

Analyse de produits pétroliers par spectroscopie Proche Infra Rouge

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TOTAL Raffinage Chimie

17^{èmes} rencontres HéliosPIR - Montpellier (France) - 7 Novembre 2016

NIR technology

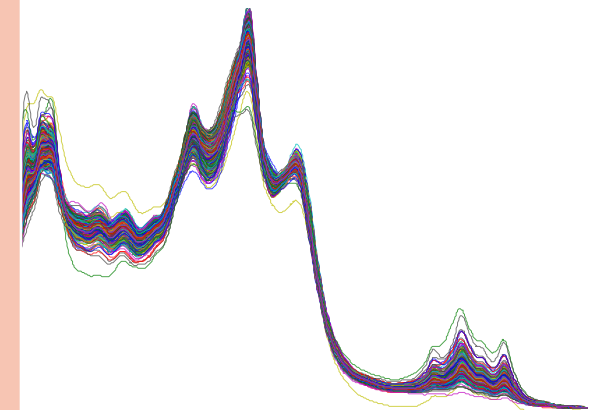
- Mature technology widely used in many industries
- Available at Total for several years
- As any technology, pros and cons

Strengths

- Rapid (near real-time)
- Little or no sample preparation (liquids, solids)
- Non-destructive
- High precision
- Multi-components/properties capability
- Can be on-line and remote (optic fibers)
- Stable and robust equipment with low maintenance available for process analysis

Limitations

- Indirect (2ndary method)
- Variations in temperature,
- Moisture, particle size and sample homogeneity can interfere
- Investment (time, money)
- Steep learning curve
- Not a trace level technology

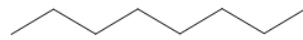


NIR technology on petroleum products

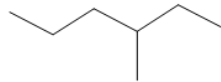
- Hydrocarbons: NIR activity of C-H bonds
- NIR spectrum of hydrocarbon product : rich information on nature, number of chemical groups and atomic environment of vibrator
- Building a specific knowledge to understand the link between NIR spectrum, the chemical structure and the physical/chemical properties to measure
- Necessity to link :
 - Products chemistry
 - Process knowledge
 - Chemometrics modelling



Spectrum: chemical fingerprint of product & process



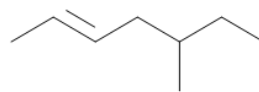
Normal
(Linear)



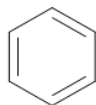
Branched
(Iso)



Cyclanic
(Naphthenic)

