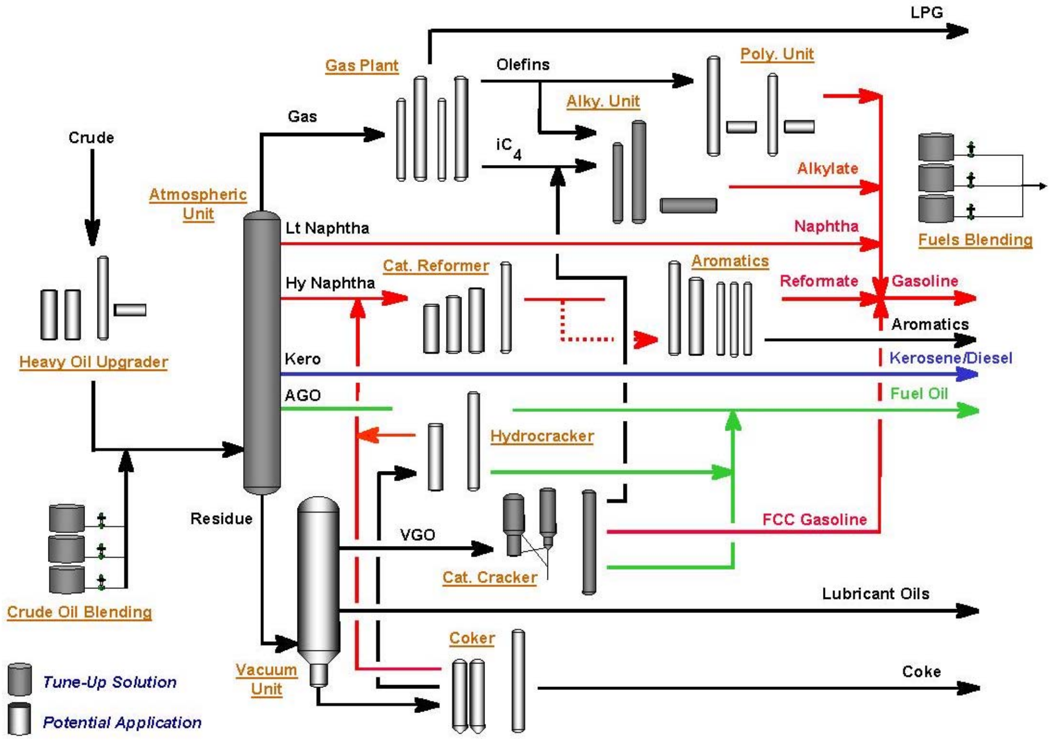
STRATEGIC REFINERY OPERATION USING NMR-ENHANCED ADVANCED PROCESS CONTROL

INTRODUCTION - NMR-Enhanced Advanced Process Control and Optimization

Advanced process control (APC) schemes frequently require near real-time stream composition information to make adjustments to controls – the faster and more reliably the better. To obtain these crucial measurements of process performance, refiners have been deploying GC, boiling point, RVP, cloud point, octane, and numerous other process analyzers. Nuclear Magnetic Resonance (NMR) spectroscopy is rapidly emerging as one of the most versatile and cost-effective technologies for process analysis.

NMR offers tremendous analytical measurement flexibility, non-invasive sampling, rapid and precise analysis, and system availability exceeding 95%, thanks to dependable system components and very low maintenance requirements. Moreover, process NMR analyzers can measure numerous chemical species, because they can be tuned for hydrogen, fluorine, or phosphorous nuclei. Figure 1 identifies potential application sites for NMR-enhanced APC systems in the refinery.

Figure 1 **- NMR-Enhanced Refinery Control Applications**



How NMR Spectroscopy Works

During an NMR analysis, a sample stream is passed through a precisely controlled magnetic field, which brings the magnetic moments of all its protons into alignment with the homogeneous magnetic field. To take a reading, an NMR analyzer transmits a pulse of 60 MHz radio frequency (RF) energy, through a tuned circuit coil, into the stream. The magnetic field component of the radio frequency energy perturbs the magnetic moments of the various protons off their aligned axes. The amount of deflection and the subsequent recovery time will vary according to the length of the applied pulse. When the RF pulse is turned off the proton magnetic moments will return to alignment with the NMR magnetic field. As the magnetic moments precess back to equilibrium, protons with different chemical environments generate alternating currents at different frequencies in the NMR irradiation coil. These currents represent protons is different environments and the magnitude of the current is proportional to the amount of that chemical proton type in the sample. Fourier transformation of the raw signal generated in the coil yields a spectrum of peaks where each peak represents a proton in a unique chemical environment. In the course of one minute the analyzer averages multiple pulses into a spectrum that reveals hydrocarbon chemical make-up, and their relative concentrations.

