab system, as shown in Figure 1, is composed of:

- An articulated arm with a syringe.
- A table for the container dedicated to the storage of samples.
- A dilution system to move the samples, performing injection and dilution.
- A system of pipes and valves for the dilution, injection or washing cycles.
- A measurement cell maintained at controlled temperature with a thermostat bath and a temperature controller, used to analyse the NIR spectra of diluted FCC feed samples.

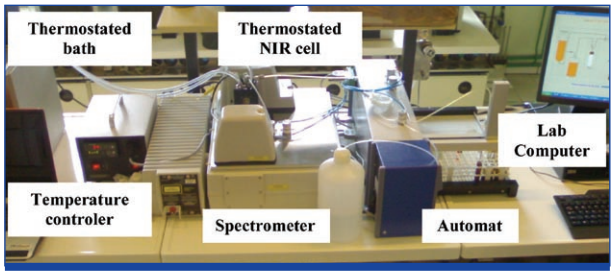


Figure 1. NIR speed system.

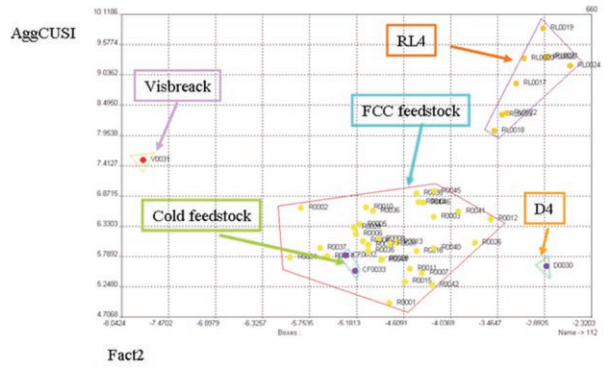


Figure 2. Top aggregate projection showing the representation of the composition of the FCC feedstock with its four main components: D4 (distillate), RL4 (long residue), visbreak, cold feedstock.

Chemical and physical characteristics of the FCC feed

Properties characteristics

The FCC feed and the long residue has an important viscosity, which can cause difficulties for its analyses. The characterisation by NIR analyses required dilution to allow injection of samples in the NIR cell.

The conventional analyses take time and results are not available for several hours after sample collection. Table 1 shows the properties characteristics of the FCC feed.

Feed and components of the FCC unit (FCCU)

The FCC feed composed of four heavy components has a main feature, the long residue (RL4). Figure 2 shows the repartitions on aggregates projection of FCC feed spectra and its components.

Modelling technique

Principles

Topnir is a chemometric software that exploits the NIR spectra in order to determine a full vector of properties attached to the hydrocarbon products.

The key feature of the Topnir technology package is the software required to carry out the analysis. This unique software enables the user to convert the information provided by the analyser into models that are used for the determination of multiple properties. It will then provide system integration to allow the transfer of properties to the advanced process control system.

Table 1. Typical specification of the long residue and the FCC feed

FCC feed specifications	Min.	Mean	Max.
Monoaromatic	49.7	57.4	67.5
Diaromatic	22.8	26.0	27.7
Triaromatic	20.6	23.0	25.8
Tetra aromatic	11.6	13.9	20.4
CCR	0.27	1.44	2.98
Sulfur	0.98	1.75	2.40
Basic nitrogen	287	440	651
Density	912	925	941
Visco @ 100	6.4	9.6	14.4
IBP	208	265	303
T10%	365	381	395
T30%	413	426	438
T50%	445	458	474
T70%	477	495	513
T90%	528	573	605
FBP	678	694	707
TAN	0.25	0.45	0.97
Long residue specifications	**Min.**	**Mean**	**Max.**
MVOL	943	955	969
CCR	6.76	7.95	9.81
Visco @ 100	48.5	71.9	115
TAN	0	0.15	0.60
SOUFRE	0.41	0.83	1.14

Topnir is based on a mathematical technique called 'topology,' which works through pattern recognition and database densification. It does not use linear modelling that would require one model per property and would not deal properly with non-linearities. Topnir instantly delivers all the properties required for a given application. Moreover, it offers the possibility of extrapolation from the initial calibration range, which is typically poor when delivered by linear models.

Concerning the treatment of outliers (samples that would not be recognised as being part of the calibration database), the classical linear methods require significant additional work in order to maintain the models. It can rapidly become a bottleneck when the application involves a lot of properties, each of these requiring a specific calibration process.

The Topnir system accounts for outliers and does not require any new calibration of the models. It is a self learning method fitting perfectly with the reality of the industrial operations. The principle of the topology is to represent the spectrum (being the absorbance along a series of multiple wavelengths) as a one point projection inside a set of two dimensional planes. These planes are defined by some markers called 'aggregates' and are representative of specific chemical characteristics (aromatic content, ratio of unsaturated to saturated hydrocarbons, etc.) With this concept, the spectral representation is condensed to a set of planes that allow a quick and accurate visualisation of the quality of the products.