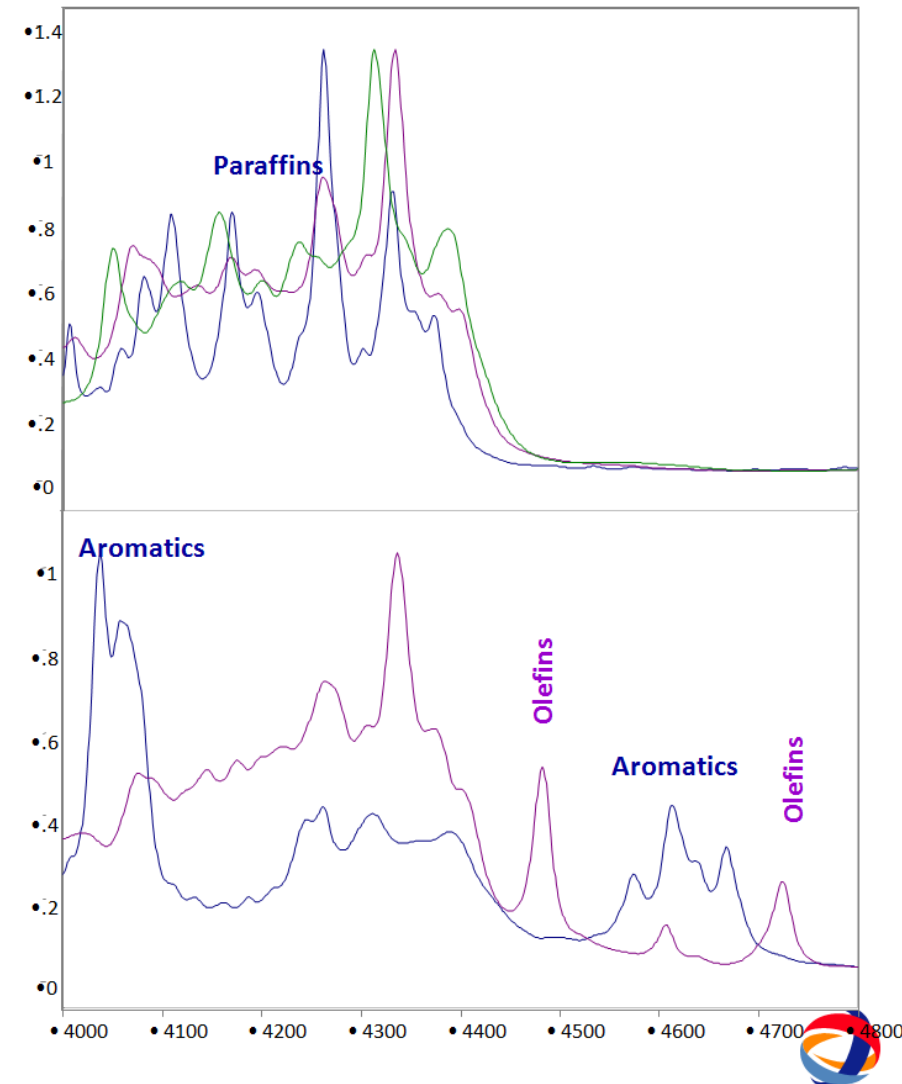


Unsaturated
(Olefins)



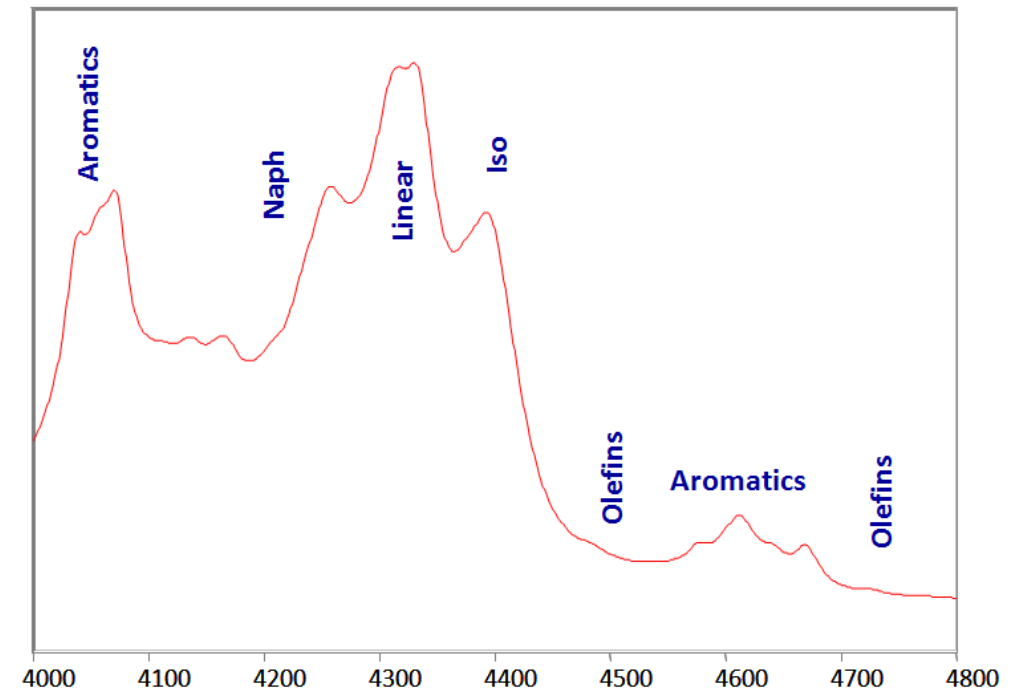
Aromatic

- Distillation
- Hydrotreater
- Hydrocracker
- Isomerase Alkylate
- Catalytic Cracker
- Reforming Platforming