This NMR spectrum can also be correlated with physical properties other than the chemical composition, enabling determination of multiple parameters from a single spectrum. And since NMR is not an optical technology, the analysis is essentially independent of sample state (e.g., solid, gas, or liquid) or physical condition. Small particulates or bubbles, for example, have little or no effect on the analysis. The sample passes through the magnetic field in a small tube, untouched and unchanged in any way, and is returned to process downstream.

REFINERY TUNE-UP SOLUTION SERIES

Advanced process control, utilizing technology ranging from simple multivariable control to model-based predictive control (MPC) and rigorous on-line modeling, generally requires near real-time stream quality information. The exceptional availability of the NMR analyzer enables this information to be supplied reliably for process control while the technology ensures accuracy and repeatability. Because this analyzer can be applied to numerous component quality measurements, a single analyzer can often alleviate the need for multiple analyzers to satisfy an APC application.

Recognizing that NMR technology is a winner for the petroleum refining industry, teaming the analyzer with appropriate Invensys advanced process control tools and control systems was a logical step. Thus, configurations of the Foxboro I/A Series NMR analyzer with Foxboro and SIMSCI software, control system hardware, and engineering services have been defined to resolve the more costly refinery process control and optimization problems. These configurations are being captured in the Refinery Tune-Up Solution Series, which currently include the following processes (Figure 1):

- Crude Oil Blending
- Atmospheric Crude Oil Distillation
- Fluid Catalytic Cracking
- Sulfuric Acid Alkylation
- Gasoline Blending
- Diesel/Distillate Blending

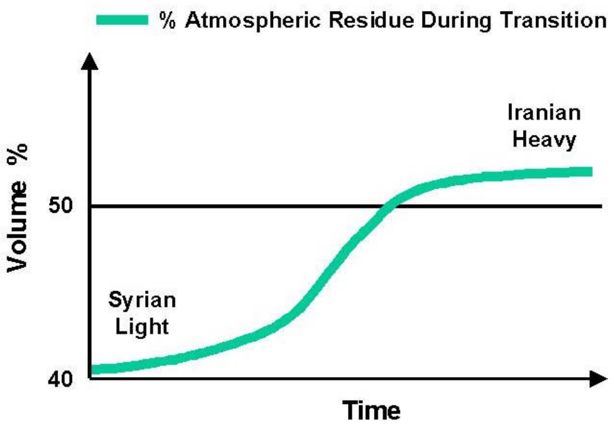
Managing Crude Transitions

Traditionally, refineries were built on the premise that crude would always come from a specific field. Supply varied little, and setpoints could be operated adequately with laboratory analysis and predictive control. Today's market is quite different. Competitive pressure to maximize profitability is driving refiners to find new ways to leverage low-cost crude feeds. They are buying more crude on the spot market, and this crude usually differs significantly from the design-crude used when the refinery was built. Managing these variations profitably requires daily revision of production schedules and continuous profitability optimization.

Figure 2 shows how variations in crude feed quality affect production of low-value atmospheric residue. As the graph shows, a feed change from a typical Syrian Light crude to an Iranian Heavy, unaccompanied by a corresponding change in the process conditions of the crude unit, will increase production of low-value atmospheric residue by about 10 percent.

Figure 2 - **Effect of Variation in Crude Feed Quality**

- **Unit operating conditions are upset by changing feed composition**
- **Product slate is not maintained at optimum**
- **User incurs significant financial penalties**



Variations in crude quality can affect cut point optimization, product quality control, feed rate maximization, and energy consumption, while also violating process equipment constraints. Without process control compensation for a crude transition, the process will experience an upset and become both less efficient and less profitable.

