Didier Lambert, Claude Saint-Martin, Bernard Ribero and Michael Sanchez, Topnir Systems, France, and Sylvie Destang, Laure Dahan and David Labatut, Innovene Manufacturing, France, discuss the advantages of Topnir in blending processes.

All in the blend

With increasing demand for oil and higher barrel prices, coupled with restrictive environmental regulations, the production of fuels such as diesel and gasoline is growing more complex. Indeed, the US and EU markets are driven by new environmental standards aimed at reducing pollution during production processes and reaching clean fuel standards within the current decade.

Refiners have to optimise their main blending operations to remain competitive. For gasoline or middle distillate blending operations, it is important to evaluate the contribution of blending components to the quality of the final blend, as well as additive response in the diesel pool. Due to the nature of properties such as octane or cetane numbers, RVP, distillation points and cold properties, this contribution is not linear. Refiners use empirical blending laws to linearise the properties and then recalculate a blending property (the blending index) for each property of a given blending component through complex mathematical functions or extensive tables.

This step has now become crucial due to the new components arriving in the refineries, such as bio-ethanol and Colza bio-ester, for which the response in a given pool is not easily assessed. Moreover, synfuels derived from sources other than oil will soon be entering refineries as blending components.

Based on 15 years of applied R&D and operations at BP Amoco Lavera, now Innovene, a procedure has been developed to transfer this complex set of non-linear laws to a Topnir model to compute easily and in real time the blending indices of any component from its NIR spectrum. Diesel additive optimisation is also provided from the Topnir model.

With Topnir technology, refiners are now able to assess quickly and accurately the response of new 'bio' blending components in their pool, as well as to characterise the commercial clean fuel products using those components in less than two minutes. Topnir blending indices and additive optimisation allow immediate characterisation leading to the optimisation of recipes, saving time and money and guaranteeing compliance with regulations. Typical benefits are approximately US$ 2 - 5 million/yr.

What is Topnir?

NIR spectra contain all the chemical information of any hydrocarbon compound but they are not easily accessible. The information is extracted by advanced statistical methods, among which the topology technique provides the most accurate and reliable results. Topnir, based on topology, works through pattern recognition and databank densification. It does not use a linear model for a set of properties (one model per property). Topnir instantly delivers all the properties required for a given application from a single model. Moreover, it offers the possibility of extrapolation from the initial calibration range.

With regards to the treatment of outliers, the classical linear methods require a very heavy amount of work to maintain the models. A bottleneck can rapidly occur when the application involves a lot of properties, each one requiring a specific calibration treatment. The Topnir system takes into account any outlier and does not require any new calibration of the models. It is a self learning method which fits perfectly with the reality of industrial operations.

Classical linear techniques require a large number of samples in the database. To overcome this problem, Topnir uses a densification technique which is one of the cornerstones of the technology. Densification is done by interpolating between the actual points, and very importantly, points outside the boxes, to determine a contour map of properties of everything within the box. This is completed when the model is initially prepared. To make the prediction even more robust, Topnir also carries out a

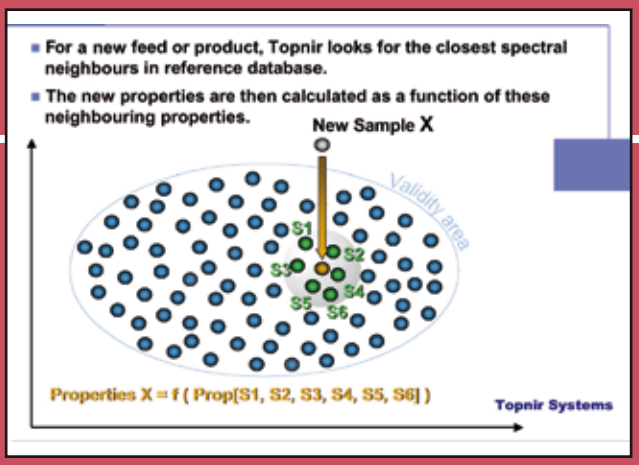

Figure 1. Topnir basic principles.