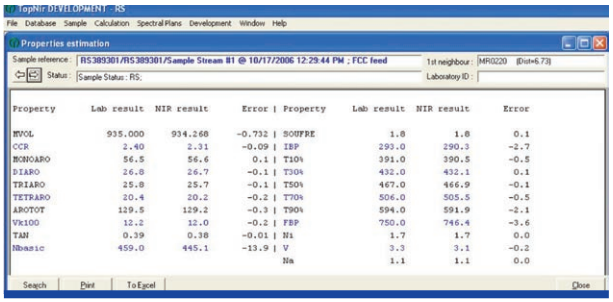


Figure 3. Topnir FCC feed characterisation screen display.

Only one single model is required to determine the full set of properties for one or several grades of products. Moreover the technique is self learning, as the model is automatically updated every time a new sample is published into the database.

For FCC feed characterisation, Topnir unique proprietary technology is particularly appropriate. Indeed, Topnir offers a real opportunity to track changes in feed quality and to optimise the FCC unit based on high frequency (eg. every 4 hours) quality determinations. Figure 3 displays a typical print screen of the Topnir results after a measurement has been performed.

As discussed earlier, the Topnir FCC feed characterisation system is able to identify outliers as shown below. The spectrum is projected onto the set of two dimensional planes and compared with the envelope of the calibration boxes. Unless the distance from the nearest neighbours present in the calibration database is too large (identifying a 'true outlier,' which would then track most likely a brand new type of FCC feed), then the prediction of the set of properties is returned to the user. Being able to predict the properties of 'pseudo outliers' is one of the main advantages of Topnir technology.

Performance

The Topnir models have been built with spectra obtained from diluted samples provided by the NIR SPEED systems. The Topnir models for the FCC feed and the residue have been calibrated over 36 samples covering a one year production period. From the spectra of the calibration population, which define spectral boxes

Table 2. Topnir and ASTM comparision

Properties	Lab methods	Units	Topnir reproducibility	Lab reference reproducibility
CCR	NF EN ISO 10370/ASTM D4530	mass%	0.38	0.34
Monoaromatic	Internal UV method	mmol/100g	8.24	NA
Diaromatic	Internal UV method	mmol/100g	1.74	NA
Triaromatic	Internal UV method	mmol/100g	1.47	NA
Tetra aromatic	Internal UV method	mmol/100g	6.9	NA
Total aromatic	Internal UV method	mmol/100g	12.93	NA
Visco @ 100	NF EN ISO 3104/ASTM D445	mm^2/s	1.38	0.7
TAN	NF ISO 6618 (NFT 60-112)	mgKOH/g	0/24	0/08
Sulfur	NF EN ISO 8754	mg/kg	0.2	0.16
Basic nitrogen	Internal potentiometric method	mg/kg	54/6	-
IBP	TBP	˚C	50.2	NA
T10%	TBP	˚C		NA
T30%	TBP	˚C	5.64	7.3
T50%	TBP	˚C	10.56	12.15
T70%	TBP	˚C	13.33	17
T90%	TBP	˚C	22.02	NA
FBP	TBP	˚C		NA
Ni	Local method ICP	mg/kg	0.22	NA
V	Local method ICP	mg/kg	0.93	NA
Na	Local method ICP	mg/kg	0.46	NA
Density	NF EN ISO 12 185	kg/m^3	2.83	1.5

shown by the aggregate projection as displayed on Figure 5, a densification of the database has been carried out by creating virtual samples. Again on Figure 5, the spectral plan allows the segregation of the standard FCC feed (magenta dots) and the imported FCC feed (red dots). Based on specific experience of Topnir Systems with mixing rules, this densification fills in the holes that would not show any neighbours. This technique improves the robustness of the model and avoids unpredicted samples within the standard area of prediction (Topnir boxes).

The Topnir model has provided accurate calibration results in accordance with the respective ASTM reference of the conventional analytical methods as shown in Table 2. From a statistical point of view, the Topnir reproducibility is compared to the reproducibility of the conventional lab methods and has to be in accordance for at least 95% of the samples present in the calibration database.

The performance of a NIR model has also to be evaluated in prediction (or validation) mode, which is computed for samples that did not participate in the calibration exercise. Figure 6 shows excellent results of such validation test for CCR property.

