Inferential Modeling for Environmental Applications: the Predictive Emission Monitoring Approach

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The Environmental Impact of Process Industries

Energy is a key component of people’s quality of life and an essential element for “driving” economies. Nowadays, we are totally dependent on an abundant and uninterrupted supply of energy for living and working. It is a key ingredient in all sectors of modern economies. But energy consumption is inseparably linked with environmental impact issues: the production, transportation, transmission and use of conventional energy have impacts on the environment, including the emission of greenhouse gases and atmospheric pollutants through the combustion of fossil fuels and flooding of lands for large hydroelectric sources.

Fig. 1 - Atmospheric pollutants produced by industrial plants

Industrial processes bear a big responsibility here. In the USA (where 25% of the World’s total energy is consumed), process industries in 2001 accounted for over 33% of all energy used [1]. This obviously reflects itself in an important impact on emission level. Considering, for example, NOx emissions for stationary combustion in the same year, the industry sector was responsible for more than 30% of the total, which rises to an astonishing 87.3% when electricity generation is included [2]. The above has caused growing concerns in the social community towards the industrial world. It has led many people to the conviction that any industrial plant sites is responsible for harmful effects and serious pathology on the public health.
The extreme wariness and criticism coming from the social community have led to the definition and enforcement of stringent constraints on the release of emissions. These constraints are nowadays among the most important factors impacting on plant performance and profitability being able, in the worst case, even to lead to the closing down of production sites. These regulations have changed and will keep on changing the rule-of-the-game in many industrial sectors.

Probably the most significant examples of “turning-age” regulations are:
- the Clean Air Act Amendment (CAAA) approved in 1990 and enforced in the following years in US, and
- the Emission Trading systems which will be established in Europe progressively starting from January 2005.

The Clean Air Act was passed in 1969 in an attempt to clean up the air in the United States. Though considered progressive at the time, the Clean Air Act of 1969 has proven insufficient and was thus amended in 1990 with sweeping revisions in an attempt to reduce acid rain, urban air pollution and toxic air emissions. Among others the acid rain program of the Clean Air Act Amendments of 1990 (CAAA) has fostered the growth of Continuous Emissions Monitoring Systems (CEMS). The overall increasing trend is far from slowing down. A recent survey from The Freedonia Group Inc., reports that demand for emission control products (hardware and software) is expected to grow at a 5.4% yearly rate, up to reach 3.9 billion dollars in 2007 [3]. The EU, in the aftermath of adopting the Kyoto protocol defined an emissions trading mechanism which is going to have a huge business impact on more than 5000 industrial installations. Companies in a variety of industries will be required to track emissions in real time, manage emissions allowances and credits across the total enterprise, optimise environmental controls, and produce compliance reports in accordance with international, national and local regulatory bodies.

Environmental Management Systems

In order to tackle the ever-increasing burden coming from regulatory compliance, process industries have started to endow themselves with Environmental Management Systems (EMS) able to provide reliable monitoring and reporting functions to the plant management and for the supervising authorities. According to ISO 14001 the goal of an EMS is “to enable an organization to establish, and assess the effectiveness of procedures to set an environmental policy and objectives, achieve conformance with them , and demonstrate such conformance to others” [4]. Among the several functions an EMS is called to provide it is possible to single out the following:
- Collecting and processing environmental-related data;
- Provide key environmental performance indicators;
- Provide Environmental Performance Evaluation planning;
- Emission Calculation & Reporting;
- Record keeping and Audit Trail functionalities;

EMS must be able to collect, re-order, store and display a wide number of data and information classes. These include [5]:
- Data for emissions inventories;
Data for assessing environmental impacts
Data to be shared with the public
Data for emissions trading programs
Data on environmental costs to be included into plant efficiency and performance reports
Data for improving plant control and operation standards
Data for early identification of possible failures and/or arriving problems

All of them are actually necessary and will become vital for understanding, managing and reporting the interaction of industrial processes with the environment and society. In Europe, EMS are expected to become more and more important in view of the enforcement of Green House Gas (GHG) regulations as a consequence of the adoption of the Kyoto Protocol.

