REFORMER MODEL-BASED INFERENTIAL PROPERTIES EMBEDDED IN APC

A major European Refiner has implemented Aspen Technology's Reformer inferred Property Package for control and optimization of their Catalytic Reformer in two of its refineries. This article highlights the methodology of execution and the benefits derived.

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Introduction

A major European Refiner is continuing working with AspenTech looking for new and promising areas to install Advanced Process Control applications and enhancing the around 50 existing applications to help improving refining margins.

Improve the usage of rigorous Models in Operations to help achieving more accurate and reliable process units quality control, is one of the areas that has been identified. This covers both open loop advisory systems area and closed loop control and optimization area.

Reformers are nowadays, in current low gasoline market scenario, even more important than in the past because of the general lack of hydrogen in Refineries and the need to often run these units either to balance gasoline or hydrogen production.
Reformers maybe operated in many different ways depending mainly on process type (continuous or semi-regenerative), market scenario and specific refinery or aromatics complex setup. RON always plays an important role: it can be a minimized till a limit to ensure proper gasoline blending, maximized to maximize hydrogen production or an optimal target to trade off with catalyst life in semi-regenerative units.
It's rare that a proper RON on-line analyzer is available in Reformers and almost never happens that information related to other properties, like coke lay down rate, is made available real time to Operations that normally rely to very infrequent Lab analysis. Not to mention the fact that important constraints like skin temperatures are often unreliable or no more available after some run time.

Some Process Licensors provide tables and correlations on their manuals and occasionally proprietary code is deployed on-line to estimate some Reformer constraints like RON. This code is a black box, difficult to maintain, tuned on a specific catalyst and not based on a commercial and open simulation tool. This code becomes unusable after changes in the process, like a secondary air added in the Regenerator tower, or the catalyst vendor changes.

This area is also non-core business for Process Licensors and these black box applications tend to be poorly maintained.

This major European Refiner decided to develop, first for one Refinery and then, given the good results obtained, also for a second Refinery, accurate, reliable and easily maintainable model based inferentials on the CCR (Continuous Catalytic Reformer) units.

Process Operations and Constraints

The Refinery CCR is equipped with a DMCplus multivariable predictive controller that in current scenario pushes the unit against constraints (basically furnaces metallurgy) maximizing feed while guarantying a minimum RON in the Reformate i.e. in the Stabilizer bottom stream.

Most active constraints in the DMCplus application are:

1. Reformate Naphtha Octane Number (RON)
2. Coke Deposition on Catalyst
3. Maximum tube skin temperatures
4. Hydrogen to hydrocarbon ratio in reactors

The Refinery is quite complex with many units that influence the H_2 and the gasoline pools.

A less than max Reformer feed or a too low or too high RON would result in an extra cost or reduced profit coming from more expensive hydrogen used in conversion and desulphurization units, suboptimal solution compared to the one coming from Refinery planning, or gasoline blending extra costs possibly because of the extra MTBE needed in case of a too low RON or simply because of a different-than-planned blending receipt in case of a too high RON.

Solution Description

Inferentials, based on rigorous models (Aspen HYSYS Reformer and related tools), have been developed for:

- Reformate Naphtha Octane Number (RON), WAIT, WABT

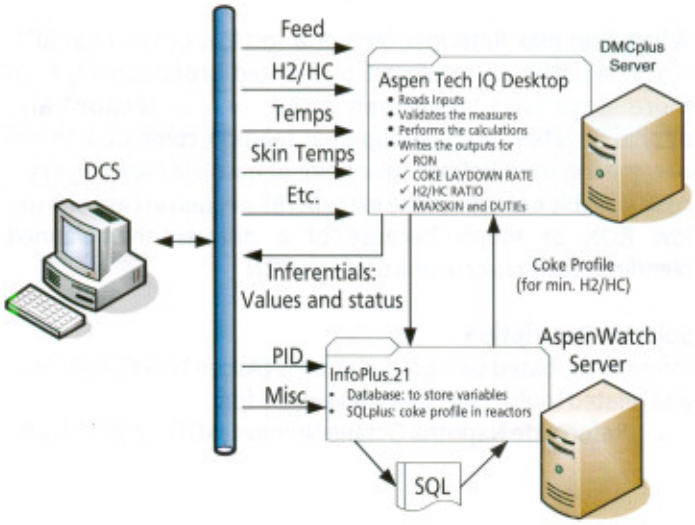
- Coke Laydown Rate (kg/h)
- Coke on catalyst (wt%)
- Coke profile in reactors
- Duties of furnaces
- Skin temperatures
- Minimum Hydrogen to Hydrocarbon ratio

The Solution development major steps are:

- Calibrate Aspen HYSYS Reformer rigorous model off-line using unit test run data
- Run case studies (4000+ cases) to exercise model over complete operating range
- Analyse model responses and build quadratic inferential models to be deployed on-line trough Aspen IQ (AspenTech tool to build and deploy inferentials on-line) and used as controlled variables within DMCplus application
- Periodically (e.g. once per year) recalibrate model to represent long-term catalyst activity decline and any other process change that may be implemented

The rigorous model is not directly deployed on line and quadratic correlations are derived instead and deployed trough Aspen IQ, the AspenTech software to build and deploy on line inferential properties.