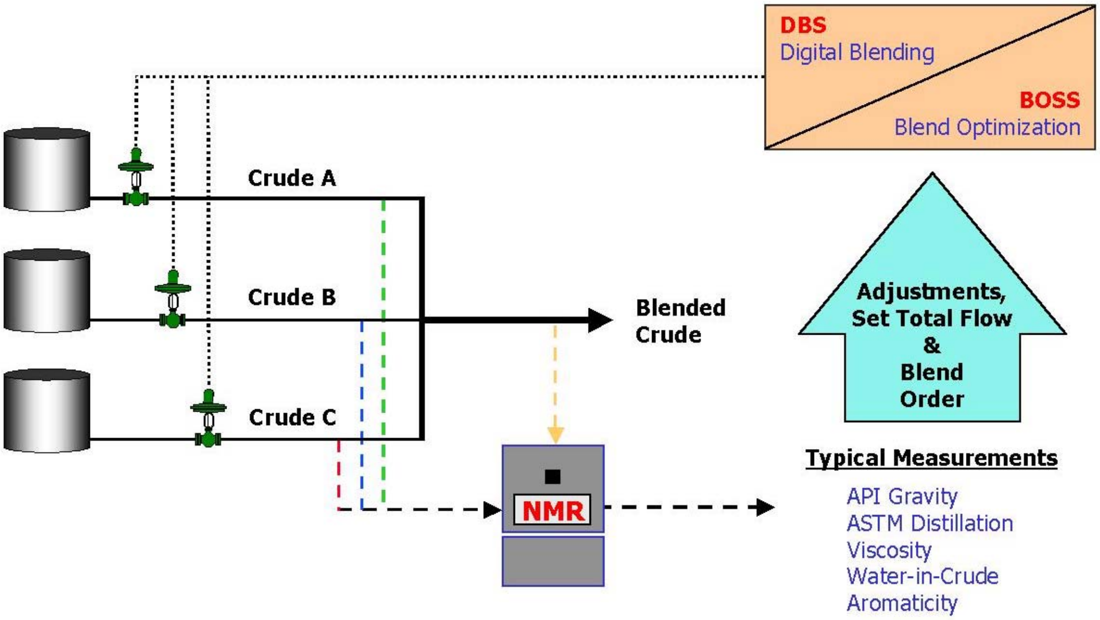
There are several options in managing the transition of crude feeds, although all options are typically not available at each refinery. Crude oil blending is very advantageous to those refiners receiving constant supplies from fields through pipelines or those with large tank farms. Refiners not so lucky must battle unit upset when transitions occur, unless they are made aware of a pending transition and have the capability to minimize the effects through process control.

Crude Oil Blending

The capability of accurately monitoring crude compositions enables precise blending of crude feeds. This means that the refiner can blend less expensive heavy, sour crudes with more expensive light, sweet crudes to achieve desired properties while maximizing profitability.

A crude oil blending system is shown in Figure 3. It is based on implementation of The Foxboro Company's I/A Series NMR Process Analyzer and Foxboro's Blend Optimization and Supervisory System (**BOSS**). A refinery information management system provides crude blend planning functionality that downloads total flow requirements, ratio limits for the crude blend components, and product quality constraints. These settings are based on refinery models that define optimal utilization of distillation and downstream units for various crude types.

Figure 3 - **Crude Oil Blending**



BOSS calculates optimal ratios based on measurements of crude component quality and blended crude quality. At the lower level is a blend ratio controller similar to the type used for gasoline and diesel blending. Foxboro can supply a digital blending system (the I/A Series **DBS**), or an existing digital blender can be used.

Depending on physical location requirements, one or more NMR analyzers are applied to the blended crude stream and to the crude component streams. The NMR analyzer measures essential qualities such as API gravity or density, true boiling point /ASTM distillation, initial and final boiling point, and water content.

Operating the refinery at optimal and constant crude composition can generate savings for major refineries on the order of 2% to 3% of the operating margin of the whole refinery. The Crude Oil Blending solution achieves this by:

> *Improved distillation unit throughput.* Constant attention to the distillation quality of the crude loads the crude distillation unit and all the other downstream units consistently. This allows refiners to operate their crude distillation unit closer to its limits, which increases throughput.
>
> *Improved refinery throughput.* If the throughput of any refinery unit is limited, a constant and optimal distillation curve for the crude oil can push all units to their limit simultaneously. This maximizes throughput for the overall refinery.
>
> *Improved performance of downstream units.* Specific characteristics of the crude will also influence performance of some of the downstream units. Changes in the ratio of paraffins to aromatics in crude,

for example, will impact/affect the benzene, toluene, and xylene output of catalytic reformers.

Improved product quality and reduced energy costs. Stability of the crude composition also eliminates one of the major disturbance factors in a refinery, resulting in more stable operation. This contributes positively to overall quality, fosters efficient energy consumption, and improves equipment reliability.