Figure 2 shows the several parts of an EMS system. The two bubbles at the lower end of the picture, are the two which have the strongest interactions with the field and which constitute the foundation for any other environmental management project. They are related to acquiring proper, reliable and timely information about the actual emission levels (the monitoring system) and to use this information to deploy adequate control actions able to drive and to keep the emissions inside the law-enforced limits. Monitoring frequencies may be divided into the following categories, according to the frequency at which the monitoring action is performed, i.e. the time between individual measurements are taken [6]:

Continuous, where there is a continuous stream of data acquired by rapid-response instruments, and displayed in real-time. It is the most expensive option and sometimes it may even not be an
option when resorting to off-line laboratory analysis is unavoidable. A typical example of this is when the required accuracy forces pre-concentration of samples, so that pollutant samples must be accumulated over a period in order to be detectable. Periodic, where measurements are taken at regular intervals, both on the spot or in order to accumulate enough samples. It is possible to have Non-continuous response monitoring, where the measurements are made in response to a given foreseeable but not-schedulable event (i.e. plant shut-down), happening at irregular intervals; Non-continuous reactive monitoring, where the measurements are made in response to a given unforeseeable event (i.e. limit trespassing), happening at irregular intervals; Non-continuous campaign monitoring, where the measurements are made in addition to routine analysis in order to acquire more detailed information on specific operative conditions. Campaign monitoring usually involves analysis so detailed and/or extensive which cannot be justified on a regular basis.

In the next section some more details will be given about the continuous approach.

**Continuous Emission Monitoring Systems.**

After the CAAA in US and the several specific regulations in Europe, Continuous Emissions Monitoring Systems have taken up a central role in most of the emission monitoring programs. A Continuous Emission Monitoring System is defined as the total equipment used to acquire data, which includes sample extraction and transport hardware, analyzer, data recording and processing hardware and software. The system consists of the following major subsystems:
- Sample Interface: that portion of the system that is used for one or more of the following: Sample acquisition, sample transportation, sample conditioning, or protection of the analyzer from the effect of the stack effluent.
- Analyzer: that portion of the system that senses component concentration and generates an output proportional to the gas concentration.
- Data Recorder: that portion of the system that records a permanent record of the measurement values, typically providing a new value at least once every 1.5 sec. and operating with an availability greater than 90% on a monthly basis [6]. The data recorder may include automatic data reduction capabilities.
- Calculation / conversion of the raw measured data to “normalized” values (at standardized conditions of atmospheric pressure, temperature, oxygen content, etc.).

CEMS can broadly be broken into three types of methods (Fig. 3, see also [7]):
- Extractive Methods,
- In-situ Instrumental Methods
- Parameter-based Methods.

Each configuration has its own strengths and weaknesses as briefly described below.

The extractive methods involves the physical extraction of the sample from the stack. Sample Gas is then fed to the analyzer through a heated sample line. Based on the used sample-processing methodology, extractive methods can be further broken into two techniques, direct source level and dilution.
As far as the direct source concerns, sample analysis can be carried out both on dry basis and wet basis.

Dry Basis. A sample pump feeds the sample gas through a cooler which cools down the gas to a temperature of 5°C. The chiller lowers the temperature of the gas causing condensation, particularly of water vapour, and thus a dry sample gas can be sent to the analyzer.

Wet basis. The sample gas path (From the sample take off point to the analyzer) is kept to high temperature in order to avoid condensation. This technique is used to carried out the gas analysis with ABB Bomem FTIR technology.

The most common techniques used for pollutant measurement are:

- Infra-red analyzer: CO, CO2, SO2, NO, HCl, NH3
- Chemilum analyzer: NO, NO2
- UV analyzer: NO, SO2 detection
- FTIR Spectrometer: CO, CO2, SO2, HCl, NH3, NO, NO2, H2O
- Flame Ionization Detectors Volatile Organic Compounds (VOCs)

Dilution systems achieve the same goal by diluting stack gas samples with clean dry air without any heating.

In-situ systems are basically automated instrumented techniques employing various detection principles for continuous or periodic emission measurements. This involves making direct measurements of pollutant concentrations with instruments able to provide immediate and continuous readings. Instruments which are permanently installed at the plant to provide continuous emission monitoring systems can be either point or cross-stack (path). Point in-situ systems measure the concentration at a specific point or over a relatively short path length through the stack gas. Cross-stack system project a light beam across the stack gas stream and obtain the emission data analyzing various spectral phenomena. They may be either single-pass or double pass, depending on whether the light source and the detector are on the same or the opposite side. The main advantages of this approach are that it gives information with a high
time-resolution and virtually no time delay. Moreover many of the sampling problems (condensation, adsorption, occurrence of chemical reactions) associated with extractive systems are eliminated. The disadvantages are mainly related to the difficulty and the cost of calibrating and maintaining instruments often placed in harsh or difficult-to-be-reached field locations. Parameter-based methods are possible alternatives (or supplement) to the installation of traditional CEM systems.