Aspen IQ has been selected as the best solution because it's robust, open and configurable, automatically interfaced to DMCplus application, it provides the capability to condition data and validate all input measures and output calculations for range, spikes and freezing. Aspen IQ can also manage laboratory or analysers bias update.
The Rigorous Model could be deployed on-line and this is actually an area being investigated to assess additional benefits that could be obtained, but the above solution, based on standard and configurable field proven tools, as been regarded as the one that better fits Refinery current needs.



Rigorous Model on line deployment would open the way to a truly adaptive inferential, given the fact that the recalibration of the model could be automated.

The following Figure describes the overall architecture deployed on line.

Rigorous Model

The Aspen HYSYS Reformer model is based on fundamental kinetics and it's integrated with HYSYS fractionation/heat exchange models providing this way a full flow sheet model which is represented in the Figure below.

Both Continuous (CCR) and Semi-Regenerative (SRR) Reformers can be modelled.

Some of the main features of the model developed are:

- Detailed feed characterisation
  separate responses have been analyzed for Feed Naphthenes and Aromatics content and not simply N+2A content
- Rigorous reactor model
  response against average bed temperature (WABT) have been analyzed and not simply inlet temperature (WAIT), obtaining this way more representative responses
- Rigorous heat balance
  "Heat sink" effect of recycle gas is modelled giving realistic Hydrogen/Hydrocarbon ratio response

Inferentials development

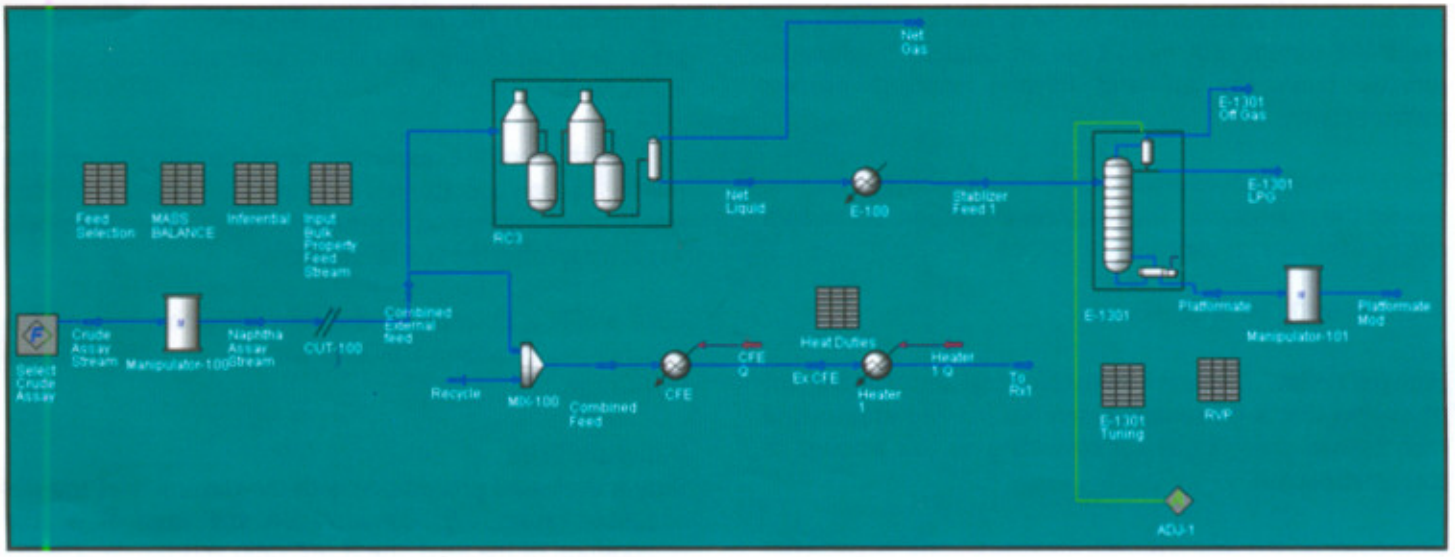
WAIT and WABT

Weight Average Inlet Temperature (WAIT) is calculated as follows:

$$WAIT = \frac{T_{IN}^{(R1)} * CW^{(R1)} + T_{IN}^{(R2)} * CW^{(R2)} + T_{IN}^{(R3)} * CW^{(R3)}}{CW^{(R1)} + CW^{(R2)} + CW^{(R3)}}$$

where T_{IN} (for R1, R2, R3) represent the inlet temperatures of the three reactors and CW the catalyst weights.
The Weight Average Bed Temperature (WABT) based on reactors Average bed temperatures ($ABT^{(R2)}$), is calculated as follows:

$$WABT = \frac{ABT^{(R1)} * CW^{(R1)} + ABT^{(R2)} * CW^{(R2)} + ABT^{(R3)} * CW^{(R3)}}{CW^{(R1)} + CW^{(R2)} + CW^{(R3)}}$$



