HYDROCARBON ENGINEERING

June 2014
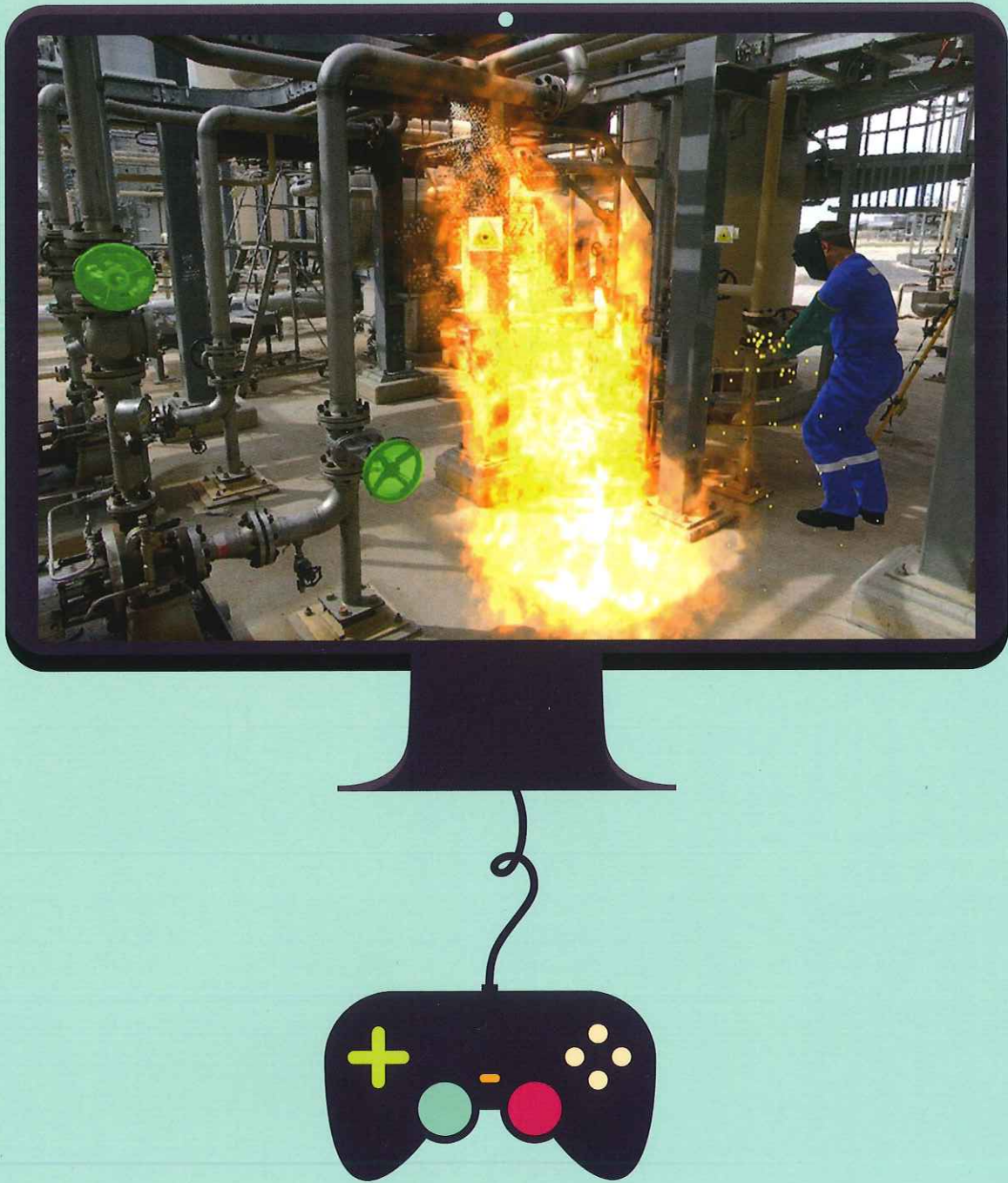
contents

June 2014 Volume 19 Number 06 ISSN 1468-9340

THE POWER OF SOFTWARE ANALYSERS

Gregorio Ciarlo, Federico Callero and Maurizio Simonelli, ABB SpA, Italy, discuss the application of predictive emission monitoring systems for applications in which fuel characteristics are variable or in a complex process plant.

Continuous acquisition of emission data is a standard, legally enforced requirement for the process industry to monitor and control the pollutants released into the atmosphere and to verify that plant emissions do not exceed the thresholds defined by the regulations.