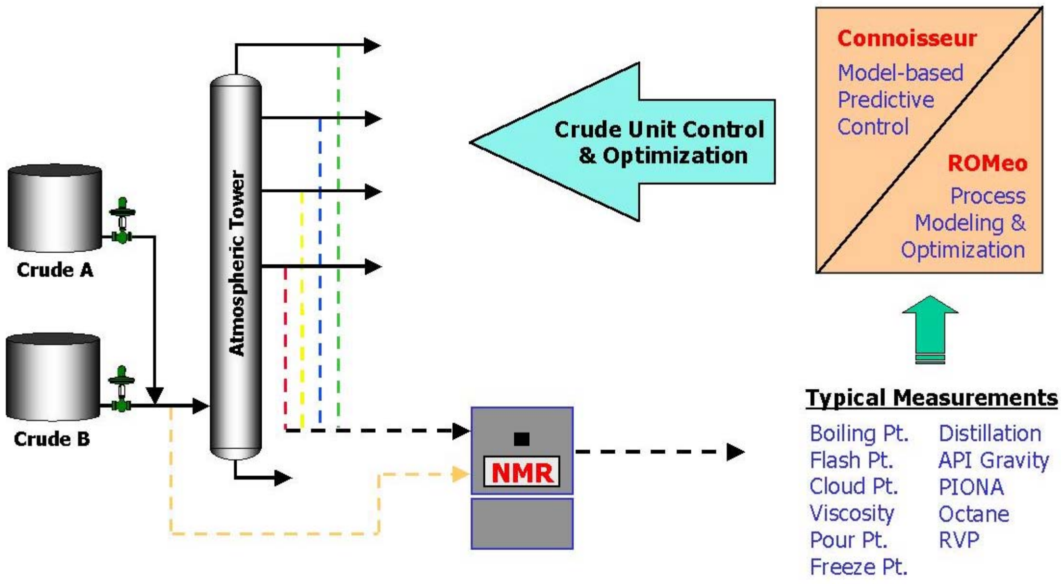
Improved management of crude changes. Maintaining optimum and constant crude quality and composition enables more efficient management of changes in crude.

Atmospheric Crude Oil Distillation

In the past, refiners would manage the transition from one crude to another by manual adjustment of various controlled variables for a given time, thus relying upon prior crude transition experience in order to minimize process upset. By using NMR-enhanced control and process optimization, however, the refiner can follow the transition from one crude to another in real-time and adjust parameters as needed to maintain maximized profit. The result can be dramatic savings per crude transition, since the typical 4 – 8 hour upset due to a transition is essentially eliminated.

Figure 4 shows how Foxboro I/A Series NMR Process Analyzer measurements would be deployed in an atmospheric crude oil distillation unit application. Because NMR technology can also monitor the distillate streams as well as crude feed, the cost benefits are substantial. It can replace complex traditional physical property and laboratory analyzers as well.

Figure 4 - **Atmospheric Crude Oil Distillation**



The crude feed analysis supplies crude characterization information to enable feed transition compensation. **ROMeo**, SIMSCI's Rigorous On-line Modeling and Equation-based Optimization software, provides a completely unified and integrated environment for on-line modeling, process simulation, data reconciliation, and optimization. Newly calculated setpoints to continue an optimized unit performance are calculated and sent to Foxboro's model-based predictive controller, **Connoisseur**, upon a crude transition. Connoisseur, using a dynamic multivariable model, makes the necessary process manipulations to attain the optimum control setpoints determined by ROMeo, while minimizing disturbance to the process.

ROMeo and Connoisseur maintain unit operation at optimum between crude transitions. Atmospheric tower overhead and sidecut product draw stream quality measurements provided by the Foxboro NMR are used in the Connoisseur model to monitor process operation performance and supply control feedback information. Common advanced control targets include:

- Maximizing unit throughput up to equipment constraints
- Maintaining product quality while maximizing yield of most valuable products
- Maximizing preheat train, pumparound, and fired heater heat transfer efficiencies

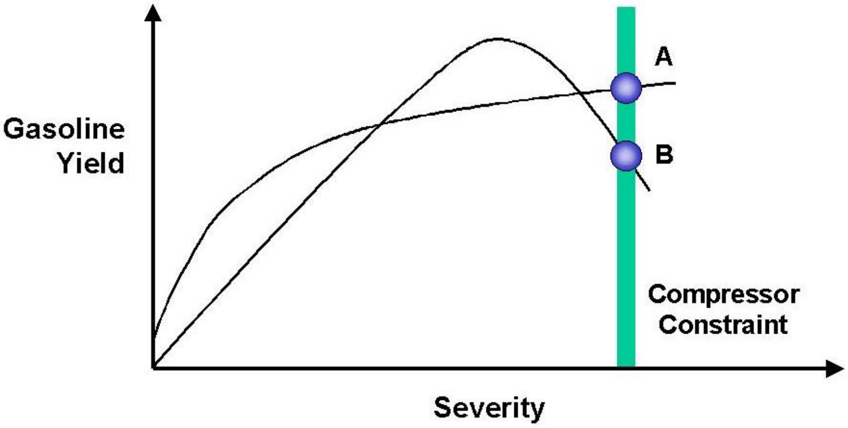
Including crude transition compensation and unit optimization, overall benefit can reach $0.12/bbl feed.