Spectrum: chemical fingerprint of product & process

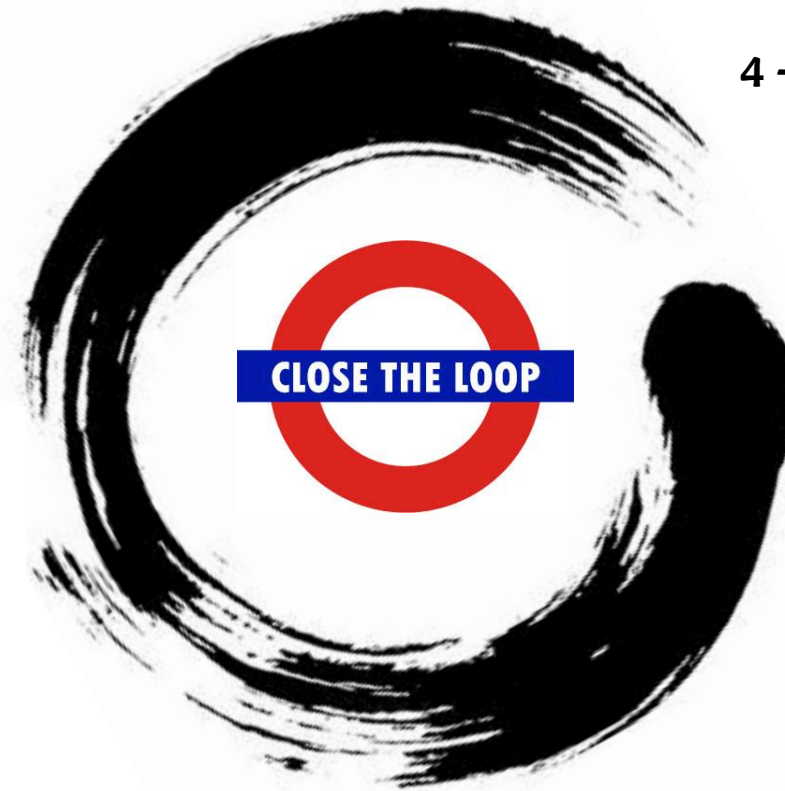
- All petroleum products are complex mixtures of these basic chemical structures
- Each product in a refinery has a specific fingerprint
 - Crude feedstock
 - Unit feed
 - Intermediate products
 - Finished products