In this context a parameter is defined as a property whose value can characterize or determine the performance of process or control equipment directly correlated with emission levels. According to EPA [7], alternative monitoring options include:

- using parameters as indicators of proper operation and maintenance practices
- using parameters as surrogates for emissions determinations
- using parameters in models that calculate emissions
- performing mass balance calculations
- employing a CEM system to monitor a more easily analyzed gas as a surrogate for one that is more difficult to analyze

As a result of the above, parameter-based methods can be split in two main categories:

1. Surrogates
2. Predictive

Surrogates are process parameters which may be used for determining directly the compliance of a source with emission standards. In this case the process owner must establish and justify the parameter values that assure the compliance with the actual regulations. This usually requires an extensive testing and validation procedure which is highly application dependent. The Predictive class applies where the relationships between process conditions and emission levels are not so straightforward to be fully described by a single parameter and involves the concept of modeling. It will be more extensively described in the next section.

**How Modeling Technologies May Help**

With over 25 years of experience both in the United States and Europe, continuous emission monitoring for many pollutants is a mature technology. In addition to the traditional approaches, new technologies are being introduced into this field at a quick pace in order to improve the plant operational efficiency with a consequent reduction of emissions to the atmosphere. On top of hardware and electronics-related innovations, modeling technologies promise to be able to take a primary role for meeting monitoring requirements for hazardous air pollutants.

They are already a proven and often used technology in modern process automation, where they are used by process engineers to develop compact mathematical expressions that describe the behavior of a process or event. Operating in real-time, models are fed with input variables values and compute resultant values for the output variables. Depending on the nature of the model, this may or may not represent a causal relationship.

It is possible to distinguish between two main approaches in modeling technology, the theoretical and the empirical [8]. A theoretical model is derived from scientific principles such as
conservation of mass, energy and species, and the laws of thermodynamics. An empirical model is mathematically derived from collected process data. Valid theoretical models always provide a causal relationship, while an empirical model may not.

Empirical modeling techniques are based on the capability to extract relevant information out of historical process data. They are able to provide accurate real-time estimate of difficult to measure quantities, exploiting otherwise hidden or neglected correlations, and providing deeper insight into the process. In this case the estimated quantity is often referred to as an *Inferential Variable* and the model is also called an *Inferential Model*. Process control applications usually employ inferential models.

Figure 4 and 5 schematically describe the relationships between input data (the available on-line measured variables), output data (the variable that needs to be estimated) and the model itself. In the *model building* stage, devoted software is used to import, pre-process and filter out historical datasets. These must include all the possible inputs and samples of the quantity that needs to be estimated (i.e. NO$_x$ or CO$_2$ content) properly collected. The output of this activity is a model, which has to be extensively tested and validated on the widest possible range of operative conditions.

Once the model has been built and validated it can be placed on-line. It is fed with the actual, “live” process data and provides accurate real-time estimates of the desired quantity. In order to do that the software has to be able to pre-process incoming input values so to filter out possible outliers, bad qualities and identify transient states. Similar treatment must be done also on the model output so as to increase its reliability and accuracy.
Modeling technologies can provide strong support to existing emission management systems, by means of what is known as a Predictive Emission Monitoring System (PEMS). These systems do not measure emissions but use a computer model to predict emission concentrations based on process data (e.g. fuel flow, load, and ambient air temperature). The model is based on measurements at either the source or from generic emission information. While lots of applications prove that software systems provide an accuracy close to that of hardware-based CEMS, virtual analyzers are able to offer additional features, like [9]:

- Trace back causes of emissions, identifying key variables;
- Validate sensors automatically
- Reconstruct emission levels from historical data, in case of failure of the hardware device
- Can be used for process optimization purposes

A successful PEMS can provide continuous information on emissions (where none existed before), as well as improve operational efficiency while reducing emissions. It will identify actions which will maintain reduced emission rates and will help to prevent limit trespassing. PEMS provide also the channel to acquire near-continuous real time feedback and to reinforce parameters necessary to operate the plant below maximum permitted emission levels by developing a mathematical relationship between operational parameters and emission rates.