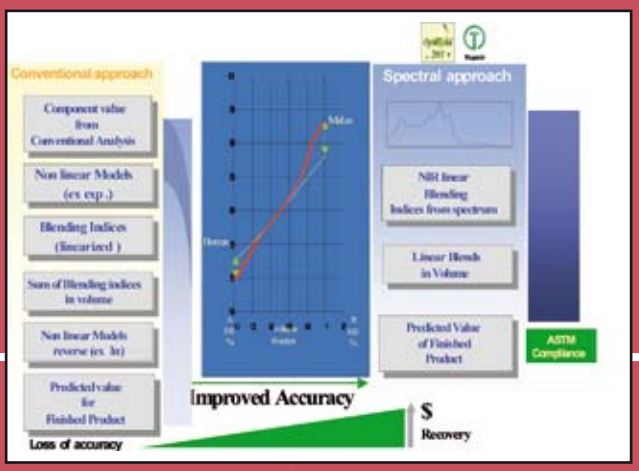

Figure 2. Advantages of Topnir blending indices compared with conventional approach.

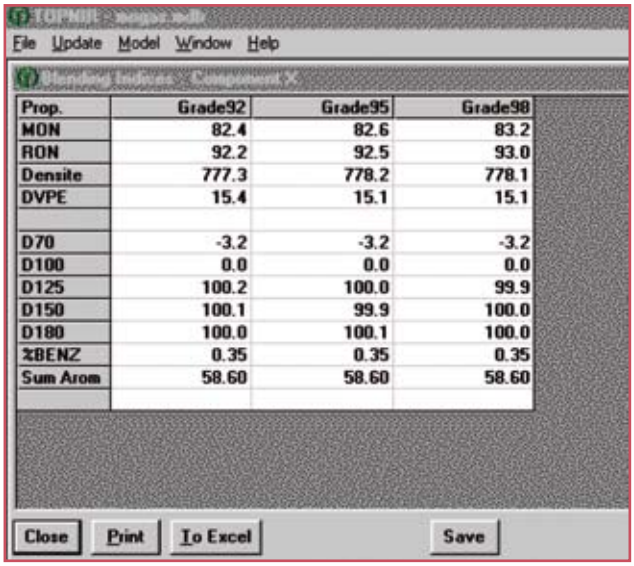

Figure 3. Blending indices calculation result matrix.

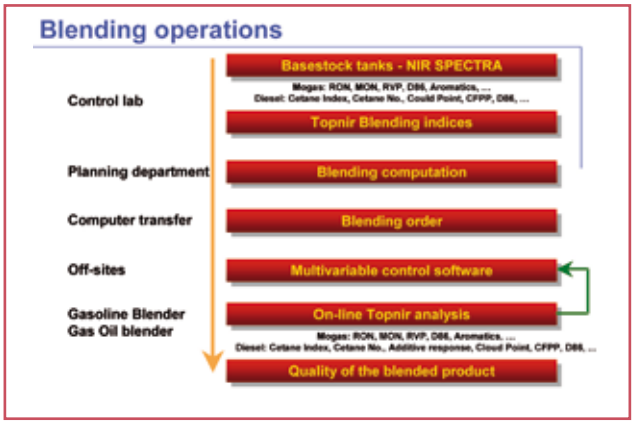

Figure 4. Gasoline and gas oil blending with Topnir blending indices.

Table 1. RON properties of blending components

Blending components	True RON	RON blending indices	Bonus RON
Isomerate	80.9	86.5	+5.6
HCK gasoline	78	84	+6
Toluene	117	113	-4
Full range reformate	98.6	98.3	-0.3
Heavy reformate	106	104	-2
SRG	79	84.5	+5.5

Table 2. Blending indices for a RON95 gasoline grade

Blending components	True RON	RON blending indices	Bonus RON	Recipe RON95 (%vol)
SRG	76	81	+5	3.1
HCK gasoline	78	82.7	+4.7	9.1
FCC gasoline	91.5	92.7	+1.2	11
Reformate	97.7	97.4	-0.3	76.8

local densification 'on the run' to ensure every prediction will be made from a large number of neighbours.

Densification uses proprietary spectral blending laws, tuned in to client site specificity. In less than two minutes, the technology returns a full array of properties, allowing efficient multivariable control of the blender and faster convergence on commercial specifications. Online process control is not constrained by long response times from traditional analysers, and integration of quality is made on hundreds of measurements during the blend.

Fibre optic wave guides allow for decentralising of measurement cells, to optimise installation costs by remote implementation and optical multiplexing. Outliers can be sampled automatically and their spectra processed and stored in the database to improve the robustness of the model.