Application development

Reference method in lab
1 - Calibration data acquisition

2 - Models development

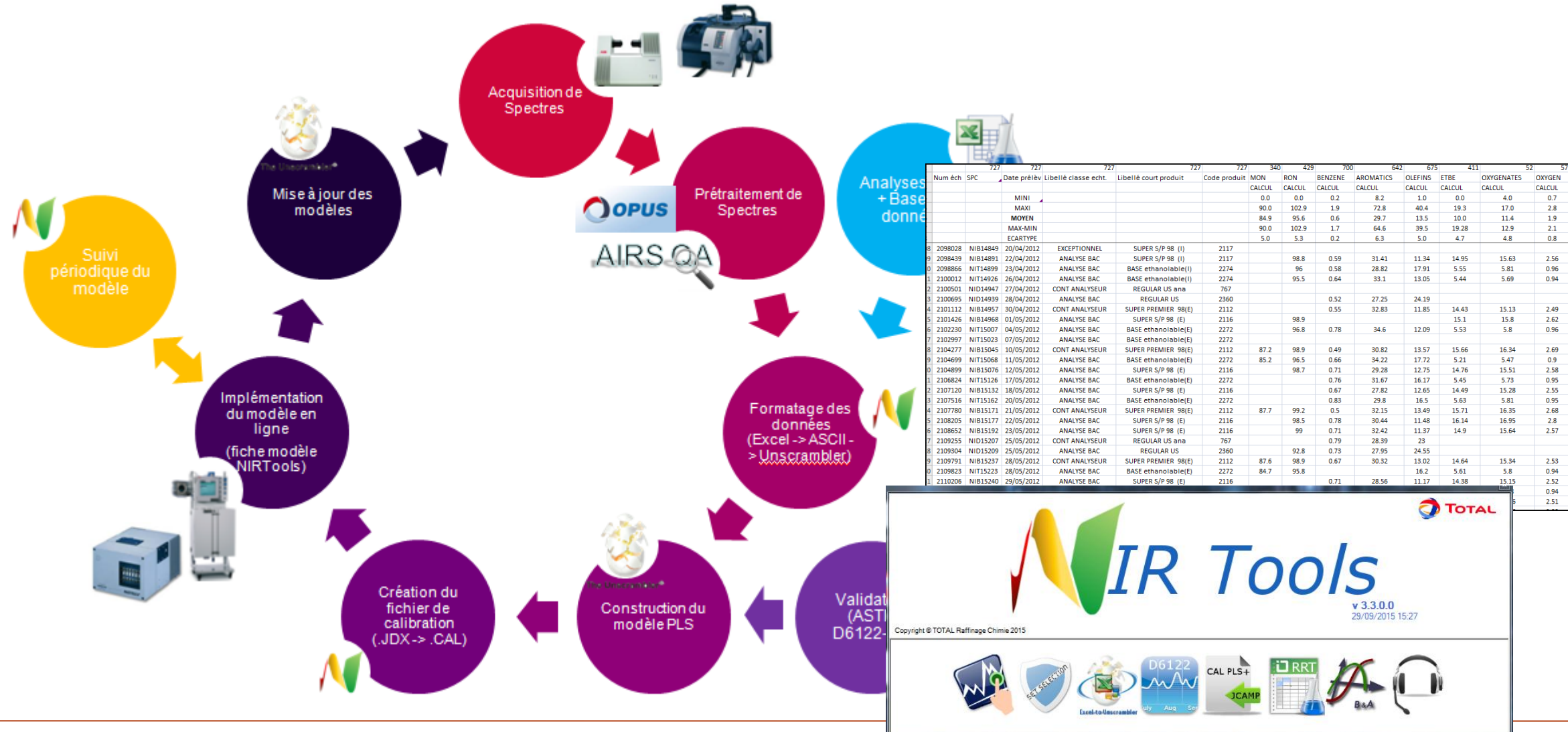