RON

RON is inferred based on the following process measurements:

- Rxj Inlet Temp
- Rxj Outlet Temp
- Feed Rate
- H/HC Ratio
- Separator Pressure
- Catalyst Circulation Rate
- Feed Naphthenes
- Feed Aromatics
- RVP specification (Reid Vapor Pressure)

The average bed temperature for each reactor is calculated as reported above using the Rxj measures and RON is then inferred based on a quadratic correlation and using these average bed temperatures and all other measures reported above.

The correlation actually uses for all measures both linear and quadratic terms.

Coke

Both coke laydown rate [kg/h] and its amount on catalyst [w%] have been calculated based on both the reactor and the regeneration operative conditions.

A coke profile in the reactor has been also calculated depending on the occasional event of not burning completely the coke in the regenerator and thus not regenerating completely the catalyst. This profile is used to evaluate the maximum amount of coke deposition in the reactor to be used to set the minimum hydrogen to hydrocarbon ratio. In other words the minimum H_2/HC ratio is calculated in order to avoid excessive coke on catalyst entering the regenerator.

It is well known that a full catalyst cycle trough reactors-regenerator is as long as 8 or 10 days but Regenerator section (i.e. CCR section of the Reformer) can stop for long time while Reformer keeps running and this events have then to be properly managed.

Current Coke Laydown Rate (i.e. the rate in kg/h at which coke is laying down on the catalyst) and the resulting equilibrium coke on catalyst (w%) are inferred based on the same process measurements used for RON (obviously apart RVP) plus Naphtha feed boiling range information and using a similar linear and quadratic correlation.

The current Coke Laydown Rate (kg/h) inferred represents the spot coke laydown rate. If the same feed and operating conditions are maintained for a complete catalyst cycle then this would represent the equilibrium coke on catalyst (w%) entering the regenerator. The regenerator entry point is where the catalyst samples are taken and then analyzed.

The catalyst cycle through all reactors in this Refinery is approximately 8 days and during this period feed quality and operating conditions normally change many times. Use then laboratory results to update this inferential would be incorrect.

Nevertheless the coke on catalyst can be calculated as:

$$Coke_{w\%} = \frac{Coke_{kg/h}}{CatalystCirculationRate_{kg/h}} \cdot 100$$

We could call the above properties equilibrium Coke Laydown Rate and Coke on Catalyst.

The actual Coke Laydown Rate to the regenerator (kg/h), and hence the current spot (w%) Coke on Catalyst, is calculated directly from the air and oxygen content process measurements.

The calculation is based on an overall mass and oxygen balance around the regenerator. The combustion reaction, assuming a chemical formula for coke equal to CH_x, is:

$$4 \cdot CH_x + (4+x) \cdot 0_2 \Leftrightarrow 4 \cdot CO_2 + 2x \cdot H_20$$

With the air flow measures it is possible to calculate the amount of oxygen that is consumed during the burning process and then burned coke (kg/h) corresponding to this amount of consumed oxygen.

Once obtained the coke laydown, the coke on catalyst (w%) can be calculated with the equation reported above.

H_2/HC ratio

The minimum hydrogen to hydrocarbon ratio, that guarantees to maintain the coke deposition over catalyst within limits, has been also calculated. This is actually the minimum hydrogen to hydrocarbon ratio that permits to maximize reformate yield while respecting the coke on catalyst constraint in regenerator capacity.

Both Reactor and Regenerator operations affect the minimum hydrogen to hydrocarbon ratio because the coke deposited over the catalyst depends on the operative conditions of the reactor but also on the coke that passes through the regeneration section without burning.

It's very important taking into account the event of coke not burning in the regenerator because of a CCR failure and passing trough, to avoid underestimating the minimum H_2/HC ratio.

Figure below reports 3 different cases that explain what happens when Regenerator Tower shuts down.

In normal operations (A) the coke deposited in the reactor is totally burned in the regeneration section, therefore the coke on catalyst depends only on the reactor operative conditions: a uniform deposition of coke along the reactor can be assumed in this case.

If the regeneration tower fails to burn completely the coke (B), a slice of catalyst not completely regenerated enters the reactor. When the regeneration tower is again operative (C), the coke is completely burned and the catalyst fully regenerated again. However the slice of catalyst covered by coke is still in the reactor, slowly moving and generating a "coke profile".