Fluid Catalytic Cracking

The fluid catalytic cracking unit (FCCU) is one of the most important units in the refinery. Few FCCUs have real-time process optimization implemented, since feeds typically have been measurable only in the laboratory. These measurements take many hours, with reports available only once or twice a day. Even the measurement of PIONA (paraffins, isoparaffins, olefins, naphthenes, and aromatics) and the distillation properties of the rundowns are difficult to achieve on-line. The Foxboro I/A Series NMR now provides a means of obtaining these measurements near real-time, thus enabling significant economic benefit to the refiner through APC and process optimization.

Like the atmospheric crude distillation units, the FCCU has been built on the supposition that the feed composition will remain near design specifications. In today's economic climate, this is no longer true. Figure 5 shows that as you change from one feed (crude type) to another, the optimal target severity changes also. In this case, maintaining the same optimization will actually reduce yield and increase costs (B).

Figure 5 **- FCCU - Gasoline Yield vs. Severity for Two Different Feedstocks**



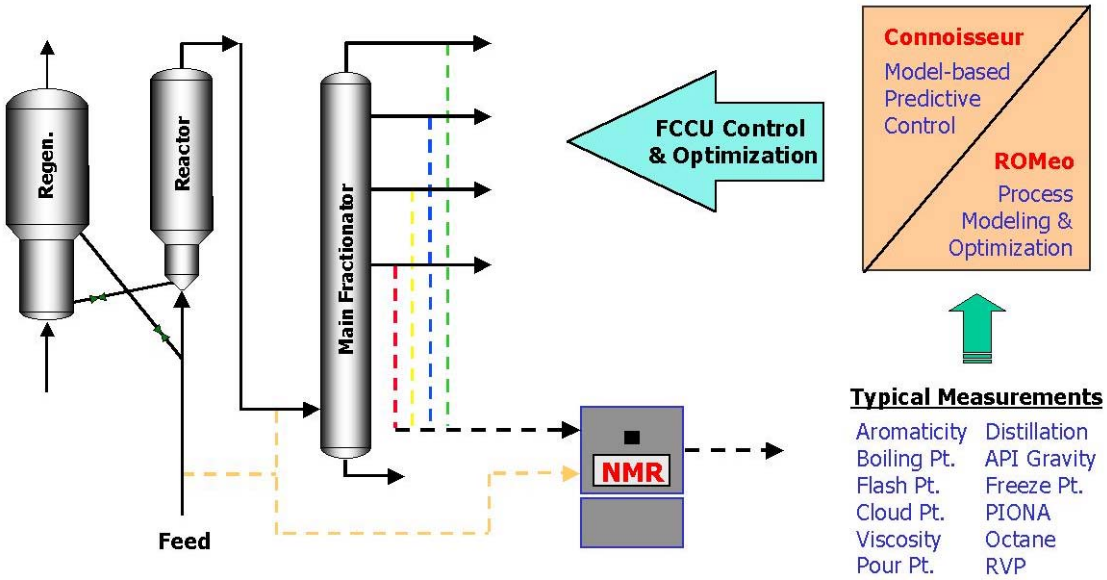
Using the Foxboro NMR to characterize the feed and coupling it to the ROMeo process model (Figure 6) helps optimize the process in the following ways:

1. If the feed has changed, the NMR analyzer provides near real-time data on changing feed properties to enable the most economical conversion of the available feed.

2. If the feed remains unchanged, the on-line analysis of the feed enables the operator to run the process closer to equipment constraints; for example, near the limits of the LPG compressor at the back end of the process. This increases the throughput of the unit at very little additional cost.

3. As with feed transitions to a crude distillation unit, ROMeo and Connoisseur maintain FCCU operation at optimum. The main fractionator overhead and sidecut product draw stream quality measurements provided by the Foxboro NMR are used in the Connoisseur dynamic model to monitor process operation performance and supply control feedback information.