4 - Monitoring, control charts,
models update



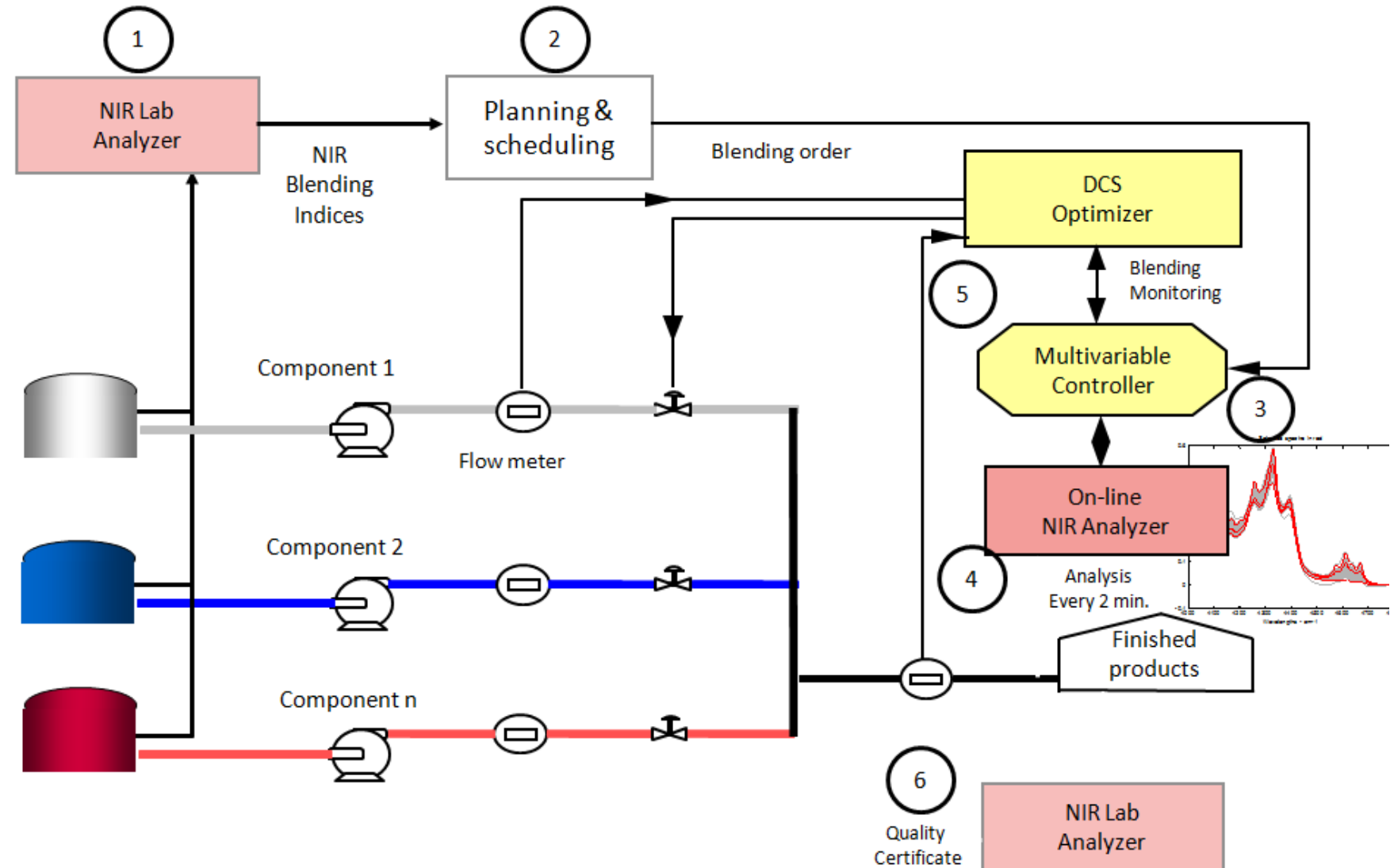
3 - Calibration models transfer

Data cycle - some effort is required !