The minimum H_2/HC ratio calculation takes into account the presence of the moving coke slice to avoid underestimating the H_2/HC ratio.

Without this accurate calculation, when the coke slice exits the reactors section operator has to reduce the catalyst circulation rate to avoid an overload of the regeneration tower. This would happen days after the CCR failure event.

Coke profile is described and monitored within the solution continuously providing DMCplus with an accurate minimum H_2/HC ratio.

Duties and Skins

Duty is evaluated process-side with the classical heat transfer equation taking into consideration the mass flow, the composition of the feed, the H_2/HC ratio and the delta in I/O temperatures.

Skin temperatures are inferred by adopting the Standard API-530 method, where the radial component of the heat flow is calculated together with the transfer heat coefficients in bulk, fouling and across the tube describing this way the temperature profile from the inner part to the skin of the tube itself.

This certified methodology it is not straightforward to implement and requires a detailed knowledge of furnace geometry and metallurgy and also of products thermodynamic properties, but permits to safely use inferred skin temperatures as closed loop controlled variables.

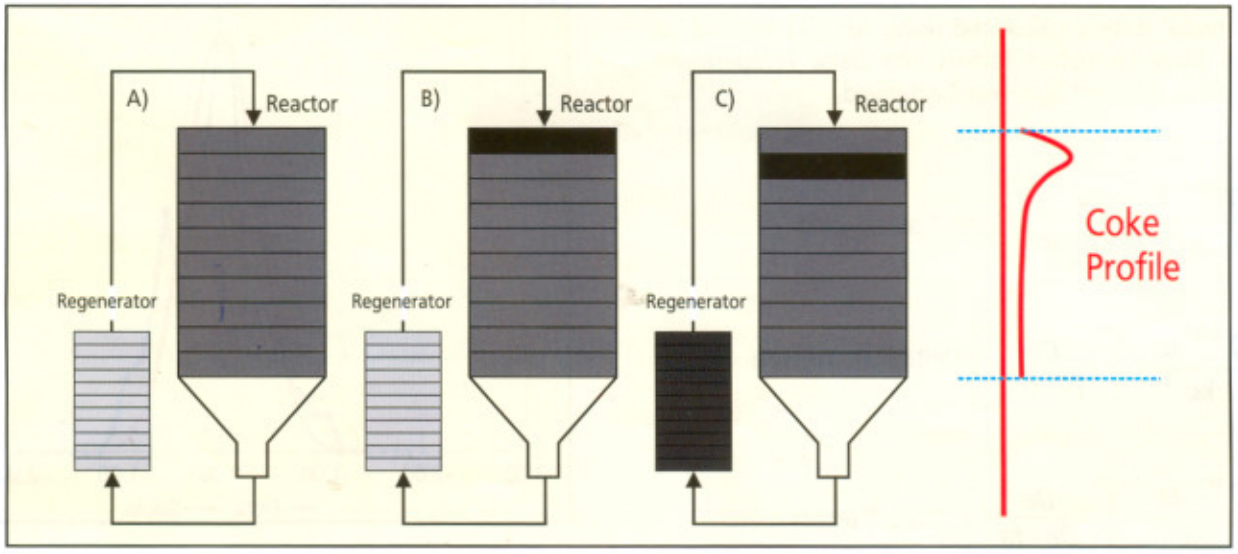
The products affecting heat exchange are naphtha and hydrogen, in a mixture in vapour phase, and also coke deposited along the walls of the tubes.

The thermodynamic properties which are required for naphtha and hydrogen are: Specific Heat, Viscosity and Thermal Conductivity while for coke the only needed property is Thermal Conductivity.

All these properties have been calculated using the Rigorous Model and then building accurate correlations; function of pressure and temperature, to be deployed on line.

Heat transfer coefficients have been calculated according to API-530 as function of Reynold (Re) and Prandtl (Pr) numbers:

$$h = f\left(Re, \mathrm{Pr}, \frac{\mathrm{Tb}}{\mathrm{Tw}}, \frac{\mu b}{\mu w}\right)$$

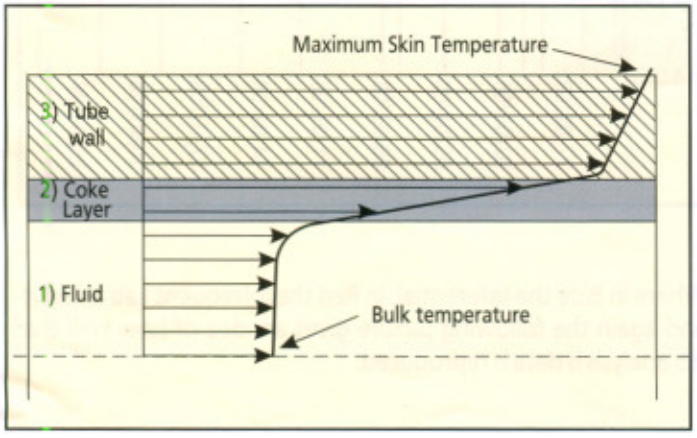


Where:
Tb, μb represents respectively the bulk temperature (coil outlet temperature) and bulk viscosity

Tw and w represent respectively the temperature of the fluid that is in direct contact with the coke layer and its viscosity
It has to be noted that Tw is unknown and it has to be found through an iterative process that has been easily implemented on line.

