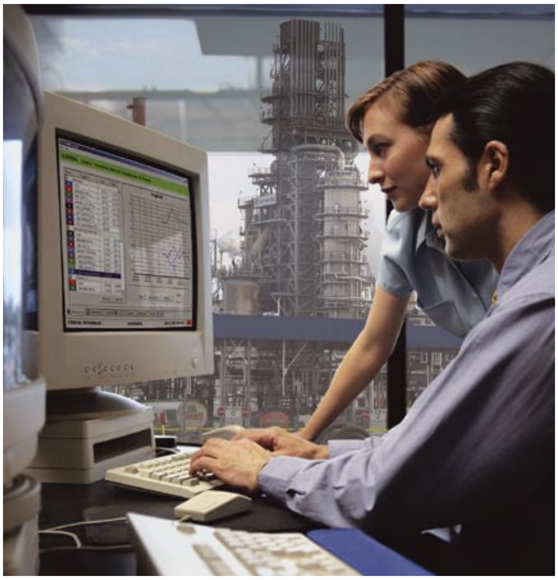
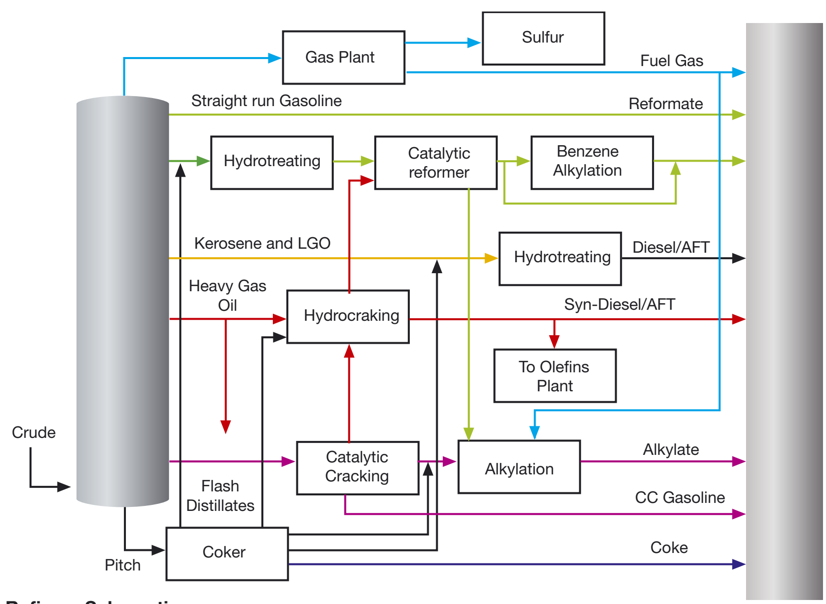
Final Product Blending for Gasoline and Gasoil



A sustained, global increase in light fuel demand, driven by the emerging economies of China and India, among others, has led to a strengthening of refining margins, even in the face of rising crude oil prices. Process analytical FT-NIR applications in refineries cover a wide range of different processes, including distillation units, conversion units and final product blend optimization. However, the availability of high production margins for final products has re-emphasized the role of process FT-NIR in high-value final product optimization applications, gasoline and diesel product blending, crude oil distillation, and, in petrochemical plants, naphtha steam cracking.

The advantages offered by process FT-NIR include multi-property, multi-stream analyses, high analysis repeatability (normally significantly better than conventional on-line analyzers), and accuracy in keeping with ASTM norms. In addition, process FT-NIR analyzers are able to model not only direct chemical compositional information, but also bulk process stream properties such as octane, distillation curves, kinematic viscosity, cetane, cloud point etc., which are often the properties most required by unit optimizers, or the most constraining in terms of product release.



Refinery Schematic

What are the defining characteristics of refinery process streams, from an analytical point of view?

Firstly, refinery streams, unit feeds, unit rundowns and blended product are remarkably complex hydrocarbon mixtures. The goals of refinery process analytics are rapid unit feed and rundown characterization to achieve unit optimization. Samples from refinery streams are normally captured very regularly for laboratory analysis using well-established methodologies. These laboratory methods may be slow, and they may have questionable repeatability, but they are the de facto criterion for product release. As such, they form the basis for on-line process analyzer validation, and also provide a rich background of analytical information for chemometric model development.