Due to its unique capability of property prediction from the overall NIR spectra, Topnir is able to deliver blending indices for any type of component. Compared with the conventional approach, Topnir is a faster, easier to use and more reliable method of comparing the quality of components for blending operations. Figure 2 shows the comparison between the classical method and the Topnir approach. For each component, Topnir delivers linear values for each property according to a dedicated finished product. If there are, for example, three different grades, the results will be a linear property matrix (blending indices matrix), as shown in Figure 3, with three vectors of blending indices.

Blending operations using Topnir blending indices

The monthly planning LP model requires adequate blending indices to predict average blend recipes, while the specialised multi blend LP model used to compute the optimal recipe also requires accurate blending indices to minimise blending costs. The traditional approach of correlations and multi-entry tables is cumbersome whenever the crude slate and refining scheme are complex. Topnir's approach to computing blending indices is well suited to a fully computerised planning/scheduling/multivariable control system (Figure 4).

This ability to predict the blending indices of blend components has three major effects on blending control:

- It allows the process to start with a very accurate blend recipe.
- It allows feed forward compensation.
- It provides a good fallback position in case of analyser failure.

Moreover, the possibility of using a customised and reliable multi stream FTIR analyser opens the way to inline determination of blending indices rather than taking samples from tanks before the blend startup. The overall cost of added sampling lines and associated instrumentation can be justified due to the possibility of inline certification blending, allowing shipment of finished product directly to customers. More elaborate strategies are possible using running gauge tanks or direct rundowns for components and blending directly into a pipeline or a ship. In such cases, blending indices are continuously monitored from the online NIR analyser.

Case study

Computation of components

Table 1 gathers the true value of gasoline blending components for the RON property as well as blending indices (i.e. the direct contribution of components in the final blend, here a grade RON95). It is easy to see the contribution of each component in the final blend for the property considered. Table 1 was produced by Topnir in less than two minutes for all relevant properties of the blending application.

The difference observed for each component between the true value and the blending indices is linked to the interaction between this component and the blend matrix, due to the synergy between the various chemical species. As Topnir works on the full NIR spectra, containing all the chemical information, it can easily obtain such information on each component.

Computation of gasoline recipe from components

To blend a RON95 gasoline grade, the Topnir blending indices are shown in Table 2. For the volumes defined on the right column of the table, corresponding to the recipe of a RON95 grade, the linear calculation would be:

81 * 3.1% + 82.7 * 9.1% + 92.7 * 11% + 97.4 * 76.8% = 95.03

Another example can be seen in Table 3 for the blending of a MON88 gasoline grade. To blend the MON88 grade shown in Table 3 with MTBE, the recipe is obtained from the calculation:

87.5 * 8% + 85 * 45% + 89.1 *35% + 97.2 * 12% = 88.1

With the Topnir approach, the sum of linearised values multiplied by volume fractions of each component is directly equal to finished product property estimation. The accuracy of this approach results from the fact the prediction is based on the whole spectral blending results and not only on property blending results. The NIR spectral domain (between 2 and 2.5 μm) is far richer in terms of information regarding aromatic, linear, olefinic and iso, explaining why Topnir blend indices are far more accurate than the conventional way of blend calculation.

Determination of blending indices for biofuels

The strong incentive from regulatory authorities to use bio components such as bio-ethanol and Colza bio-ester bring new challenges to the refiners in terms of component characterisation and fuel blending. Topnir can quickly and accurately determine both the blending indices and recipes using those components. An example is given in Table 4 where Colza bio-ester is used to produce a 50 ppm diesel grade with a constraint on the flash point. By computing the blending indices by the ratio of each component, a flash point of 60.1 ˚C for a real blend value measured at 60 ˚C is obtained.

Blend results

Table 5 shows some statistics from eight months of Lavera gasoline blender monitoring in 1999, for blends without online monitoring. One of the constraints in the refinery at that time was the four small tanks with a capacity lower than 3000 m^3. With a 1200 m^3/h blender, it was not possible to start a real monitoring of the blends. In this case it was absolutely necessary to use accurate recipes from initial blending orders to avoid producing any extra giveaway, or to increase the reblends rate.

If Topnir is not used online, Topnir blending indices are so efficient that it is possible to start the blend with the initial blending order with the same rate of success. The reblend rate is less than 5%.