The temperature profile across tubes is defined by the three layers described in Figure below.

1. the fluid as mixture of naphtha and hydrogen
2. the coke layer
3. the tube wall



The duty generated in the furnace must be decomposed in an axial duty flow and radiant duty flow; therefore the global generated duty is multiplied by corrective factors: FC a factor accounting for circumferential heat flux variations; FL for longitudinal heat flux variations; FT to take into consideration the effect of tube metal temperature on the radial heat flux.

$Q^{RAD}=DUTY \cdot F_C \cdot F_T \cdot F_L$

Once the radial duty is calculated using API-530 method to obtain the three correction factors, the Delta Temperature across the three different layers can be derived.

$$\Delta T_f = \frac{Q^{RAD}}{h} \cdot \left[\frac{De}{Di - 2 \cdot tc} \right]$$ Delta T across fluid

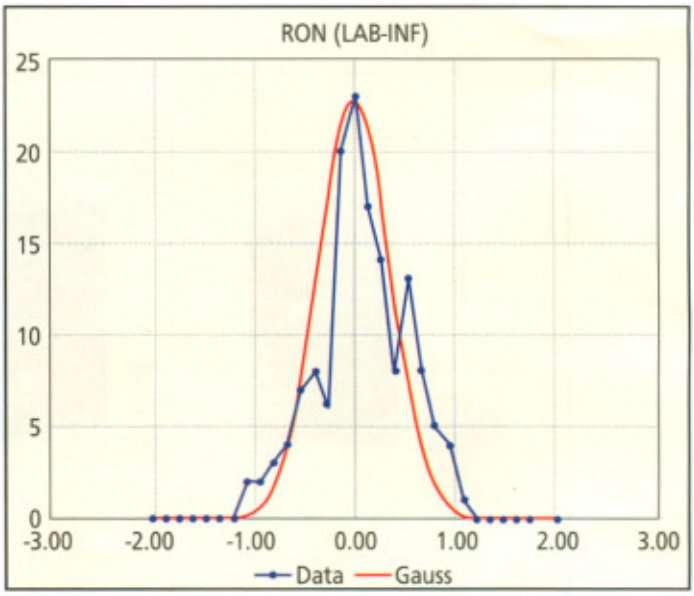
$$\Delta T_c = \frac{Q^{RAD} \cdot tc}{kc} \cdot \left[\frac{De}{Di - tc} \right]$$ Delta T across coke

$$\Delta T_m = \frac{Q^{RAD} \cdot ta}{kw} \cdot \left[\frac{De}{De - ta} \right]$$ Delta T across metal

where:
De and Di are external and internal diameter of the tubes
tc is the coke layer thickness
ta is the tube thickness
kc and kw the thermal conductivities of coke and metal respectively
The maximum skin temperature can be then calculated adding the above ΔT's to bulk temperature.