From a plant owner's perspective, the availability of efficient and reliable tools for the acquisition of emission data is of paramount importance as environmental constraints can affect production. Additionally, if a plant fails to provide emission values for extended periods, environmental authorities may impose plant shutdown.
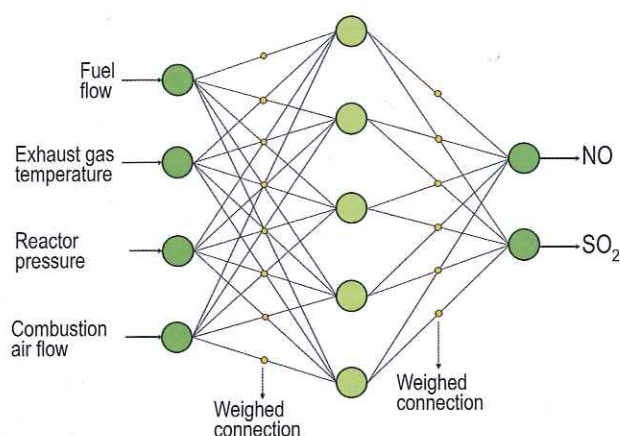
Figure 1. Artificial neural network schematic.

The traditional solution employed by the industry to comply with the legislation is hardware based continuous emission monitoring systems (CEMS); such systems normally comprise analysers (to sample and identify the compositions of released flue gas) and an IT infrastructure (to manage, record and store the emissions values).[1]

Artificial intelligence (AI) offers an alternative to hardware based analytical solutions for measuring and recording air pollutant emissions that is recognised and accepted by most of the environmental authorities.[2] Predictive emission monitoring systems (PEMS) are an innovative technology able to estimate emissions on the base of the values of relevant process parameters to an accuracy comparable with hardware instrumentation. Depending on local regulation, PEMS usage is permitted as:

- A back up to traditional CEMS to increase the availability of emissions data (applies to most European countries).
- A primary source for emission monitoring (applies to US and the Middle East Area).

This article describes a successful application at a major European refinery, where a PEMS was introduced to act as a back up to the traditional analysers, providing an estimate of the emissions from two very complex processes: the fluid catalytic cracking (FCC) and sulfur recovery units (SRU).

PEMS technology

PEMS are software based technologies developed to estimate pollutant concentration through advanced mathematical models. Given their capability to provide the same information as analytical instrumentation, they are also defined as software analysers.

Modelling techniques can be divided into two main categories:

- Fundamental modelling that relies on first principles (for example, conservation of energy/mass and thermodynamics laws).
- Empirical (sometimes referred also as data driven or inferential) modelling that exploits the capability to extract significant information from historical process data (for example, pressure, temperature and flow) and reconstruct the behaviour of the estimated property (the pollutant emissions).

Within these two categories, inferential techniques have proven to be the most effective in creating reliable models

able to estimate emission values accurately. Advanced modelling techniques (for example, multi linear regressions (MLR), artificial neural networks (ANN) and genetic algorithms) are the typical tools behind data driven predictions.

ANN (Figure 1) in particular provides the flexibility needed to optimise the balance between performance and robustness of the model.[3]

A challenging yet successful implementation

In order to enhance the performance of the existing monitoring system and not to be forced to reduce plant production due to emission related issues, the customer, a major European oil refinery, chose to install PEMS to back up traditional CEMS in two fundamental areas of their refinery: fluid catalytic cracking (FCC) and sulfur recovery units (SRUs).

These plants are crucial from a production perspective but also play a substantial role in emissions production. To make matters worse, their operations (that include the treatment of acid and other environmentally hazardous compounds) sometimes have adverse effects on CEMS equipment.

The customer had two main requirements:

- To increase the uptime of the analysis system to above 97.5%, enabling them to comply with the requirements in terms of the availability of the emissions data.
- To reduce the necessity, imposed by regulation, to engage a third party company to monitor emissions continuously when the CEMS equipment was offline.

The predictive system was designed to provide a redundant measurement of key pollutant components:

- SO_2.
- CO.
- NO.
- O_2.
- Flue gas flowrate.
- Particulate.

Process overview

FCCs can be considered the 'heart of modern refineries' as it is there where the heavy hydrocarbon feeds are upgraded to lighter and more valuable products, generating most of the gasoline in the refining process.[4]

A cracking plant comprises two key subunits:
- The reactor: where heavy compounds are broken down in the presence of a catalyst (typically zeolites).
- The regenerator: where the coke deposited on the catalyst during the cracking process is burned off in order to recycle the catalyst.