The PEMS can also be used to optimize operations by reducing emissions while increasing power production.
As discussed, current regulations require traditional end-of-pipe periodic stack testing and continuous emissions monitoring (CEM) systems which are designed to record compliance with permit limits and exceeding when a violation actually occurs. With this system, there is no opportunity to prevent or lower emissions at the time of measurement. Conversely, the proposed implementation of the PEM could allow plant engineers to directly correlate the relationship between varying operational parameters, predict emissions at its plant in advance, and to take action to adjust emissions before the violations actually occur. The ability will prevent the emission of pollutants at levels which approach or exceed permit limits.

An additional benefit of PEMS is that the emissions models can be used with model based control strategies for optimization of the process with respect to operational costs and compliance margins. Examples are available in literature (see for example [10], [11])

Inferential analyzers can provide different benefits according to the several different situations. Several US states allow PEMS as an alternative monitoring technique for certain programs and regulations. In this case the plant is allowed to lease a portable CEM for some weeks to gather emissions data, to build and validate the adequate models and then, after a proper certification procedure, to remove the hardware analyzer and to rely only on the inferential ones [12]. Alternatively, PEMS can provide the only way to obtain a continuous stream of (estimated) emission values where CEMS are not present. This applies to units where either the in-situ (i.e. periodic) analysis approach is used or the campaign approach is present.

But even when a CEM system is already in place and working, the addition of an inferential system back-up may unleash wide and somehow unexpected benefits. They offer the possibility to increase the Operative Availability (OA\(^1\)), providing:
- an early warning about possible performance degradation;
- an alternative way to estimate emission content, when the CEMS is not available (because on failure or under maintenance).

Although they differ by country, many European national regulations, explicitly call for software-based, redundancy emission monitoring systems. In Italy, for example, the 1995 Government Directive [13] states that: “... in case of unavailability of the continuous measurement [system], the owner, whereas possible, is to implement alternative emissions control actions. These have to be based on non-continuous measurements or correlations with operative parameters and/or with specific raw material composition [data]. .... Data measured or estimated by means of such techniques will be accepted and fully used in the compliance assessment procedure”. Moreover they offer a possibility to save on maintenance contract allowing more relaxed intervention time (i.e. 48-72 hours instead of the typical 24 hours) because of the presence of the software sensor acting as a back-up.

Fig. 6 summarizes schematically how emissions modeling can be profitably exploited, even in countries where PEMS are not legally-accepted as an alternative to CEMS surrogates. In the next section, a proposed solution is described and details are given on how to exploit all the related benefit from this technology.

\(^1\) OA = \( \frac{TBF}{TBF + RT} \times 100 \) where: TBF = Time Between Failures; RT = Repair Time.
Model-Enhanced Emission Monitoring Systems

On the basis of many years of experience in applying inferential methods in process control projects, a new product has been designed to develop and deploy empirical models.

OptimizeIT Inferential Modeling Platform (IMP) is an innovative software package for the development and deployment of data-driven advanced applications. It is based on two separate environments:

- IMP Model Builder for application design and development
- IMP On-line for on-line project deployment and monitoring

IMP features latest generation data analysis and modeling technologies developed in house or selected from technology leaders around the world. The user is able to exploit a rich collection of highly sophisticated tools for data analysis and pre-processing available at his fingertips [14]. All the different tools are embedded in an intuitive working environment based on the latest HMI concepts, which remove any hurdle for the inexperienced user.

IMP features some latest generation toolkits, which allow building models through several technologies including:

- Neural Networks
- Multiple Linear Regressions
- Calculation Scripts

One of the most time-consuming tasks in developing neural models is the iterative training and testing procedure, needed to identify the model with the best performance, which does not over-fit the data. One of the salient advantages of the IMP neural method is that it can actually be tuned after it is trained in order to provide more or less generalization. This allows the user to decouple the training activity from the testing activity, offering a big advantage both in development time and in the accuracy and reproducibility of the method.

IMP embeds empirical modelling technologies in a process control oriented environment, unleashing all the power of neural network modelling, without most of the related drawbacks and
nuisances. Highly automated, yet very simple procedures allow the user to simultaneously build several models and then to compare the results. In this way, most of the model building activity is completely automatic, even to the point of executing overnight. The engineer needs to check the results and accept the most convenient and best performing models, using the many available comparison facilities. Additionally IMP includes powerful tools for process and quality monitoring, allowing the user to quickly implement SPC control charts and even MvSPC. This is particularly efficient in monitoring complex processes with just a single number, the Hotelling $T^2$ statistic [15].