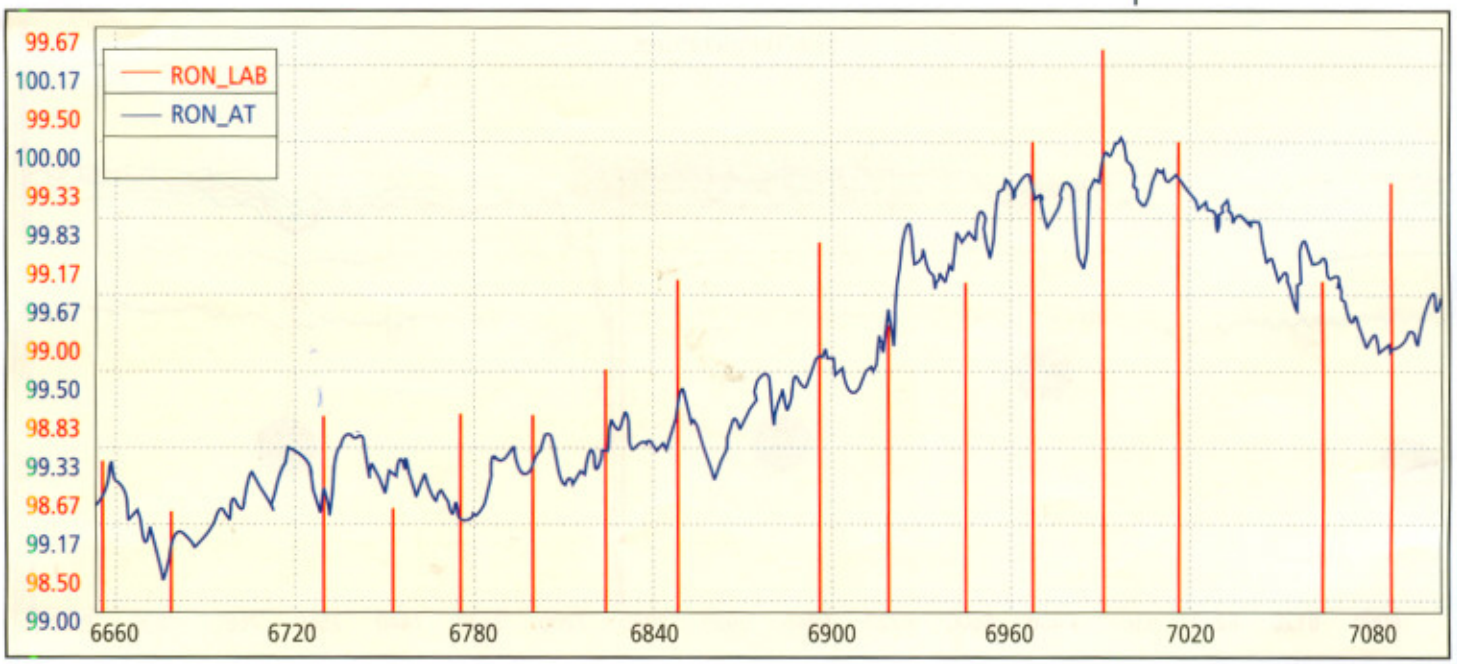
Results
In the following some of the results obtained are reported.

RON
- 1 year data (2008)
- 160 lab analysis,
- 11 outliers (plant shutdown-startup),
- 149 used samples



Coke
- 1 year data (2008)
- 97 lab analysis,
- 6 outliers (regeneration tower OUT),
- 86 used samples

Where in Blue the Inferential, in Red the infrequent Lab analysis and again the following picture gives an idea of how well the lab analysis is data is reproduced.

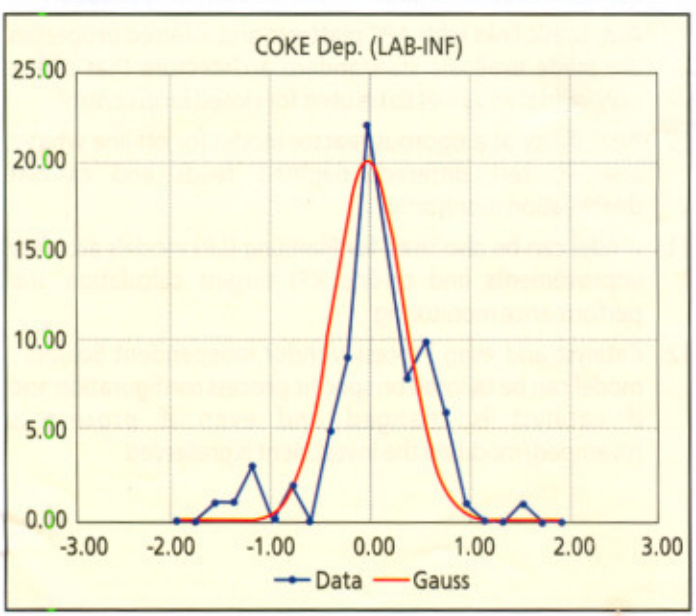


Where in Blue the Inferential, in Red the Infrequent Lab.

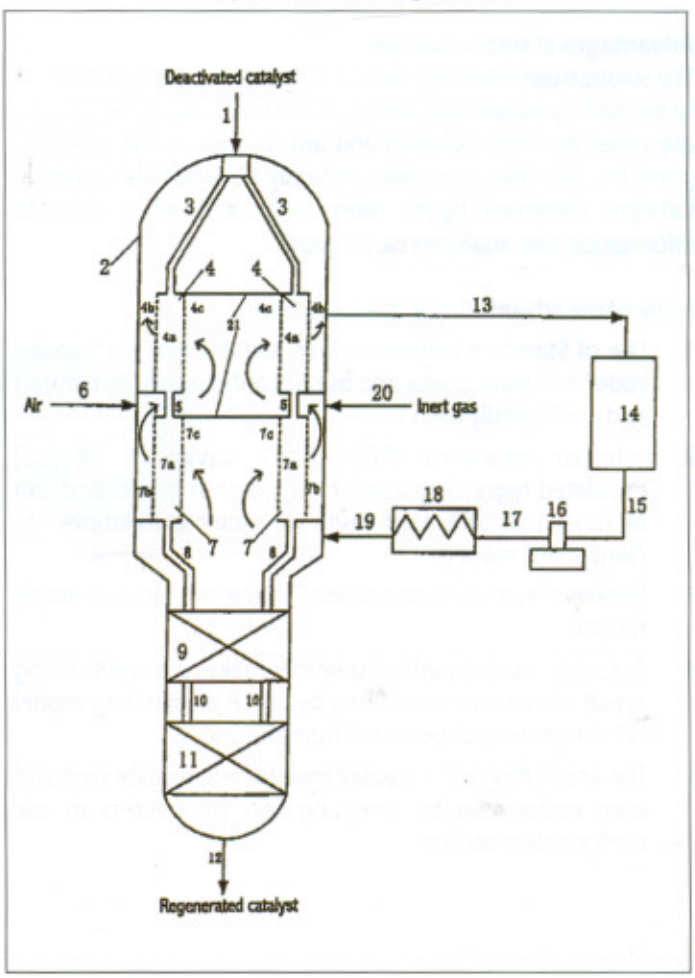
The Process Licensor correlation was based mainly on the WAIT measure and the N+2A feed analysis was required to update the measure (this analysis is performed once per week) to take into account the feed quality changes.