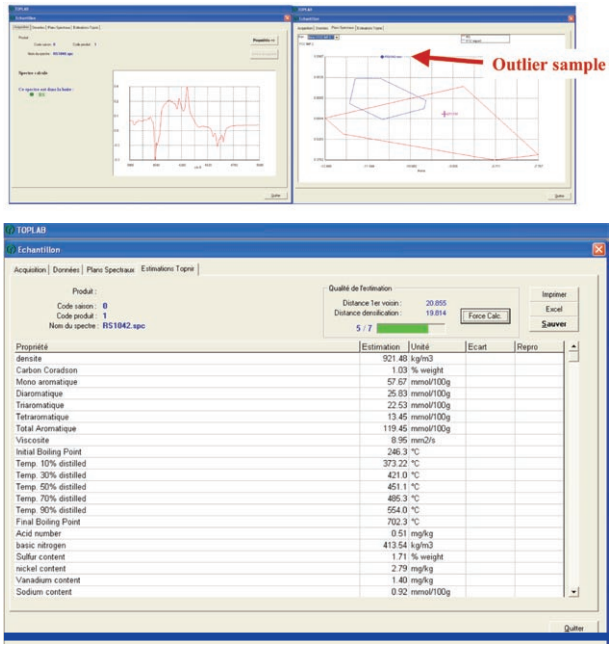


Figure 4. Toplab FCC feed characterisation screen display.

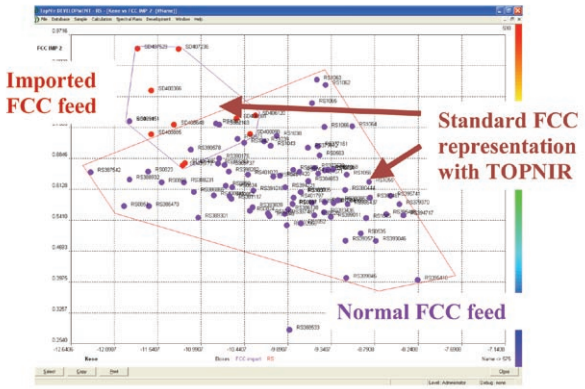


Figure 5. Projection of spectra inside aggregate planed and boxes.

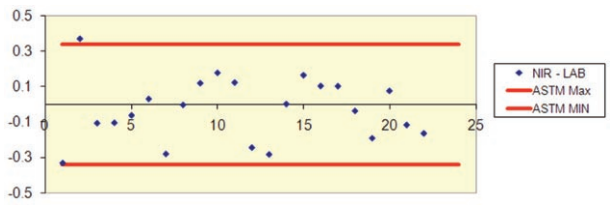


Figure 6. Comparison of Topnir and ASTM performance for CCR measurement on validation samples.

Characterisation for FCC unit optimisation

The FCC feed characterisation is used as a key input to the optimisation of the FCC unit.

FCC unit optimisation with Topnir prediction

The advanced and rigorous FCCU cracking model is an advanced process model that helps the operation of FCC units in two possible ways. It is capable of predicting the economic impact of a change in the feed composition, and it can be used to optimise the performance of the unit on a continuous (online) or regular (offline) basis.

The FCC feed characterisation by the Topnir system is now used to feed the model in order to:

- Quantify the effects on yields and product properties from the changes in feedstock quality, catalyst addition rate and operating conditions.
- Perform marginal feed evaluations, benefit from the ability to select the right additional feed at the right price.
- Help select the best catalyst for use in the unit, given particular operating constraints and economic goals.
- Monitor and optimise the performance of the unit on a continuous basis. The model is easily integrated with online optimisation systems.
- Assess ways of pushing the throughput of the unit to its limit.
- Combine the process control model with refinery information systems and planning and scheduling tools to enhance the overall hydrocarbon management capability.
- Identify opportunities to improve unit performance; alternatively function as an investment decision support tool to assess the effects of revamps.
- Evaluate the improvements in unit performance after changes in FCC hardware, such as feed nozzles and stripper internals.

Conclusion

All FCCU process models require detailed characteristics of the FCC feed, combining ASTM analytical methods with additional specific analysis such as mass spectroscopy, nuclear magnetic resonance (NMR) and high performance liquid chromatography (HPLC). The turnover for measuring all properties is, in most cases, not short enough that the results of the rigorous process model can be used efficiently as part of an online optimisation of the process conditions. With a high frequency of measurement for the entire set of properties, Topnir is a unique solution enabling an online and offline optimisation of FCC units. Some key properties such as aromatics, basic nitrogen and CCR are extremely well predicted from the Topnir models, and these are the key properties for the FCC feed optimisation model. From the successful application of Topnir NIR automated lab system to FCC feedstocks, Topnir Systems is confident that the methodology can be deployed across a wide range of heavy feedstocks, such as hydrocrackers, visbreakers, integrated gasification combined cycle (IGCC) units and cokers feeds.