Secondly, in marked contrast to the chemicals sector, the key product quality criteria for most refinery process streams are not straightforward chemical component concentrations. Indeed for some applications, the traditional GC-based methodology is weak, precisely because it is a separation-based technique better suited to discrete component measurements. For even a relatively simple refinery unit-feed stream such as naphtha, there are at least 50 to 60 discrete components present at above trace levels. Collective and bulk properties, such as boiling point or viscosity are often of great significance in unit optimization.

Refinery process streams, whether feeds or rundowns, normally flow in pipes from which sample take-offs can easily be arranged, and to which samples can normally be returned into a pump-suction. Thus extractive sampling into a fast-loop sample conditioning system is the accepted norm in the refinery context, and for good reason. It allows for appropriate sample flow control, filtration to remove particulates, and water, if hydrophobic self-cleaning filter membranes are used. In addition, exact temperature control of the sample is very easily achieved.

However, this does not imply always using the same analyzer configuration. Indeed there are roles in FT-NIR-based refinery process analytics for a range of analyzer formats, including integrated units located in a full-specification analyzer shelter, field-mounted units located close to sample take-offs to limit fast-loop run lengths, and fiber-optic based units allowing for discrete sample flow cells per stream where the application requires a variety of sample temperatures for different streams.

Process Unit	Stream	Analyser Format	Properties
Crude Distillation	Feed	Fieldmount, Extractive	TBP, TAN, Density
Crude Distillation	Rundowns	Shelter, F-Optic, Extractive (local)	ASTM D86, PINA, CP, FP, Aro%
Naphtha Cracker	Feed	Fieldmount, Extractive	PINA, C-number, ASTM D86
Reformer Unit	Feed & Rundown	Fieldmount, Extractive	PINA, RON, Aro%, Bnz%
Alkylation Unit	HF Acid Recycle	Shelter, F-Optic, Extractive (remote)	HF%, Water%, ASO%
Alkylation Unit	iC4 Recycle etc	Shelter, F-Optic, Extractive (remote)	iC4%, nC4/C3 ratio
Gasoil Hydrotreating Unit	Rundown	Fieldmount, Extractive	Cetane, Aro%, ASTM D86
FCC Gasoline Hydrotreating Unit	Rundown	Fieldmount, Extractive	RON, ASTM D86
Gasoil Blender	Feed & Rundown	Shelter, Extractive	Cetane, Aro%, ASTM D86, CP, PP etc
Gasoline Blender	Feed & Rundown	Shelter, Extractive	RON, MON, ASTM D86, Bnz% etc

Example Analyser Applications

Extractive Analyser Sample System for Final Product Blending Application

Final Product Blending

Gasoline or diesel blending is a complex refining process as operating personnel are required to meet fuel quality and legislative targets while operating at the lowest possible cost. To meet these operating targets, typical properties that are measured and controlled include RON, MON, RVP, aromatics, benzene, olefins, ASTM-D86 distillation points, and oxygenates for gasoline, and for diesel, cetane index, cloud point, pour point and ASTM-D86 distillation or recovery points. Traditionally, these measurements have been obtained by periodically stopping the blend and removing samples to the laboratory, or have been provided by a host of classical on-line analytical techniques, e.g. Octane Engines and Gas Chromatographs. There are, however, a number of problems associated with these approaches. These include the high capital and operating costs of multiple techniques, slow response time and, in many cases, poor analytical repeatability. These disadvantages are especially evident in the utilization of octane engines. These performance issues can lead to significantly higher blending costs due to unavoidable "property giveaway", as well as reduced blender throughput, coupled with increased inventory and demurrage costs. The financial incentive to blend continuously and faster is therefore very significant, which means that rapid on-line analysis of key product properties is highly desirable. FT-NIR spectroscopy has proved to be a reliable and cost-efficient technique for this purpose. A further development in the use of this technique is analyzer technology that allows calibration transfer between analyzers, i.e. using the same predictive models on different instruments without re-calibration. This is particularly useful for a refinery that operates parallel blenders and also wishes to use FT-NIR in the laboratory as an off-line check or to provide redundant analyses.