It is the regenerator that is responsible for most of the emissions from FCC units.

SRUs are very complex processes designed to remove and recover sulfur from refinery exhaust gases before their release into the atmosphere.

They are important from both profitability and environmental compliance perspectives:
- Profitability: SRUs are able to recuperate up to 99.9 % of the sulfur (a valuable product) that can then be sold on the market.
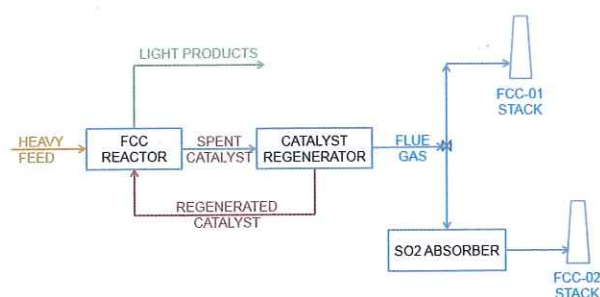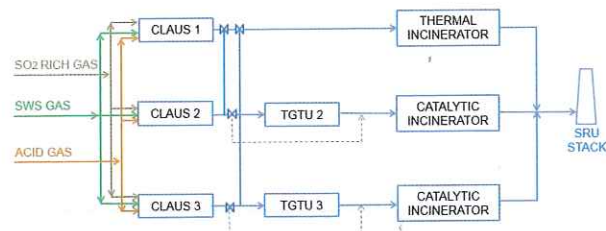
Figure 2. Layout of the FCC and absorption units.
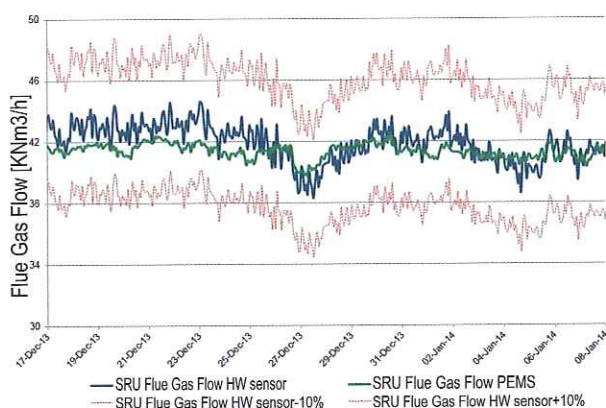

Figure 3. Layout of SRUs.

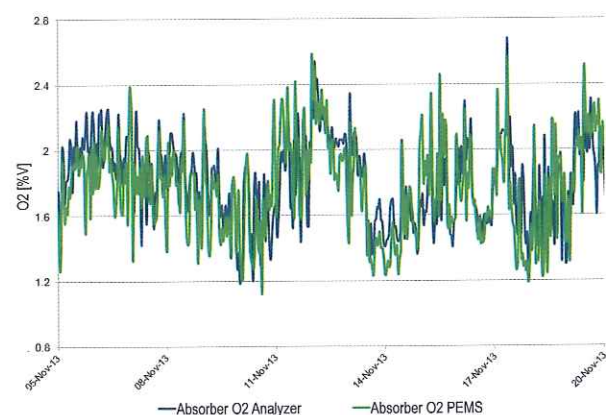**Figure 4.** Comparison between PEMs and CEMs for SRUs flue gas flow.

Figure 5. Comparison between PEMS and CEMS measurements of O_2 from the absorption unit.

■ Environmental compliance: SRUs transform the residual H_2S into SO_2, a much less harmful compound that is tolerated by legislation.

Sulfur recovery is normally accomplished through several treatment stages designed to reduce final sulfur content below the limits imposed by regulation. The Claus process, tail gas treatment unit (TGTU) and final incineration are typical subprocesses within a SRU.

Plant layout at refinery site

At the customer's site, the FCC and SRU plants have undergone a series of upgrades and modifications, enlarging the number of units involved to increase refinery capacity and to limit the impact of emissions.

Downstream of the traditional FCC unit, a patented absorption process with its own stack (FCC-02) was commissioned to reduce the SO_2 released into the atmosphere (Figure 2). A valve can be positioned to divert the exhaust gas from the cracking unit to the absorber or directly to the previous stack (FCC-01).

The SRU comprises three, parallel desulfurisation trains, each characterised by different treatment technologies and process units. The trains are equipped with a number of bypass valves that enable the process gas to be diverted among them as required (Figure 3). Each train comprises a Claus process that is largely identical. However, the second and the third trains are each equipped with different, patented downstream TGTUs and the final incineration stages for each train are not identical; the first train has a thermal incinerator but trains two and three use a catalytic process with a higher sulfur removal capacity.