Example of NIR application

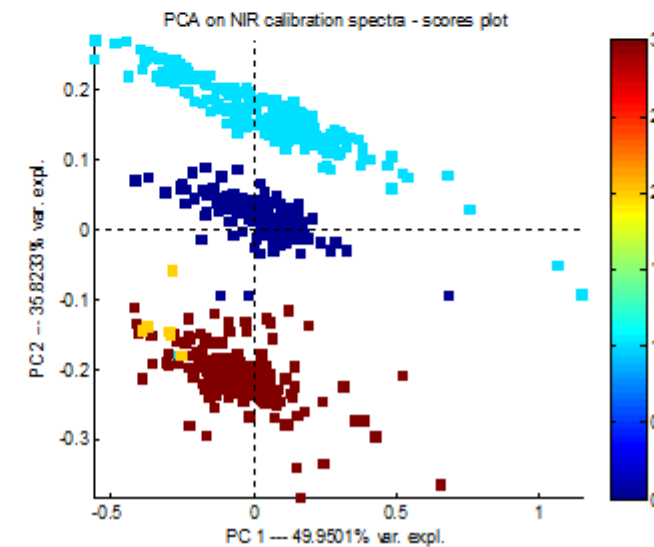
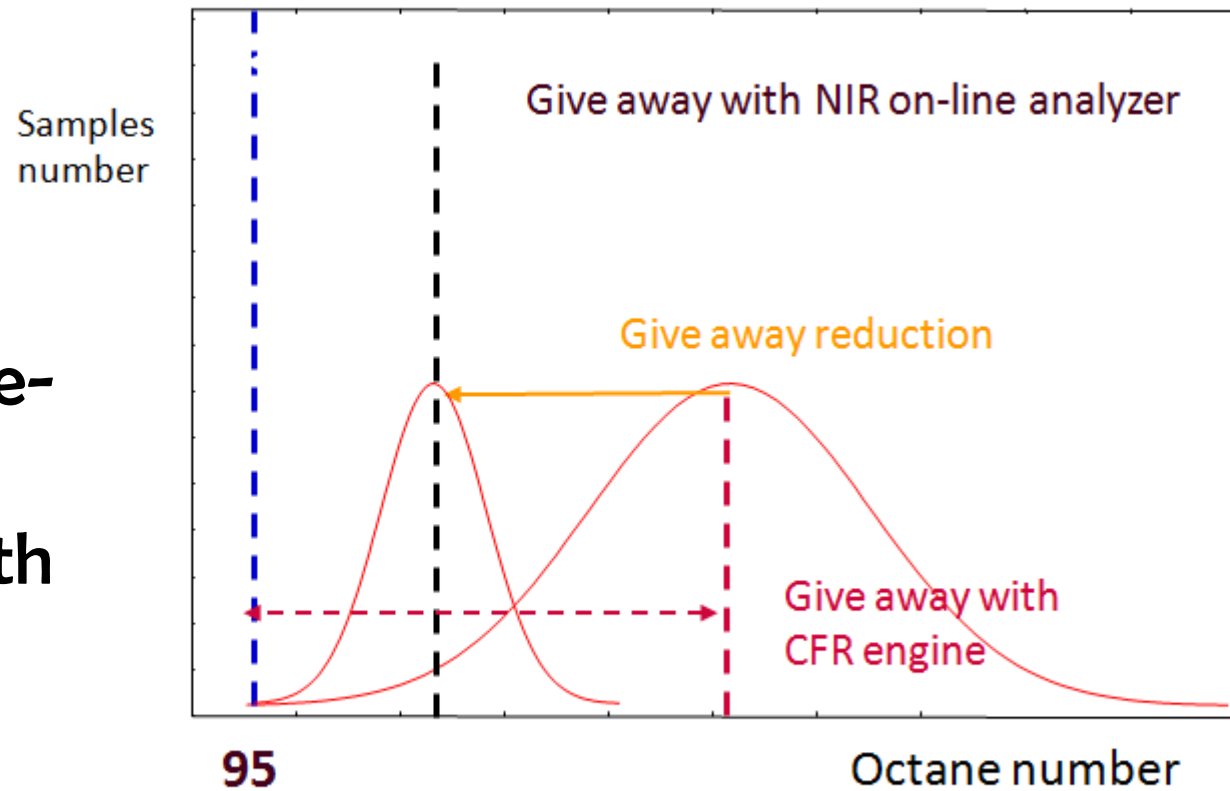
- Gasoline blending optimization



Example of NIR application

Minimum specification

- Blending give-away reduction with on-line NIR analyzer



Some hurdles

- Volatility of products
- High absorbance
- Complex sample matrix, not known and not constant
- Lack of variability
- Evolving process
- Temperature
- Water !

Best practices

- Homogeneity of hardware
- Controlled hardware
- Acquisition methods homogeneity across the branch
- Chemometrics (central support for models)
- In-house software
- In-house training (acquisition and modelling)
- Continuous evaluation of new hardware/accessories



Future ?

- Better models with multi-sources data ?! (data fusion, data merging, data cleaning) NIR + PI data ?
- Machine learning - different models ? Globalize models accross sites
- Data transferred automatically
- More sensors, micro (nano ?) equipment



TECHNOLOGY

How it Works

The SCiO solution combines two powerful technological components, the revolutionary SCiO Sensor, and the SCiO Cloud. Together these two disruptive technologies provide a fully integrated end to end solution that gives you everything your business needs for instant molecular analysis

[CONTACT US](#)



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**THANKS FOR
YOUR ATTENTION
AND
PLEASE DON'T ASK
TOO MUCH**