The profitability of a gasoline blending operation is determined by many elements. Major factors include optimization of blending component production, inventory control, and minimization of property giveaway. Refiners are also faced with ever tightening legislative regulations governing the quality of gasoline products. These economic, fuel quality and regulatory constraints result in a complex task for the blending operator.

FT-NIR technology can provide fast, reliable and accurate analyses of these blended gasoline product and component streams. This analytical capability can assist in reducing blending costs while meeting product property specifications as part of an overall recipe optimization. FT-NIR analysis can provide Gasoline, Diesel or Jet fuel properties such as RON, MON, Cetane Index, RVP, aromatics, cloud point, D86 distillation points, benzene, and oxygenates, among others, in essentially real-time. All of these properties can be extracted from a single FT-NIR spectrum. Typical FT-NIR calibration model performance on gasoline and gasoil data, for a refinery with a good reference laboratory are shown in the tables below:

Typical FT- NIR Analyser Performance Data for Final Product Gasoline		
Property	**Accuracy (SECV) at 1σ**	**Precision (r) at 1σ**
RON	0.28	0.01
MON	0.32	0.01
% Aromatics	0.8	0.02
% Olefins	1.2	0.03
% Benzene	0.1	0.005
% Oxygenates	0.2	0.01
RVP (kPa)	0.9	0.16
D10% (degC)	1.8	0.1
D50% (degC)	2.1	0.1
D90% (degC)	3.2	0.1
E170	1.6	0.08

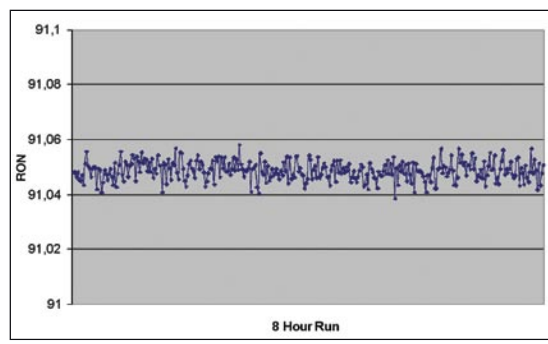
Typical FT- NIR Analyser Performance Data for Final product Diesel		
Property	**Accuracy (SECV) at 1σ**	**Precision (r) at 1σ**
Cetane Number	0.33	0.08
Cetane Improver Vol%	0.0034	0.0015
Aromatics Vol%	0.23	0.06
PAH Wt %	0.18	0.05
API Gravity	0.16	0.04
10% Rec	2.2	0.3
50% Rec	2.0	0.6
90% Rec	5.2	0.5
Cloud Point	2.1	0.3
Flash Point	1.7	0.4
Viscosity(cSt at 40°C)	0.032	0.009

Typical FT-NIR Calibration Performance Data for a Refinery with a good Reference Laboratory

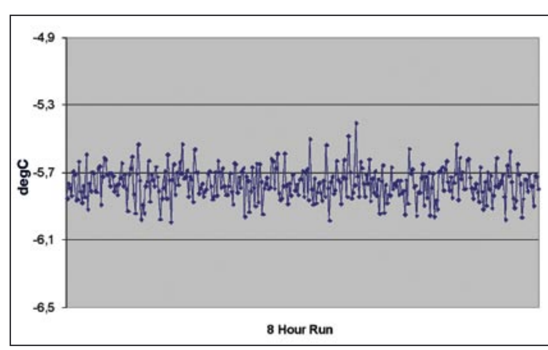
Process FTIR Analyser Repeatability

As a correlational technique, process FT-NIR will yield an analytical accuracy exactly as good as the ASTM laboratory reference data used to develop the calibration models, provided good statistical practices are followed. However, it is perhaps not always fully appreciated how much the analytical repeatability and analyzer availability can be improved by using process FT-NIR as compared with conventional multi-analyzer blend optimization schemes. For light hydrocarbon streams, which can be easily and successfully prepared for analysis by simple sample-conditioning filtered fast-loops, the inherently ultra-low-noise optical technology of FT-NIR can yield exceptional analytical repeatability compared with conventional physical analyzers.

