Topnir, the refining optimization solution

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Introduction

The increase of environmental restriction and the constantly international business competition constrain the refiners to adopt specialize analytics techniques. Less give away and efficient yield are the keywords of success in the petrochemical world. As a leading supplier of advanced technology tools, ABB provides complete solution allowing the intuitive management and optimization of the global refining chain. Based on a multidimensional technology approach combining mathematics (Topology), chemometry and Near-infra red spectrophotometry, ABB solutions are unique offers including analyses, control and optimisation.

Quick and accurate the Near-infrared analysis is very appropriate to hydrocarbon identification so qualitatively as quantitatively. A spectrum is a fingerprint of a refining product. It contains all the chemical information required for its identification. TOPNIR software has been developed within ABB to provide rapidly a full vector of properties. The predictions accuracy is moreover guaranteed within the ASTM worldwide criteria. Coming from 25 years of applied R&D and operation in BP Amoco, ABB has developed a unique patented approach of measurement in refining product properties.

History

Near infrared spectroscopy takes more and more interest within the petrochemical refining since the last 30 years. A BP team based at Lavéra in France, composed of mathematicians, chemist, opticians, chemical and process engineer has start in 1974 to work on the application of the NIR apply to the hydrocarbons products. Their expertise within the refining industry as enhanced the development towards the area in which the application where the most effective; the blending operation and optimization, process control and supply chain optimization. After year of studies, the first model on the MON property was achieved in 1986. The next year, the first patents were registered. Since when, the technology evolved and further new add ins were implemented to improve the system. Going through the spectral discrimination, then by a fiber interface, the concept was running well on laboratory. In 1990, the first Gasoline model was transfer directly to the blending unit. Hence all the advantages of the system were visible to refiner's people. The technology can be use on line that mean that control and advanced process control tools can be directly implemented to automate (reduce laboratory use (costly and time consuming) and improve the products production.

The licensing activity start in 1994 and the first applications were therefore install in other refinery than BP Lavéra as for example, Shell DEA Wesseling in Germany or again BP Grangemouth in Scotland. TOPNIR™ was then created. TOP for Topology and NIR for Near infrared spectroscopy. Other variant modulus was then added like Optiblend (blending optimization), Simblend (Simulation of finished products blending) or Simcrude (simulation of crude product blending), to make the Software package complete and attractive for refiners.

Near Infrared Spectroscopy: Proceedings of the 11th International Conference.

In 1999 the activity was transfer to ABB group, which is the leading supplier of advanced technology tools. ABB provides complete solutions allowing the intuitive management and optimization of the global refining chain. Nowadays the ABB team is based in Aix en Provence in France. Composed of 14 engineers the group is become center of excellence

Hydrocarbon identification by NIR

The Near infrared region of electromagnetic spectrum is spread from 4000cm^{-1} to 14500cm^{-1}.

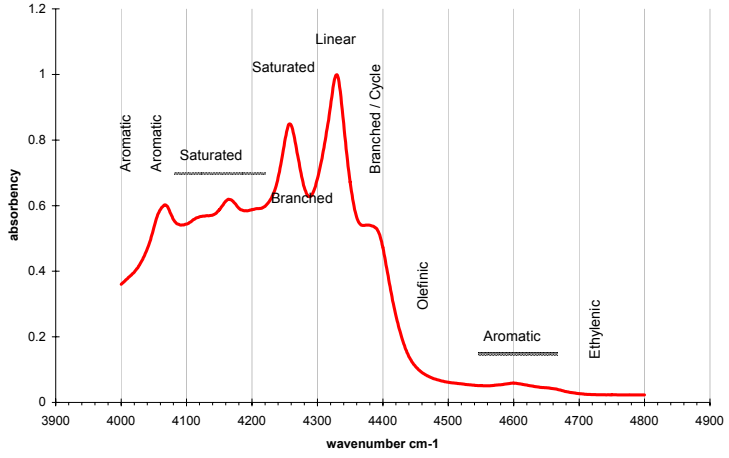
The NIR absorption is composed of a combination band adjacent to the fundamental band (MIR) and three overtones region. Our interest has been focus on the combination region where the frequencies of vibrations between the bonds of the atoms is higher than in the overtones. The region of our concerned is from 4000cm^{-1} to 4800 cm^{-1}. The spectra signal is mostly sensitive to C-H, O-H, S-H and N-H bonds.