Figure 6 - **Fluid Catalytic Cracking**



FCCU controls and optimization include feed preparation, the reactor/regenerator, the main fractionator, the wet gas compressor, and the downstream gas plant. Typical operating objectives are

- Maximizing unit capacity
- Maintaining product quality while maximizing yields of most valuable products
- Optimizing energy utilization
- Controlling conversion
- Improving safety and reliability via operational stability

Total economic benefit can approach $0.30/bbl feed.

Sulfuric Acid Alkylation

The alkylation unit control system provides composition measurement and control solutions to reduce or eliminate problems characteristic of sulfuric acid alkylation unit operation. The system applies NMR technology for stream composition analyses with tightly integrated advanced process control to deliver optimum unit performance.

The Foxboro NMR analyzer is used to determine acid strength for the optimization of acid use, the emulsion character (acid-to-HC ratio), the isoparaffin-to-olefins ratio, and the acid-soluble oil content. Secondary applications include safety, quality control, and additional chemometrics uses.

Connoisseur is applied to improve the control of total feed composition and operating conditions to reduce the production of side products such as acid-soluble oil and heavy alkylate. Control improvements in the distillation section assure RVP control of the alkylate product, reduce propane and normal butane diluents in the reactor recycle streams, reduce isobutane losses in product streams, and reduce utility costs. In general, distillation column controls are enhanced to accommodate changing feed composition, temperature, and flow rates, with minimum disturbance to product quality. Reboilers, preheaters, and particular condensers are controlled to maintain required heat transfer rate, thus aiding column operation stability and preserving product yield. Furnace firing controls reduce fuel consumption.

Model-based predictive control targets include:

- Maintaining isoparaffin-to-olefins ratio at optimum
- Maintaining acid-to-hydrocarbon ratio at optimum
- Maintaining optimum overall reactor temperature profile
- Maximizing throughput within feed availability, fractionation capacity, or other constraints

Connoisseur's LP optimizer can be used to drive the process towards an economically optimum set of process constraints. The optimum strategy is determined by the product and utility costs applied in the LP objective function. These costs can be adjusted on line to reflect changing market conditions.

Achieving the following objectives maximizes alkylation unit profitability:

- Maximize alkylate make
- Maximize isobutane/olefin ratio
- Maximize the use of low cost feed in preference to higher cost feed when alternative fresh feedstocks are available
- Maximize propane recovery
- Minimize isobutane losses in product streams

The benefit contributed by the NMR analyzer alone can amount to 10 - 15% of acid costs. The additional benefits acquired from the Connoisseur application range from $0.10 to $0.20 per barrel of feed.

Refinery Blending Systems

To satisfy new gasoline reformulation requirements, blend header complexity is increasing with the increasing number of blend components. Diesel and other blended fuels are also subjected to more severe blending requirements in order to comply with environmental mandates. As a result, refiners are compelled to evaluate the effectiveness of their blending operations and are adding or improving blend optimization to boost profitability. Common blending operation targets are

- to reduce reblends and improve profitability
- to meet product specifications while conforming to environmental requirements

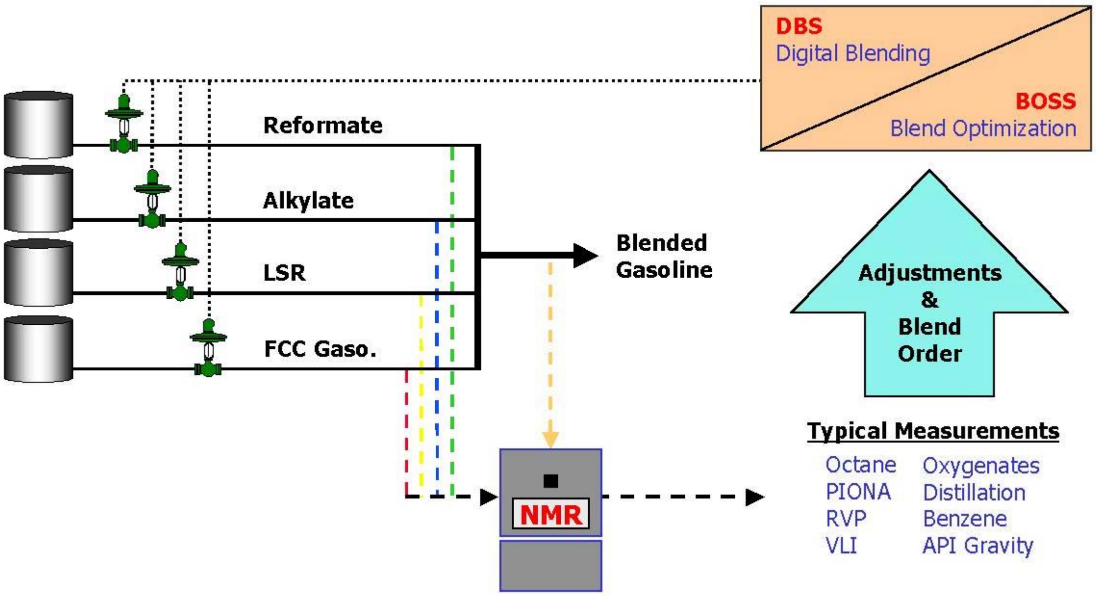
- to enhance effective inventory capability
- to lower risk of missed export schedules
- to improve refinery planning/scheduling accuracy