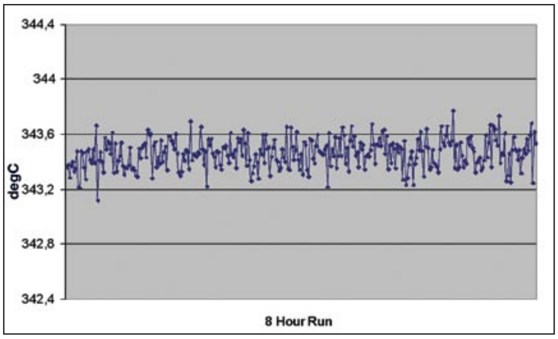
The outstanding repeatability of FT-NIR gasoline or gasoil property measurement is of significant benefit to the blend operator. True changes in blend properties can be tracked precisely during a blend, changes that would be otherwise 'lost' in the noisy or infrequent results obtained from classical analyses. The operator or multi-variable control scheme can then make process decisions to maintain optimized blending with the assurance that the property deviation is real. In addition, this increased repeatability over the traditional lab method means that property giveaway can be reduced.



Gasoline Property Repeatability (RON)



Diesel Property Repeatability (Cloud Point)

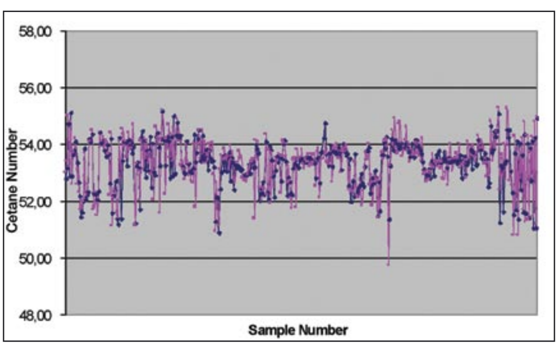


Gasoil Property Repeatability (T95)

Tracking the Laboratory Reference Standard

Since the process FT-NIR analyzers used for refinery process stream analysis and unit optimization are secondary analyzers, dependent for their operation on correlational models using laboratory reference data, it is important for validation purposes that an on-going SQC track-record of performance relative to laboratory standards is maintained. There are useful ASTM guidelines to this practice covered in ASTM D6122 and ASTM E1655.

The attached Figure shows such a laboratory reference method vs. process FT-NIR control chart comparison for a diesel blending application (cetane number).



Tracking the Laboratory Reference Standard

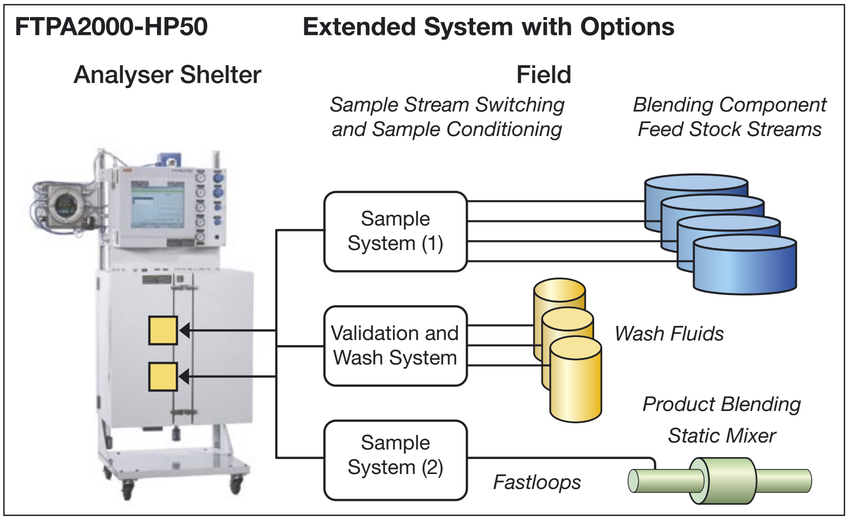
This is a very important aspect of maintaining the reliability and credibility of an installed process FT-NIR analyzer, and is of particular significance for critical optimization and quality giveaway applications. The discipline of monitoring the on-line analyzer performance versus the site laboratory reference allows for rapid detection and adjustment in case of divergence. Medium-term drift and offset of the laboratory reference needs to be compensated, and calibration modeling impacts caused by significant changes in blend order or blending component availability need to addressed.