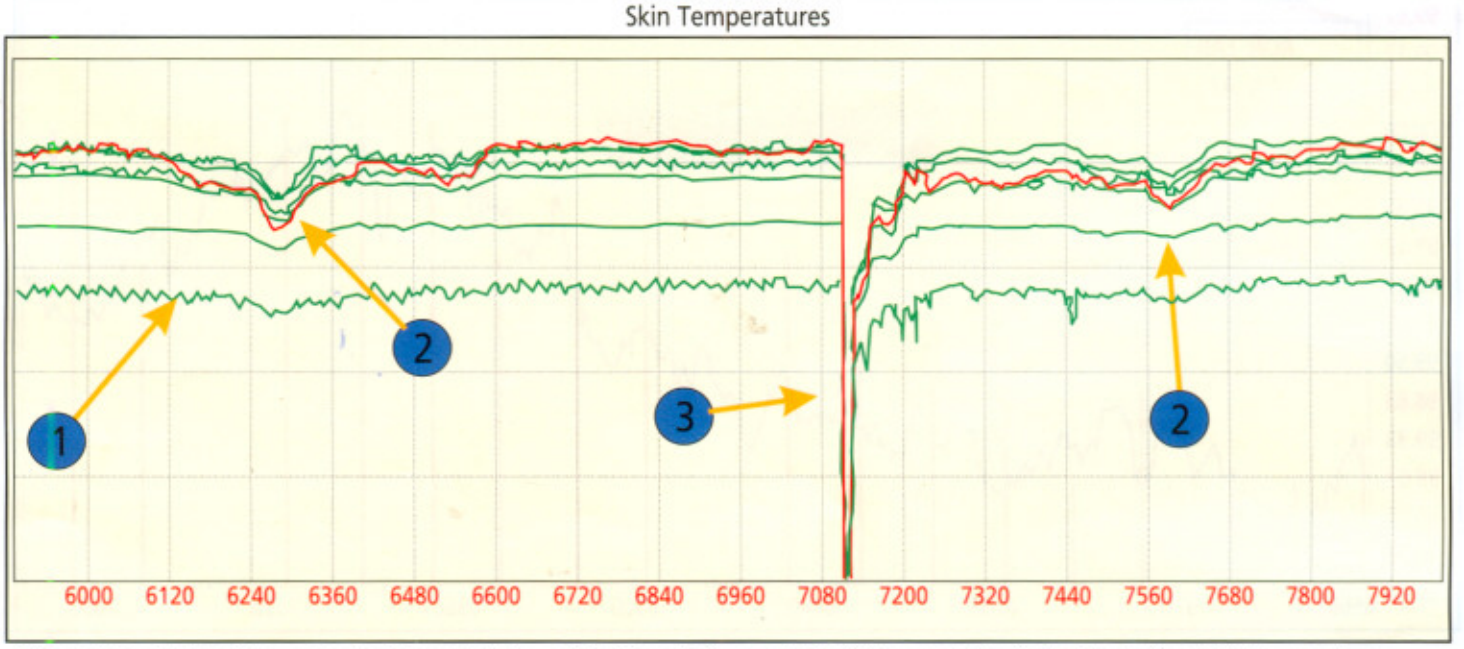
The blue line RON inferred measure takes into account the feed quality changes, by including in the calculation the WABT, which is a measure of the reaction progress.

The following picture gives an idea of how well the lab analysis data are reproduced: 99% of the data falls within ± 0.45 range and the official lab analysis ASTM reproducibility is ± 0.70.