Topnir was also used online during the blending for other tanks with a volume over 3000 m^3. All component tanks were in running gauge mode and the blending time was approximately 15 - 20 hours.

Table 6 shows a case history over eight months of gasoline blending in 1999 at the Lavera Refinery, for blends with the Topnir online monitoring. Figure 5 shows the comparison blending per blending along the same period.

When measuring RON on a blending component, a value is obtained (for example, 92). However, with this value, all the information related to the chemical hydrocarbon structure of the component is lost as well as the synergetic effects with the other components, depending on the hydrocarbon matrix of the finished product.

With Topnir blending indices, the solution is easy as the complexity of linearisation has been overcome. NIR is a very accurate method because it contains all chemical information such as aromatic, linear and double bounds. Figure 6 shows the reduction of laboratory workload effort on CFR MON and RON measurements with a parallel increase of information access; as Topnir blending indices delivery takes less than two minutes, blending component quality is checked more often in the laboratory.

Diesel additives optimisation

Surprisingly, the additives put in diesel blends for Cetane booster and CFPP flow improver (MDFI) have been considered as a 'basic commodity' until now.

Even experienced operatives sometimes use an excess of additives because of the strongly non-linear and complex

Table 3. Blending indicies for MON85 and MON88 gasoline grade

Blending components	True MON	MON85 blending indices	MON88 blending indices	Recipe (% vol)
C4 FCC	85	87.1	87.5	8
ISOM	86.5	84.3	85.0	45
REF100	91	89	89.1	35
MTBE		96.7	97.2	12

Table 4. Blending indices of components in Colza bio-ester

Blending components	Flash point (˚C) true value	Flash point (˚C) blending indices	Recipe (%vol)
HDS light gas oil	60	61.2	30.7
HDS medium gas oil	75	63.7	43.2
N/P	42	20	4.8
HCK gas oil	58	54	17.3
EMC (Colza bio-ester)	ND	88	4

Table 5. Blending target achievement with blending order only

Grade	Number of blends	Volume (m^3)	MON	Target	Delta
RON98 ULG	14	39 438	88.12	88.1	0.02
RON95 ULG	31	86 201	85.06	85.0	0.06
RON97 Leaded	18	70 916	86.15	86.1	0.05

Table 6. Blending target achievement with online Topnir monitoring

Grade	Number of blends	Volume (m^3)	MON lab	P&S target	Delta
Premium	19	69 938	88.06	88.1	0.0
Regular	37	132 879	85.13	85.0	0.13
Leaded	28	186 986	86.13	86.1	0.03

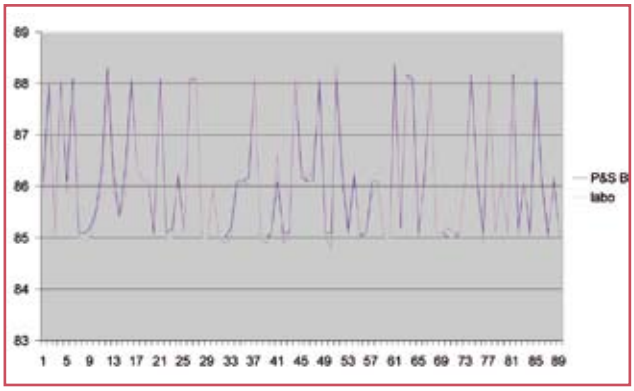

Figure 5. Comparison blending per blending.

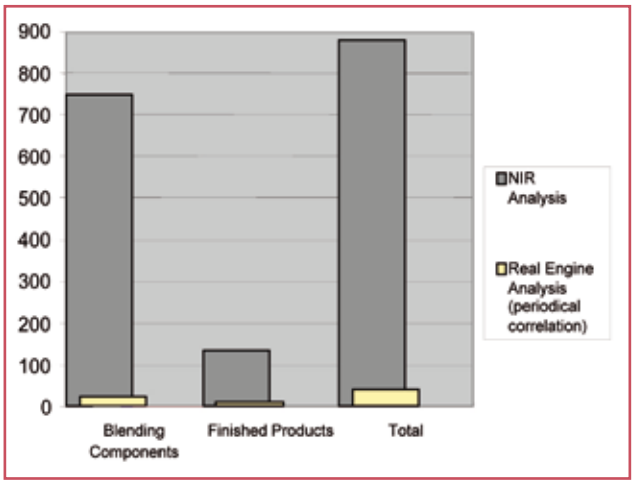

Figure 6. Six months statistics of effects on lab workload from using NIR blending indices.