To realize the greatest profitability in refinery blending operations, a blend optimization system is used to provide management of the component and product tanks, blend header, on-line and laboratory analytical systems, and planning/scheduling activities. This optimizer, Foxboro's Blend Optimization and Supervisory System (BOSS), produces blended products with a high degree of precision to meet specifications while minimizing quality giveaway, maximizing the use of the lowest cost components in the blend, increasing the flexibility of the tank farm operation, and minimizing the frequency of reblends. A flexible objective function permits component cost, inventory constraints, or product specification to direct the optimizer.

Providing BOSS with near real-time component stream and blended product chemical quality information is the NMR analyzer (Figures 7 & 8). This information enables multivariable analyzer-directed control including:

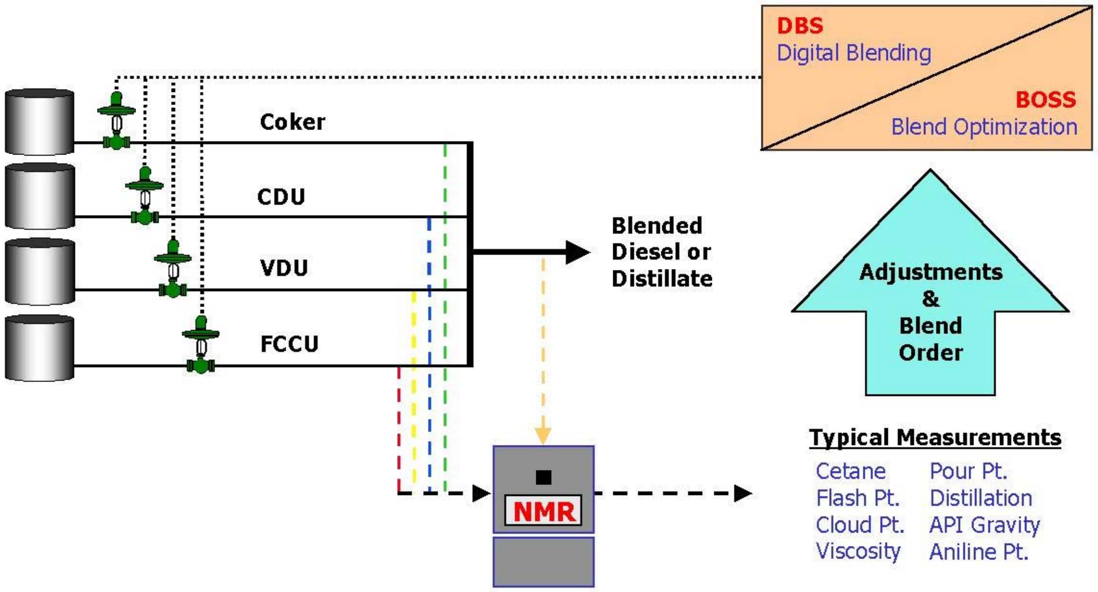
- Feedforward control for component quality variations
- Feedback control for product quality variations
- Quality integration of product and component tanks
- Projected product qualities at the blend header

Figure 7 - **Gasoline Blending**



Actual process manipulations are made by existing digital blend controllers or a Foxboro-supplied Digital Blending System (DBS). DBS features include uniform ramping, continuous pacing, analyzer trim, temperature-compensated flow measurement, and flexible loop configurations. It may be configured to include an automated procedure for manipulating the equipment involved in blending, transfer, flushing, and pigging operations.