Process FTIR Field Installations for Gasoline and Gasoil Blending

When all of these various aspects are properly considered, process analytical FT-NIR for refineries offers very specific advantages. It is a rapid, low-maintenance, multi-stream, multi-property, on-line analytical technique, providing exactly the type of fast analytical response required for on-line process unit optimization schemes. If correctly implemented, validated and monitored, it has been shown capable, when installed on high added value refinery processes, of yielding multi-million dollar return-on-investment (ROI) year on year.

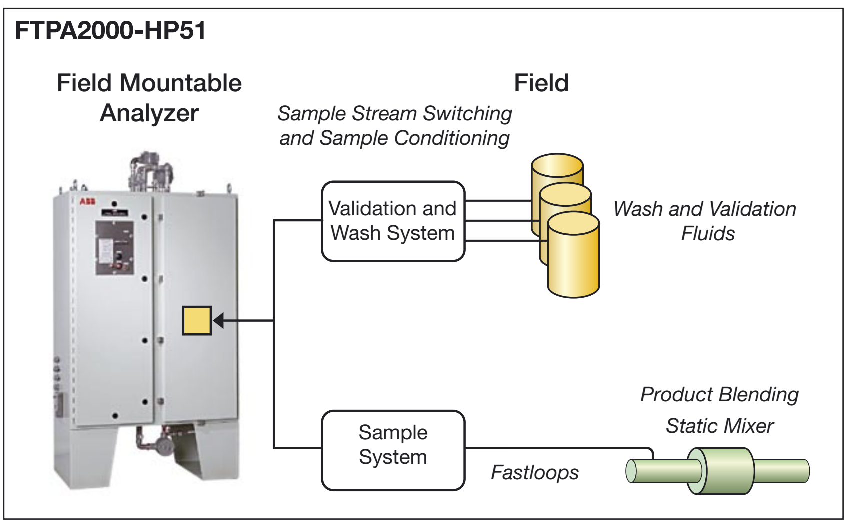
Field installations for process FT-NIR analyzers in final product blending applications can assume a number of configurations. The classical format analogous to a process GC analyzer configuration, sees the process FT-NIR analyzer as a fully integrated unit complete with appropriate hazardous zone certification for installation in an analyzer shelter. In just the same way as a GC, this analyzer is fed by one or more fast-loop sample conditioning systems. Also, as in advanced process GC configurations with parallel columns, the process FT-NIR analyzer can be fitted with dual cells to allow maximum cycle time efficiency and to limit physical stream switching. This approach has the advantage of absolute control over the sample condition and temperature at the point of measurement, along with the simplest optical arrangement, and the widest range of NIR wavelengths available for calibration purposes. Where the physical layout of the off-site blend header and tank farm allows this configuration to be selected, it is the method of choice. This configuration can also be made available in a field-mountable analyzer package, requiring only limited climate and anti-frost protection (Examples A and B).

However in some circumstances this arrangement can lead to the requirement for very long sample fast-loop runs. This is perhaps especially so when a large number of final product blending components are to be measured as part of the optimization scheme. In this case it may be convenient to locate one or more field-mounted sampling cabinets in the region of the tapping points for the blending components, as well as a separate arrangement for the blended final product. This configuration is very flexible in terms of the balance between individual sample cells per stream and physical stream switching into common sample cells, which can be selected on the basis of stream compatibility. This approach possibly offers the optimum in cycle time for a multi-stream final product blending application, and allows, if required, for complete sample stream segregation., However, it is normally limited to a narrower range of available NIR wavelengths for calibration purposes, and imposes a not inconsiderable civil-engineering cost, in terms of fiber-optic cable installation. Also, it loses the elegant optical simplicity of the first approach, with some consequent risk of complicating the calibration process. It can however be implemented in either safe area or hazardous area multi-channel fiber-optic analyzer packages (Example C and D).