As this is the main constituent among the hydrocarbon product, this makes the technique suitable to identify them (ex: the size of the peak is directly proportional to the amount of material present). Each component is a unique mixture of atoms, no consecutive analyzed will therefore give the same near infrared spectrum. Studies have highlighted the characterization of chemical groups and atomic environment of vibrator in function of the wavelength.

Wavenumber (cm-1)	Group
4720	Ethylenic
4670	Aromatic
4640	Aromatic
4615	Aromatic
4585	Aromatic
4485	Ethylenic
4460	Branched
4385	Branched/Cyclanic
4330	Linear
4305	Branched
4260	Saturated
4210	Saturated
4170	Saturated
4135	Saturated
4100	Saturated
4060	Aromatic
4040	Aromatic

In the table on the right side, some of the chemical characteristics or group have been identify. For each on, the wavenumber represents the region where the groups can be find.

The spectra is so a **fingerprints** of a product (Picture 1).



Picture 1. Wavelength/ wave number area.

Moreover, the NIR signal is not only sensitive to the composition of the components, but also to the physical properties such as crystallinity; crystal shape and particle size. NIR is an excellent tool for the qualitative and quantitative analysis.

The technique is rapid, accurate, and reliable and can be transfer on site.

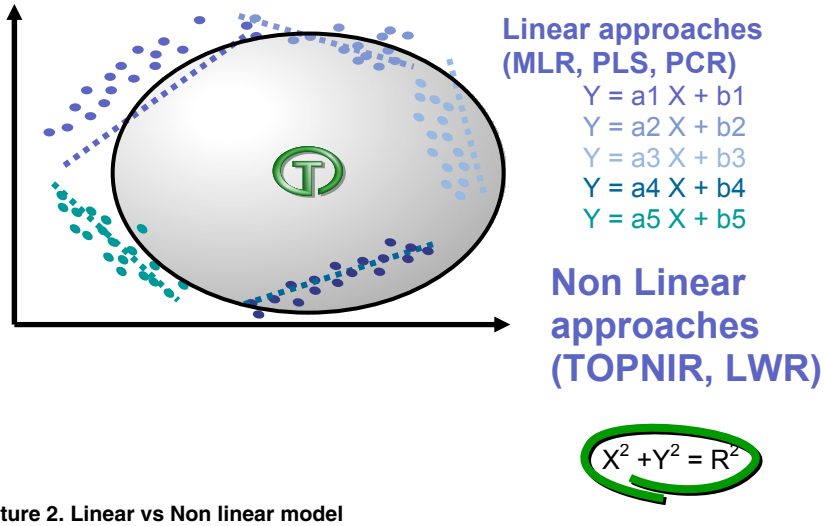
Now that we know that the spectra have an abundance of information, we need to extrapolate this absorbencies/ wavelength to obtain real products properties like MON, RON, flash point, density and so on. The main job is not yet done, the key point in the success of the implementation of NIR model rely on the use of chemometrics tools; data mining and reconciliation, discrimination and properties characterizations.

Linear versus Non linear models

PLS is the most spread technique in the analytical area. Most of the application running nowadays is using this technique. Its application is straightforward. The possibility to choose more or less latent variable, make of it a versatile tool for the representation of non-linear process. A large amount of application is running with PLS all over the world. This gives to the technique a great advantage.

However this technique has seen many limitations, among the modelling experience. To be more robust a model cannot be used for different properties. It increase considerably the size of the database if for each properties (RON, MON, density, DVPE/RVP, distillation cuts, %aromatic, % benzene, …) a model have to be calculated.

Imagine that you want to symbolize a circle by line. This will be impossible. The best you could get is by multiplying the segment by a large number. This is what happens when you want to use linear model. The number of model have to be proportional to the number of properties analyzes. The best results will be obtain by using directly an appropriate model (non linear)



Picture 2. Linear vs Non linear model

The best properties predictions with a PLS model are obtained when the unknown sample is representative of the overall database. The average of its properties must then be similar to the mean of property point used to create the model. This disadvantage is very important, cause for example anytime a sample is deviated form the mean, the model will tend to minimize this gap. The evaluation of real properties is then false.