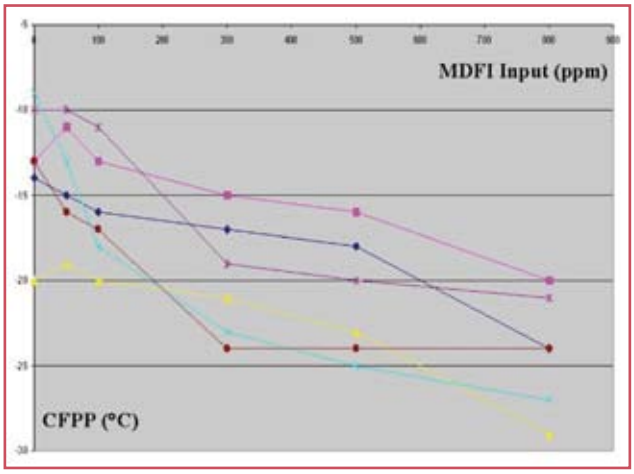

Figure 7. Different MDFI response curves for the same finished product.

nature of additive response curves. The goal of the refiner is to reach the commercial specification first time round; to avoid costly reblending operations, quite often at the expense of the additives. Indeed, additives were not accounted for in the linear program, neither in the scheduling nor in the blending optimiser and controller. Figure 7 shows different MDFI response curves for the same finished product grade, with the same MDFI additive, and is drawn from real data from a European refinery laboratory.

It is interesting to note that for the same product grade and additive, the MDFI response curves are very different and strongly correlated to the blending recipe and blending component qualities.

The implementation of Topnir optiblend additive module allows accurate gauging of the additive response and the adding of the required amount to reach specifications. Figure 8 illustrates the methods of operation before and after Topnir optiblend implementation.

Three areas must be considered for a typical MDFI response curve:

- The potential none effective area, where the additive has little or no effect on the product CFPP.
- The slope area, where the slope is very important.
- The safe area, where the maximum effect of the additive is reached or almost reached.

Topnir's Optiblend module allows safe and accurate operation in the 'slope area', the risk of producing off-spec product being minimised thanks to the safety CFPP target (-23 ˚C, for a specification, -20 ˚C). The additive optimisation could drive the average MDFI input from 273 ppm down to 74 ppm (approximately 200 ppm; 70% of additive saved) for each blend.

As an average, the MDFI input decreases 200 ppm thanks to Optiblend. With a production of 400 000 m^{3}/yr, the global saving is approximately US$ 130 000/yr for the grade considered above. For all the diesel grades produced, the overall benefits are approximately US$ 350 000.

Hardware

The FTIR process analysis integrated system includes an analyser cabinet and a sample conditioning system. It is completely integrated and executes all the functions required by the Topnir/FTIR process applications, for example:

- Sample preconditioning assemblies.
- Outliers auto grabbing.
- Optical cell assembly.
- Multi channel arrangement.
- Cell flushing and validation.
- Utilities control bloc assembly.
- System and analyser control unit interfacing module.
- Model data base interfacing.
- Data interchanges.
- System packaging.

It is specially designed for supporting the Topnir/FTIR process application. 10 definitive benefits over the other existing systems have been considered in this article:

- System and analyser processing, model database interfacing and data interchanges integrated in the same remote PC supplied by customer in safe area.
- Architecture designed around PC hardware and Windows operating system.
- Users can change, modify or edit remotely all analyser and calibration parameters. Maintenance graphic displays allow full visibility of the flow sheet and offers fast learning circuitry with minimum training.
- Two levels of data interchanges to customer DCS (CDCS) and process/lab benchtop. Inter spectrometer supported by data highway.
- Digital temperature control of the optical cell operated by a chiller compressor. No vortex cooler requiring huge instrument air consumption.
- System integrates up to eight channels, featuring independent optical flow cell when sample segregation is required.
- Three styles of sample preconditioning systems designed for crude, white and yellow/black products and installed on sample fast loops.

- Flushing and auto validation systems feature piston floating cylinders for full integrity.
- Rugged Atex certified cabinet in carbon steel, 30/10 mm sheet and IP64 rating. Can work outdoors and in harsh environments.
- Improved calibration transferability from benchtop analyser.