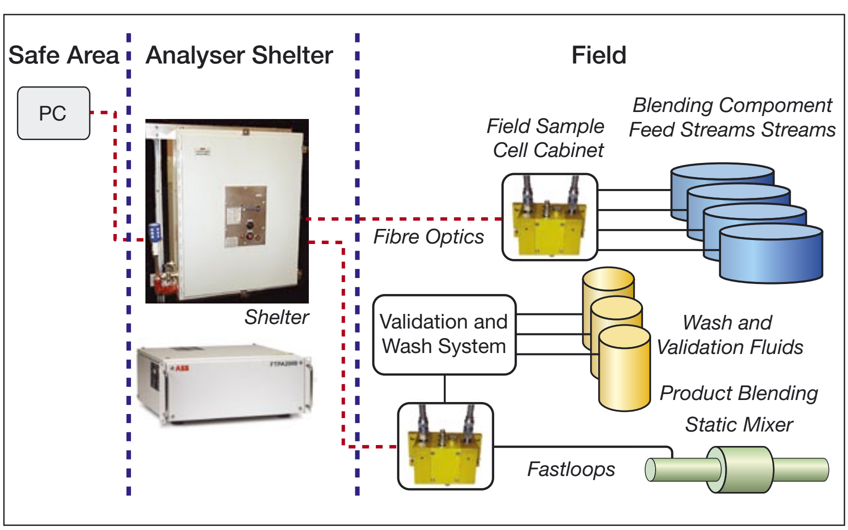
Field Analyser Installation for Gasoline and Gasoil Blending (A)

Example A: Final Product Blending Analyzer configuration, showing a Process FT-NIR analyzer system installed in an Analyzer House, with fast-loop sample conditioning systems and wash/validation fluid systems for sample cell maintenance and analyzer validation. Uses physical stream switching to select streams for analysis



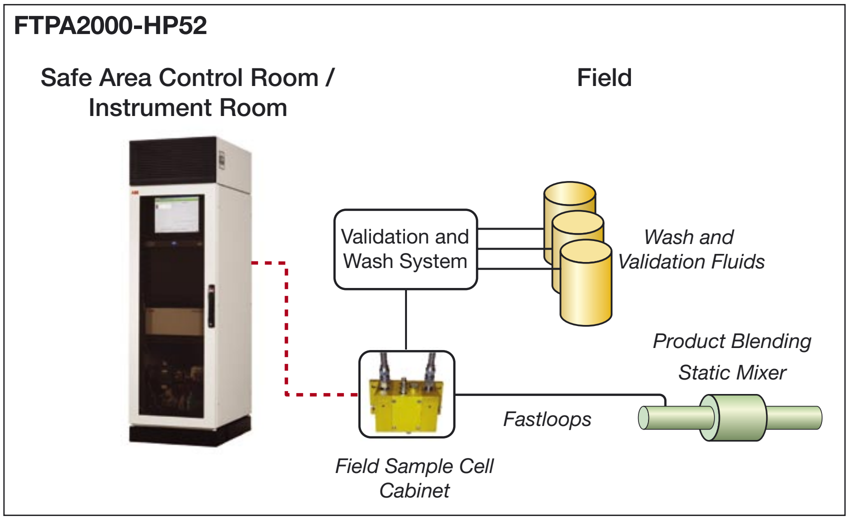
Field Analyser Installation for Gasoline and Gasoil Blending (B)

Example B: Final Product Blending Analyzer configuration, showing an FT-NIR analyzer system for Field-Mounting without the need for a full-specification Analyzer House. Uses fast-loop sample conditioning systems and wash/validation fluid systems for sample cell maintenance and analyzer validation. Uses physical stream switching to select streams for analysis



Fibre-optic Analyser Installation for Gasoline and Gasoil Blending (C)

Example C: Final Product Blending Analyzer configuration, showing a fiber-optic process FT-NIR analyzer system with Hazardous Area enclosure installed in an Analyzer House, with remote PC controller. Uses separate cells for blending components and final product streams, and can use multiple cells where physical stream switching is to be avoided. Sample cell cabinets can be remote or local to sample take-offs..



Fibre-optic Analyser Installation for Gasoline and Gasoil Blending (D)

Example D: Final Product Blending Analyzer configuration, showing a remote fiber-optic process FT-NIR analyzer system installed in an Control Room or Instrument Room, with integral rack-mount PC controller. Uses separate cells for blending components and final product streams, and can use multiple cells where physical stream switching is to be avoided. Sample cell cabinets can be remote or local to sample take-offs.