Moreover, the maintenance of the model is heavy as it have to be re-calculated each time a new sample is use for updating.

The not satisfactory result obtain with PLS model have push the BP team to work on a new approach based on Topology techniques.

Topology

We have seen previously that the spectrum of a product allows its discrimination among other products. The spectrum is the "fingerprints of the sample". The postulate that ensues to this, around which the topology turn is that, when two samples have the same spectra, they are automatically identical. And therefore, same spectra mean that the samples have the same properties

In the topology, the principal feature of the technique is the representation in plans of the spectra. The aim of this representation is to visualize easily the sample represented by a point. Hence when each point is plot in such planes, they can be compared.

Topnir is software develop within the team to create and develop the model.

Model building

The example below described the development of a finished product model

Once the process of the refinery have been study, and after that the future analyzed products have been well identify, a series of analyzes are achieved by the refinery laboratory under the supervision of one member of our team. For the corresponding product, the conventional laboratory analyzes are obtain simultaneously with the NIR spectra (MB 160). The database hence construct must be representative of the divers change of product feed, operating condition (season campaigns), product import that will affect directly the composition and properties of the product. The number of samples does not be automatically important, from 20 samples, the model can be constructed.

The next stage is the densification of the database. This consists of filling up the database with synthetic samples by using blending laws (blending of the initial components) or inter-finished products. The size of the database grows up from 20 samples to 2000 samples. The densification has for objectives to fill up the gaps within the validation area (delimited by boxes). Then each time a new sample has to be analyzes, its spectra is compare to those enter in the database. As far as a spectra match the one of the unknown sample, therefore, the new sample can be identified.

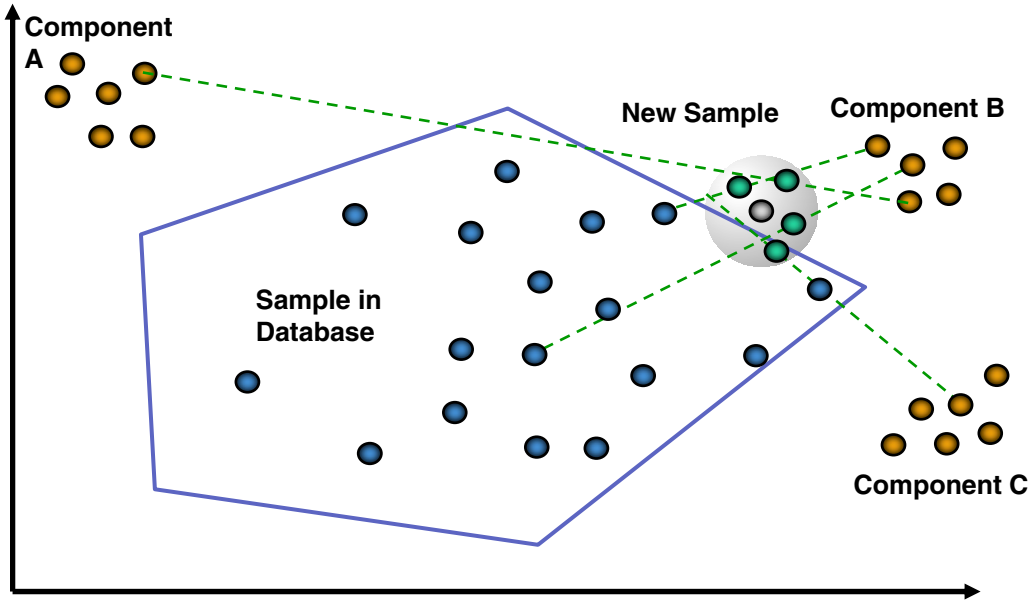
This is the theory, and as we know it is almost impossible to have two times the same spectra. Therefore, the neighborhood of the new spectra is also considered. An identity sphere is defined to delimit the range of sample to select in the neighborhood. The properties will then be calculated as a function of these neighbours. The radius of this sphere is defined in accordance with the robustness and the accuracy of the model.