Figure 8 - **Diesel or Distillate Blending**



A refinery blending system upgrade project is often more expansive than blend optimization. Blend optimization demands accurate tank information, and automating the tank farm is prerequisite in order to gain most benefit. Then, to maximize blend operation performance, Foxboro can complement blend optimization with the Tank Information System (**TIS**) and the Oil Movement Information System (**OMIS**) software applications.

TIS provides tank inventory information, tank monitoring functions, and tank status and information reports that satisfy internal and regulatory information reporting requirements. This system compiles data provided by tank gauging systems, and is usually an integral part of a blend optimization control scheme.

The tank information system database contains static and dynamic configuration data as well as calculated and measured data. Static data includes information such as tank ID, tank contents ID, API table ID, reference temperature, and tank strapping table values. Dynamic data includes level and temperature alarm limits, and calculated data includes volume correction factor, tank volume, thermal expansion coefficient, dry volume, available volume, ullage, net weight, and more. Accurate tank information allows operation with lower inventories, and the material balancing capability can be used to detect tank leakage. Particularly useful for blend scheduling, it can alert the planner of a potential conflict.

OMIS supplies the engine for automating the tank farm. This system provides resource management of equipment, sequencing and logic functions to control equipment, and flow path selection. System functions include movement planning, automatic movement control, equipment monitoring and management, and product movement and storage reporting and archiving. The equipment database covers tanks, pumps, valves, pipelines, and mixers.

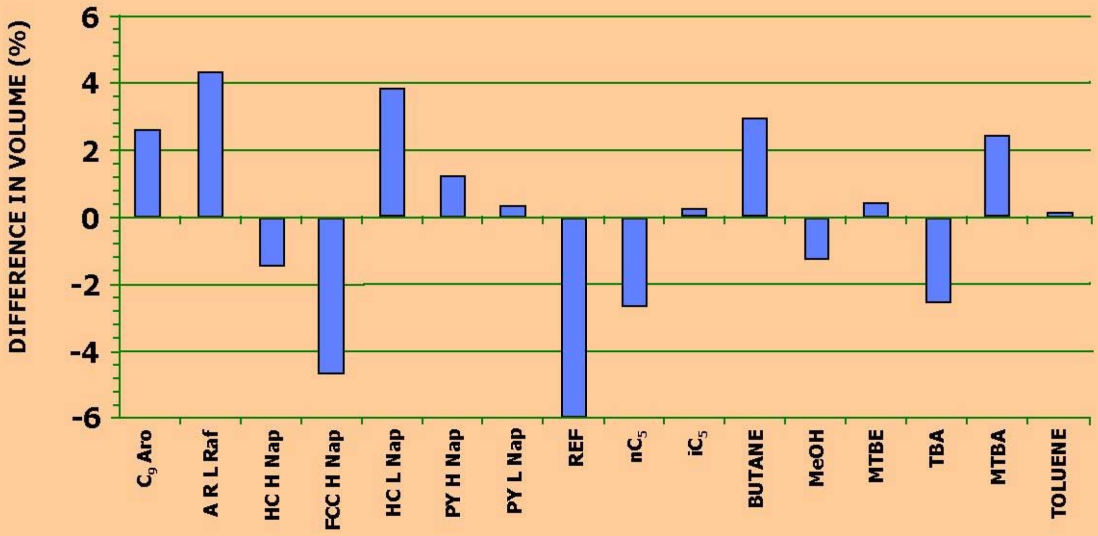
An expert system-based guidance system directs the operator to minimize the potential for human error, protecting equipment from damage, and avoiding stream cross-contamination. The system's "illegal" tank level change information provides a leak detection capability, using both level and flow measurement data. Another system feature is the option to select a swing tank or another pump without the need of a shutdown.

Setting up an oil movement involves selecting the appropriate tanks, pumps, pipelines, etc. from an oil movement planning display. Once the selection is made and the selected path and equipment is validated by the system, the flow path is established. Operation of the flow path equipment can be performed in either an automatic or semi-automatic mode, depending on a need for operator intervention.

A refinery gasoline blending system upgrade project including blend optimization can provide benefits amounting to $0.10 to $0.25/bbl gasoline. Including the cost of engineering studies, new field equipment, and new instrumentation in a tank farm automation and blend optimization project, the payback period is typically less than 18 months. This is true for gasoline, diesel, and fuel oil blending operations.

Benefit From Process Analyzer-Enhanced Blend Optimization

Maximized use of the lower value components



A notable benefit reported by a BOSS user was a significant reduction in use of the more expensive components reformate and FCC heavy naphtha, afforded by increases in use of the cheaper C_9 aromatics, aromex light raffinate, and butane.