Analyser Performance for Final Product Optimization

Why is analyzer accuracy and repeatability so important for blend optimization? There are various ways in which real-time on-line analytical data for the final blended product can be used in an optimization scheme to improve the economics of blending (and thus boost refining margin). These include minimizing re-blends (and thus improving overall refining capacity), as well as cost reduction in blend feedstocks usage. If the blend quality target can be met while maximizing the contribution of lower cost components, this can be a major contribution to improved blending economies. It should be said that a key part of the overall scheme to achieve these benefits is played by the Advanced Blend Control optimizer itself. This is critical, but will be undermined if not supplied with the best available on-line analytical data.

Profit Improvement Through Better Analytical Accuracy

The calculation below represents the “baseline” giveaway associated with an analytical uncertainty of 0.1 PON (Pump Octane Num)ber). This can never be reduced to zero, of course, but a crucial impact on overall refinery margin can be obtained by minimizing it as much as possible. What the numbers show is that for a very conservative improvement in analytical precision of 0.02 to 0.05 PON, consequent upon operation of real-time on-line process FT-NIR final product analysis, annual ROI can realistically be expected to be in the $1.5M to $3.0M range.

Cost of Octane Giveaway, $M per year 0.1 PON (Pump Octane) per 200,000 bbl/day CDU Capacity		
Item	Factor	Value
A	Octane Giveaway	0.1 PON
B	Multiplier for APC 99% Confidence Level	2,58
C	Refinery Margin, $/Octane-Gallon	0,015
D	CDU to FPB Conversion Ratio	0,562
E	Average Throughput (CDU) bbl/day	200 000
F	Average Throughput (CDU) gals/day	8 400 000
	Lost Profit, Octane Giveaway/day	$18 270
	Lost Profit, Octane Giveaway/year	$6 668 550

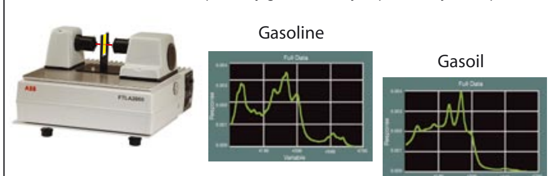
Analyser Calibration

Modeling Techniques

The technique of using NIR spectroscopy for property prediction is a correlative secondary method which can ultimately be only as accurate as the reference methods that provide primary calibration data, e.g. a laboratory gas chromatograph analysis for olefins or aromatics content. This data from the reference method is fed into mathematical modeling software along with the spectra to generate a model. This model correlates the spectra to the list of properties to be predicted. ABB offers several modeling techniques including PLS, PCR, Peak height and topographical models appropriate to the needs of each specific project and site application.

FTNIR Optical Measurement

- Measures complex hydrocarbon mixtures without separation
- Uses a calibration method to determine chemical and bulk physical sample properties (eg PINA, ASTM D86 Distillation, RON, MON...)
- It's a secondary method – relies on Lab reference data for calibration, but has exceptionally good stability, repeatability and speed