If a large radius is choose, then more neighbours will be selected and use for the properties estimation. In that case, the possibility to take a non-corresponding sample is greater. The model will be robust, that mean that at any time properties estimation will be given but the accuracy of the prediction will not be good enough, Otherwise, if the radius is small the neighbour will be less numerous but their physical and chemical properties will be closer than from the unknown sample. The prediction will then be accurate; the properties guarantee according to the ASTM is one of our requirements. Too small, the radius will create instability on the prediction.

A good compromise is choosing to get a prediction of all the points that are situated within the model range and within ASTM guarantee. For the atypical point, out of the range of validity of the model, the process is push further with a second densification.

According to the postulate first enumerated, once the neighbourhood has been well defined the properties of the new point is calculated by a weight average of the properties of theses surrounding points.

The weights are defined following the specificity of the wavelength to the properties estimated.



Picture 3. Real time densification

Real time densification

In order to improve the prediction with the neighbourhood, a second densification is made. This time, it is achieved in real time. Once a new point is projected in the spectral plans, its closest region is fill up by virtual point that are obtained with the blending of components sample. This second densification can be used either or not the point is within or out of the validity range. The figure above shows this process:

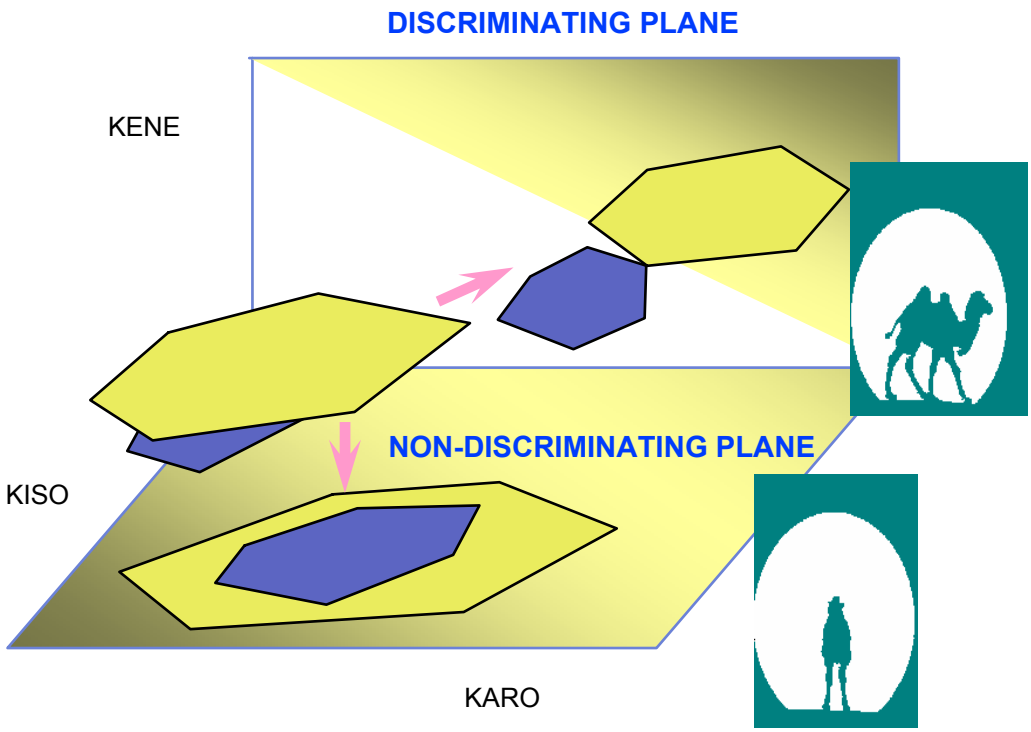
A new sample is plot and appears to be out of the validity area. Then, one points from each component A, B and C is taken. A new blend is then achieved that will be plot within the identity sphere. This process will fill up the sphere and generate enough neighbours to allow good properties predictions.

As we can see the representation of the spectra to one point per aggregates plan is very important. One of the main work, is to determine which plan will be the more suitable to represent the family of hydrocarbon analyzed. This is achieved in discrimination work.