The SRU is fed with the gases from the different refinery treatments and production units. The composition and ratios of these gases are neither well known nor fixed over time: essentially, the feed comprises three H_2S, CO_2 and NH_3 rich streams of variable concentration.

Relevant challenges

The plant layout and the complexity of the different processes involved presented significant engineering challenges to the development of an effective PEMS solution:

■ Feedstocks variable composition:
  ▪ FCC feed characteristics depend directly on the initial raw hydrocarbons processed by the refinery and by the performance of the upstream units and is not controlled by the operators.
  ▪ In SRUs, a similar variability in the composition of the feed gases is observed, along with variation between the ratios of the different streams.

■ Unit layout:
  ▪ Although the FCC unit is in almost continuous operation, the SO_2 absorption unit is not; its usage is often directly related to environmental constraints. When active, up to 50% of the FCC off gases are diverted to the SO_2 absorber and then to the FCC-02 stack. When the SO_2 absorption unit is inactive, all the gases are sent to the FCC-01 stack.
  ▪ The different subprocesses involved in the SRUs create a large combination of different operating conditions. The standard scenario is represented by TGTU2 and TGTU3 operating independently with the tail gas from the first unit diverted to TGTU2. This is also the operating layout that ensures the best sulfur removal efficiency. However,

for maintenance activities and load variation several other scenarios can apply.

The above mentioned characteristics of refinery units have a huge impact on the design and implementation of a PEMS solution; the degrees of complexity encountered required very deep analysis of process behaviour together with close liaison with the customer's technicians in order to develop a robust solution able to monitor the emissions efficiently.

In accordance with customer requirements, the PEMS application was tailored to ensure optimal performance for the most typical operating modes. For the SRUs, models were developed to provide the best performance during the high sulfur removal scenario.

For the cracking and the absorption units, emissions were modelled in order to provide an accurate inferential measurement for both stacks, using the valve open position values to identify shutdown of the SO_2 absorber.

PEMS solution

Developing data driven models requires extensive process knowledge and sound automation skills. Additionally, a deep understanding of process dynamics and behaviour is fundamental for implementing an effective PEMS solution. Therefore, the very first step of the project was a technical alignment with plant personnel in order to understand the different ways the units are operated, to share relevant process documentation and evaluate available instrumentation.

Once the key components of the plants were identified, a data collection campaign was arranged to obtain an adequate baseline of data to train the models: this was performed by extracting six
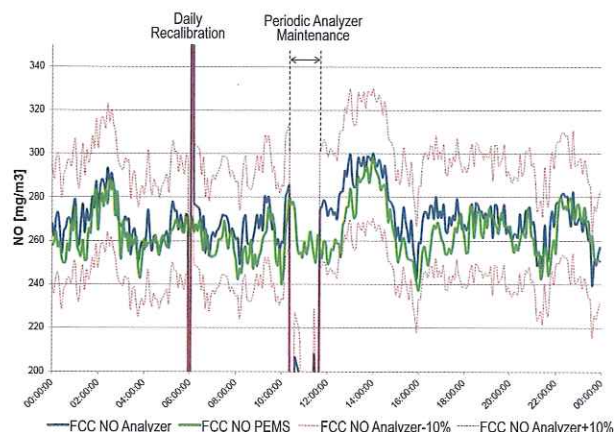
Figure 6. Model is able to extend system availability during analyser recalibrations or maintenance or recalibration.

months worth of synchronised process and emission values from plant historian and emission data acquisition system.

After data collection, data analysis and advanced data processing activities were performed to:
- Remove 'bad quality' data and outliers.
- Evaluate the basic process dynamics.
- Identify the relevant process variables that impact on the emission values.

The prerequisite for model building is the creation of a representative dataset, a set of variables that are able to describe process dynamics and that cover all the different operating

conditions. Identification of the correct sampling time is the key to the balance between overtraining the models and the loss of important information concerning process variability.

The SRUs' dynamics proved to be substantially slower than the FCC; this impacted on the final subsets used for inferential creation:

- SRUs: 70 variables and approximately 3500 records at 60 mins sampling rate.
- FCC and absorber: 50 variables and approximately 7000 records at 30 mins sampling rate.

In order to identify the final variables for each model, the engineers relied on two key ingredients:

- Their process expertise supported by interaction with the plant operators.
- Advanced mathematical tools, (for example, principle component analysis (PCA), to identify hidden correlations between process parameters and emission values.