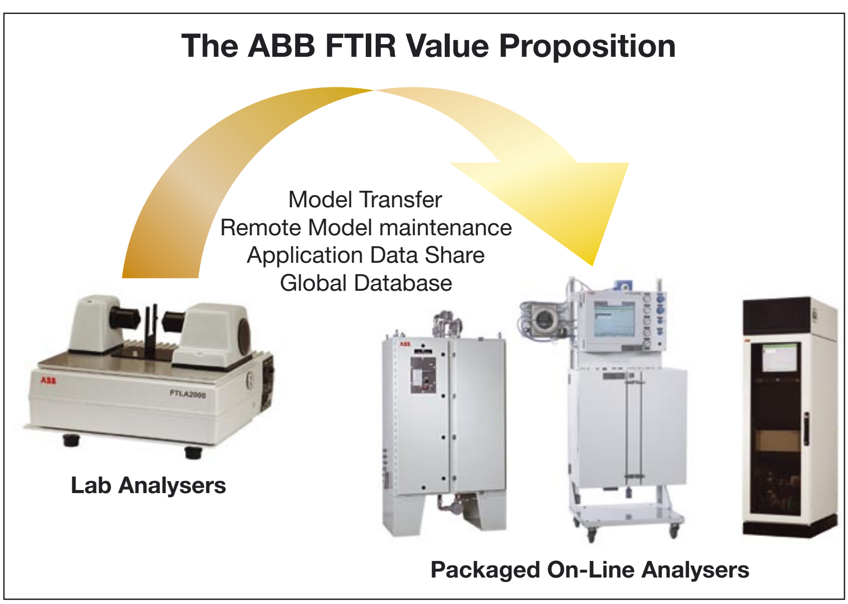
Model Generation

The calibration data should cover the range of product variability expected for that site, including variation both in the property to be measured (Octane, Total Aromatics, etc.) as well as the variability in the stream due to recipe, specification and process changes. This means that obtaining periodic data for a complete calibration for a gasoline blender for all conditions could take as long as six months to a year because of seasonal specification changes. Due to ABB's use of a large amount of global data, startup and preliminary models with good performance can be achieved much sooner. Modeling for process and seasonal variations usually involves fewer spectra than the initial data collection period. It is therefore usual for the frequency of data collection to diminish after the first few months to regular but less frequent sampling.

Calibration Transfer between Analyzers

Calibration spectral data can be obtained either using a laboratory FT-NIR or the on-line process FT-NIR. A lab FT-NIR analyzer, used in combination with an on-line system, can ease this calibration burden. Even when an on-line spectrometer installation is planned, an FT-NIR lab analyzer can be used to collect sample spectra ahead of on-line start-up. This greatly accelerates process implementation and minimizes lab effort, as routine QA/QC gasoline samples can be simultaneously characterized by conventional ASTM and lab FT-NIR methods. This allows model building to take place while the on-line spectrometer is under construction or while process installation is under way. Even when the on-line spectrometer is implemented, the FT-NIR lab analyzer is very valuable, as it provides redundancy for the process analyzer and can be used to extend on-line calibrations for blend recipe changes. For all steps in a project, be it feasibility, calibration, validation or process operation, the lab FT-NIR spectrometer is a critical support instrument for the on-line FT-NIR spectrometer. The use of an FT-NIR lab analyzer with an on-line analyzer is more simple and straightforward if the two FT-NIR analyzers, using the same calibration file, give statistically indistinguishable results when analyzing the same set of gasoline samples. This capability is equally valuable when refiners wish to use the same NIR calibration model on multiple analyzers on parallel blenders. The production of a calibration model is too costly and involved to allow instrument-to-instrument variations to affect or inhibit multiple use of the same model, or indeed to render uncertain the maintenance over time of a calibration model.

ABB's close tolerances and unique spectrometer design mean that calibration transfer among and between lab FT-NIRs and process FT-NIRs is possible without re-calibration.



The ABB Solution

ABB Bomem has the predominant NIR technology position in the global petroleum refining market. We have implemented over 100 analyzers in gasoline/gasoil applications and a host of other refinery process installations. These range across the entire refinery from Crude Oil analysis to Sulfur Recovery Unit feed characterization.

ABB has installed gasoline projects in partnership with many of the global players in the petroleum refining industry. These companies include Shell, BP, Total, Chevron, Texaco, Mobil, KOA Oil, Preem, Ultramar, Saudi Aramco, Tesoro, LG Caltex, Conoco Phillips and many others during many years in the NIR gasoline business. We are respectfully proud to say that ABB is the number one choice for many of the pre-eminent refining companies.

Global Support

We have invested in a truly global support team of refining industry application specialists. They are located in all of the major refining regions around the globe. We are committed to serving our customers with regional teams to most efficiently serve their needs. This structure enables closer partnerships with operators, which in turn improves the success of any NIR project.

Summary

FT-NIR is the technology, which currently offers the best price-performance-value-risk trade-off for on-line final product blend optimization. As an optically-based technology it allows for the most flexibility in terms of multi-stream, multi-property applications since it is compatible with both local, fully extractive sampling and remote, multi-cell extractive fiber-optic based analyzer systems. It offers multi-property analysis with rapid analysis cycle times well tuned to the requirements of an Advanced Blend Control optimizer. It is also well-established with hundreds of installations globally providing examples of successful implementation. Historically, the limitation to any spectroscopic measurement for on-line final blended product control has been the difficulty in developing, and more particularly maintaining, robust and stable calibration models. This has been to a large extent mitigated by recent developments including very well-controlled analyzer-to-analyzer variability, allowing easy maintenance and transferability of developed calibrations, the use of globally applicable product databases to speed up calibration development, and the exploitation of sound modeling procedures to minimize the sensitivity of developed calibrations to changes in blending recipes.

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