Discrimination

The discrimination is used in all model work to allow the identification of the analyzed samples. This distinction has to be done in an efficient manner that each time a new sample is analyzed (out

of the set of validation or calibration) it appears in the good area, within its homologues. Axes called aggregates delimit the discrimination planes. These aggregates are very specific, as they are



Picture 4. Aggregates discrimination

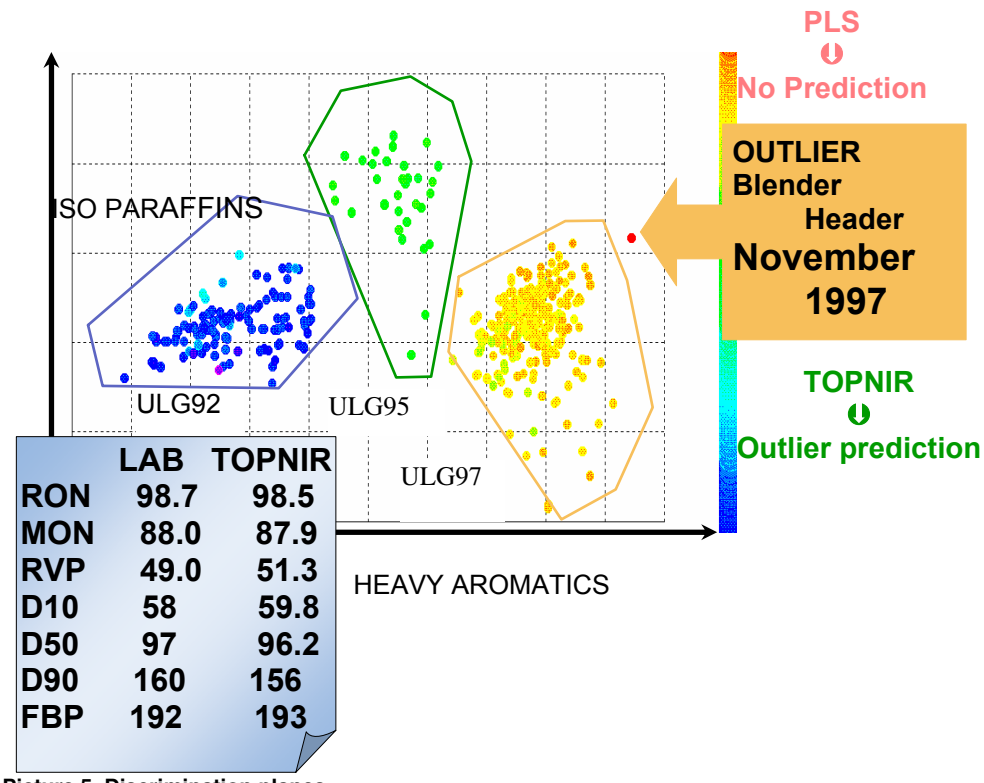
representative of physical and chemical characteristics. We must not forget the chemistry behind the spectra, and therefore, laboratory analyzes have been carrying out to determine within the spectra, the area that are marker of for example the aromatic characteristics, the unsaturated or saturated components, etc… (Confer table above in the second page)

So each axes delimited an affinity to a particular chemical characteristics. These aggregates allow us to define an average of four plans per models (product) that discriminate the family of sample. A good discrimination gives us a good identification (Picture 5)

Conclusion

A topology method has been applied to NIR spectra on petroleum refining product. It has been proven that the NIR is of good performance within the hydrocarbon product and the advantage bring by this method are very attractive to the refiners people, as the technique allow a large number of analyzes with a minimum of time, minimum of cost and with a high accuracy. The continuous improve in technology, better quality of optic fibbers, analysing cells, NIR detector and source will help and enhanced the success of the technique that require very accurate analyses. The implementation of such technology within the advanced process control of a petroleum refinery has

been done and succeeds. Nowadays many applications are running within the world in many fields (From the CDU.



Picture 5. Discrimination planes.

Some of the worldwide application:

- Petronor Spain (Gasoline blender),
- Aramco Yanbu (CDU),
- Sasol South Africa (Gasoil Blender),
- Copene Brazil (Steam cracker),
- and many other