Catalytic Reformer regenerator





1.Green lines: installed thermocouples (low reliability, particularly with furnace in End Of Run conditions); Red line: inferred skin temperature
2.Change in Process operative condition: inferred measure was responding properly, following the most reliable thermocouples indications
3.Plant shut-down: during start-up the inferred measure followed the thermocouples signal

Similar impressive results have been obtained for H2/HC ratio, Duties and other estimated properties

Advantages of such a solution

The solution described in previous sections and deployed on line to be used by closed loop DMCplus control, is by far superior to any other available Solution and also to any on-line analyzer, given the fact that it provides not only RON but also Coke on Catalyst, minimum H_2/HC ratio, Skins and other accurate information that analyzers can't supply.

Some of the advantages of this Solution are:

1. Use of Standard Software: open architecture, no "hidden code" nor black boxes and use of configurable, integrated and user friendly tools
2. Inferred measures (RON, Coke Laydown, Skins...) calculated regressing a Reformer rigorous model that can be tuned and calibrated easily. No simple correlations nor "simplified" models
3. Detailed feed characterization in the model (not simply N+2A)
4. Accuracy in constraints calculations makes it possible riding actual constraints as defined by an LP or blending model i.e. obtain the true potential from the unit
5. The application can be easily maintained, recalibrated and even customized by changing few parameters in the configuration section
6. The deployment on-line is made trough a standard and field-proven tool that provides validation for both input and output signals guarantying a safe DCS interfacing
7. The operator interface used for on-line deployment is standard, web based, auto-configurable, i.e. does not need any effort to be maintained and modified in case of application changes: it reads the configuration files and updates automatically
8. Inferred measures updates with lab analysis or analyzers to correct bias are embedded in the web based application
9. Automatic links with APC platform and inferred properties are made available via standard architecture that allows only validated values to be used for closed loop control
10. Availability of a rigorous reactor model for off-line what-if analysis, test different naphtha feeds and catalyst deactivation monitoring
11. Model can be also used for Planning (LP) models accuracy improvements and on-line KPI targets calculation and performance monitoring
12. Catalyst and even Process Vendor independent Solution: model can be tailored on specific process configuration and if catalyst is changed and even if process is revamped/modified the investment is preserved

Benefits

The benefits related to more accurate, reliable and real time information on quality depend on the use that is made of such information. Certainly using RON, Skins, H_2/HC, Coke Laydown as controlled variable within a DMCplus application that is designed to continuously push the unit, permits to make the best use of such information.

Obtainable benefits obviously depend also on market scenario, the way Reformer is operated and specific Refinery constraints.

Nowadays H_2 cost is well above 1000 €/t and a less than max H_2 production from a Reformer because of constraints, like skins or coke, not truly represented can result in huge profit losses from Hydrocracking or Desulphurization units.

Just 200 kg/h H_2 not available for Refinery conversion and desulphurization units could mean more than 2 M€/y loss.

The gasoline pool plays a role even in current diesel oriented market, because gasoline is one of crude cuts and has to be sold.

Being able to run closer to a RON target, minimizing giveaway, permits to avoid downgrading too much Gasoline to LPG.

On the other side, a too low RON leads to the need of more expensive blending receipts and mainly to an increased consumption of MTBE. Typical savings, even if strongly depending on specific Refinery layout and blending pool, could range from 0.5 up to 1.5 M€/year for each Reformate RON point.

It has been verified that efficient Reformer inferentials embedded in a closed loop application led to a feed increase of 3.7% in the Refinery were the project was first executed.

These came with:

- Increased H_2 production being able to push truly represented constraints
- Reduced RON giveaway
- Reduced MTBE consumptions
- Better CCR temperature profile

In a SRR, Semi Regenerative Reformer, where Catalyst Life Cycle is driving operations having accurate RON and Coke, i.e. catalyst life, estimates is even more important and benefits can be much higher particularly in a pro-Aromatics Reformer. This because Reformer severity is normally maximized, pushing feed and/or RON depending on market, but making sure to maximize profit true the all catalyst cycle, avoiding on one side to get end of cycle without full capacity, and on the other side to leave end of cycle some capacity on the table.

Conclusions

The proposed application for Continuous and Semi Regenerative Reformer inferentials, developed with a rigorous model and deployed on line true a standard field proven tool, is by far superior to any other solution currently available. It is based on open architecture, accurate, reliable, easy to configure and maintain. The investment is always preserved also in case of process or catalyst changes.

The use of such inferentials in closed loop control applications permitted to obtain additional benefits, if compared to poor estimates, and repay the investment in just a few months.

The availability of a rigorous Reformer model permits also to use it for other purposes like what-if analysis and test different feed types, maximizing this way the investment.

The next step is deploy on-line directly the rigorous model and move to a truly adaptive inferential..

About the authors

Stefano Lodolo is Senior Advisor and Industry Consultant with Aspen Technology in Italy. He has around 25 years field experience in Advanced Process Control in Refining, Chemical and Petrochemical industry. Stefano has successfully implemented tens of MPC and other automation projects and he holds a master's degree in Chemical Engineering for Bologna University, Italy.

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