Given the large number of units involved, SRU models required, on average, a set of 10 - 12 input parameters to ensure proper accuracy, while models for the cracking unit needed just seven or eight input variables.

Feed forward neural networks were chosen as the model architecture, since they have proved to be the most robust and effective for emission monitoring purposes.

Once developed and carefully validated, the models were installed onsite in a dedicated server and fed with real time process values from the control system; the parameters are processed within the software calculation engine to produce the emission estimations.

The PEMS system was then integrated with the existing emission data acquisition system to make it accessible by plant personnel. A devoted strategy was implemented to employ PEMS values for the 'refinery bubble limit' when emission data from the traditional instrumentation were not available.

Results

In order to obtain the customer's final acceptance, the PEMS estimations were compared with data generated by the hardware analysers; predictions from the PEMS software analysers proved to be well aligned with the values provided by the physical instrumentation (Figure 4).

In Figure 4, predicted SRU flow values are charted against real time data obtained from the flowmeter mounted in the stack. The red lines identify an interval of +/-10% from the physical measurement. In the 20 day period reported, the behaviour or the PEMS proved consistent with the physical device and the discrepancy between estimated and field measured values was very small and well below acceptance thresholds.

The same high performance level was achieved for the other two stacks monitored. Figure 5 shows predicted O_2 values from the FCC-02 stack. The PEMS also proved able to very accurately predict the behaviour of emission properties from the absorption unit.

The accuracy of the PEMS models revealed their importance during maintenance activities on the traditional CEMS; in fact, the redundant measurement provided by the back up system was able to cover the blank periods during hardware out of service times.

As an example, Figure 6 reports a daily chart of NO emissions (predicted and measured) from the FCC unit. Note that during the day, there are two periods where the analytical values are not available; for some minutes during daily automatic recalibration and for around an hour due to a periodic recalibration activity, performed by field technicians.

The PEMS NO estimation, that remains well aligned with the CEMS measurement, enables the availability of emission data to be maintained even during hardware based system recalibration, extending the overall in service factor of the emission monitoring system well above 99%.

Conclusion

Until now, PEMS were generally considered a reliable alternative to CEMS for emission monitoring from simple process units only (for example, gas turbines and boilers); they were thought unsuitable for use in applications where fuel characteristics are variable or in complex process plant.

This project dealt with critical processes, where complex layouts and undetermined, unfixed feedstocks presented additional challenges. Despite these issues, PEMS proved to be a very accurate solution that was able to act as a reliable back up to the traditional CEMS used in this kind of application.

In addition, when acting as back up, the discrepancy between the PEMS model output and analytical instrument measurement can be used by plant personnel as an early warning to identify any potential measurement drift or malfunction of the hardware devices and to validate maintenance activities. In other words, the software analyser can be used as a maintenance trigger, enabling timely corrective actions when a problem occurs, or as a benchmark to evaluate if the hardware analyer has been correctly retuned.

The robustness and reliability of predictive systems make them perfectly suitable to back up conventional hardware based systems. It has been demonstrated that they can increase the overall uptime of the emission monitoring system by allowing the substitution of CEMS values in case of malfunction or maintenance. In addition, inferential technology has been shown to be robust enough to be used as the primary emission monitoring source[5], ensuring comparable performance to conventional hardware based systems.

Finally, a well trained PEMs model provides plant operators a unique opportunity, unavailable with traditional analysers; they can perform off line simulation of emission behaviour at varying operating conditions. This 'what if' analysis enables technicians to investigate how emissions respond to changes in input variables and the role of each operating parameter in final emissions values.

References

1. ARIONI, E., BONAVITA, N., PACO, M., 'Keeping an eye on emissions', Hydrocarbon Engineering, pp 43 - 47, October 2013.
2. 'Continuous Emission Monitoring Systems for Non-criteria Pollutant', EPA Handbook August 1997.
3. MEIRELES, M.R.G, ALMEIDA, P.E.M., SIMOES, M.G., 'A Comprehensive Review for Industrial Applicability of Artificial Neural Networks', IEEE Transactions on Industrial Electronics, Vol.50, No.3 pp 585 - 601, June 2003.
4. ANCHEYTA, J., 'Modeling and Simulation of Catalytic Reactors for Petroleum Refining', John Wiley and Sons Inc., pp 27 - 29, 2011.
5. BONAVITA, N., CALLERO, F., 'Model-based emission monitoring', ABB Review 3/11 pp. 58 - 63, 2011.