The online process IR analyser, comprising the FTIR Bomem NetworkIR fibre optic based spectrometer, and the PC and the utilities controller (UC), are located within a complete cabinet, which is air purged by Monitor ATEX II2G certified EExpII. Sampling preconditioning systems are provided to ensure integrity of samples flowing from sample take off to the NIR cells.

The IR analyser is a Fourier Transform NIR analyser using interferometer technology and is microprocessor based. The fibre optics are in fluoride glass and designed for industrial use for the process analyser. No reference channel is required as the reference spectrum is directly obtained periodically through the automatic cell flushing and validation cycle.

The operating wavelength range for the Topnir model is between 2000 - 2500 nanometers (5000 - 4000cm^{-1}). The measurement cell is designed for online process analysis with a path length of 500 μm. Area classification for the online process analyser is Group IIB (IEC) corresponding to class 1, Div.1, Groups C/D NEC Code certified by ATEX CE II 2 G EEx pdem ib IIB T3.

For refineries without DCS or online connectivity, a specific version for exline application is available through Topnir. The laboratory spectrometer and isosample device collects consolidated samples during the blend with periodical checking.

Benefits

The property predictions obtained from Topnir are at least equal to ASTM standard and quite often better, allowing drastically reduced giveaway on commercial products. Typical benefits achieved with the Topnir blending optimisation system are as follows:

- Minimise quality giveaway on constrained properties such as octane and cetane number (CN), aromatics, flash point, RVP, cloud point, distillation etc.
- Elimination of reblends.
- Increased throughput.
- Reduction in demurrage.
- Reduction in component inventory.
- Improved capital deployment.
- Maintenance cost reduction as only one single analyser and one single model need be maintained.

Savings are US$ 2 - 5 million/yr for a 150 000 bpd refinery, with most of the benefits being in giveaway reduction, representing more than 50% of the total saving.

Additionally, the integration of the additive management in the refinery production chain is proven to bring additional savings of approximately US$ 1 million/yr. This includes additive input saving itself, product shipment optimisation and demurrage minimisation.

Conclusion

FTIR Topnir technology displays in one place all the properties required for blending monitoring and control such as aromatics, cetane number, flash point, pour point, distillation for diesel as well as octane numbers, RVP, etc.

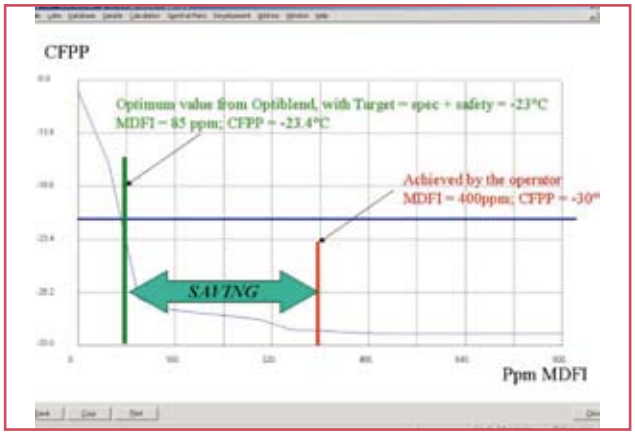

Figure 8. Before and after Topnir Optiblend implementation.

Figure 9. Online FTIR/Topnir analyser.

Indeed, the full vector of properties is available from one single online analyser, one single platform (the laboratory and online analyser are the same spectrometer) and one single calibration platform, dealing with all the blender streams. Moreover, Topnir provides accurate and updated blending indices that can be used as the single source of real time information for the refinery.

Topnir blending indices are also the unique tool available for characterising quickly the response of new clean fuel components such as bio-ethanol and Colza bio-ester in the very complex and changing hydrocarbon matrix. ■

Topnir Systems

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Enjoy the Benefits

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Field-proven technology
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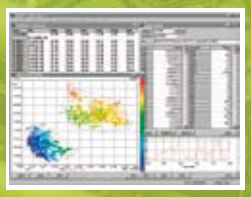

Unique patented proprietary technology

Developed in BP
More than 20 years of experience

Beyond analytic !

- Additive response determination
- Blend simulation facility
- Blending indices calculation
- Crude identification & characterization

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