IMP On-line is designed to quickly and efficiently implement applications involving process models. The engineer only needs to physically connect his PC to the network, browse the OPC Servers available and select the tags he wants to read or write back to the DCS. With no need to write a single line of code, he may specify the preferred options concerning a large number of possible configuration details, including bad quality management, tag limits, engineering units/conversions and tag filtering. Integration of bias update strategies was given particular attention. Any online implementation of inferential models is usually coupled with a periodic recalibration strategy. This strategy computes the difference between the prediction and available physical measurements (like lab analysis) and treats it statistically to determine the inferential model bias. The bias is then added to the model output, to improve its accuracy and avoid any model drift in case of failure in input sensors. The system is designed to be seamlessly integrated with existing control instrumentation (DCS, LIMS, historians) so to ease process operators access and interactions. For example, predicted emission values can be displayed, further than on IMP On-Line Monitoring screens, via DCS operator display graphics. Graphics to assist operators in determining the cause of NOx non-compliance, facilitating periodic calibration, and for reporting purposes can be also developed, including audible and visual alarms to alert operators of sensor, hardware, or software component failures. Depending on the actual instrumentation and needs, the PEM system could and should be configured in different ways. For the sake of simplicity, in the following section the description of the typical HW analyser back-up and validation is given.

Typical Hardware and Software Architecture.

The hardware architecture is very simple: the inferential system is loaded on a PC able to communicate through OPC with the DCS where all the process variable and the analyser data are available (in the reference case, shown in Figure 7, the interface between the analyser and the DCS is realized through Modbus).

The basic goal of the system is to:
- allow a continuous validation of the readings coming from the HW analyser;
- spot periods when analyser re-calibration and/or maintenance is needed;
- act as a back-up of the analyser when it is out-of-service, in maintenance or simply unreliable.
**HW Architecture**

Fig. 7 – Example of OptimizeIT IMP hardware architecture

**Fig. 8 - Example of OptimizeIT IMP software architecture**
To fulfill this scope the SW architecture shown in Fig. 8 has been designed. The model calculates the emission predicted values, on the ground of the actual process data. These values are compared with the values measured by the analyser: the discrepancy is sent to a logic which generates a signal when it is greater (in absolute value) of a pre-defined, configurable threshold. Following the plant policy and habits the signal may trigger an alarm on the Operator Console, on the maintenance station or on both.

Figure 9 shows how the operator can be informed by the system with a simple, intuitive trend display: when the two values drift apart, the event is considered to be a maintenance trigger which could be used to activate a checking action on the analyser. If the analyser is recognized as the origin of the drift, the maintenance may be activated while the inferential system provides a back-up value which could be used as a substitute of the HW read-out.

It should be noted that the system not only gives indication about when maintenance actions could be required, but also provides a way to validate them, that is demonstrating the effectiveness of the maintenance action in removing the problem.

Figure 10 describes the main stages of a project involving a model-based PEM system. The project usually starts with a kick-off meeting (KOM) where a detailed description of the plant is given by the process owner, highlighting all the relevant information both on equipment and
operative practices. If possible at the end of the KOM, historical process and emission data are made available for model building purposes. After a careful analysis and subsequent cleaning of the data, the inferential model is developed and thoroughly tested in order to assess and validate its performances and robustness. Meanwhile proper on-line data processing are also designed based on historical data statistics and characterization. The last step is the commissioning of the application in the control room following what agreed and defined with the customer at the KOM. Usually a 1 month validation period is foreseen before final acceptance. In the figure orange boxes identify off-line activities (involving IMP Model Builder) and blue on-line ones.

As an example about how modeling techniques can be easily and effectively implemented on process units, a test application on a polymer plant is briefly described in the following paragraphs.

The customer in question had a problem with the final stage of the process where the finite, extruded product is steam-stripped to remove hexane. Mobile analyzers are used in “monitoring campaigns” (so falling in category B.3 following the classification given in section 2.) to assess the amount of pollution vented into atmosphere with the steam. Obviously this is far from optimum because the analyzers are connected to the plant no more than 20% of the operating time. However using the data stored during these campaigns, it has been quite simple to identify a model, which could be easily put on-line for real-time continuous emission monitoring purposes. Figure 11 shows the excellent accuracy the Neural Network model is able to provide.
Environmental-Constrained Process Control

The model-based system described in the previous section could be also seen as the basic layer on which a real environmental-constrained process control strategy could be realized. Having a continuous, validated stream of reliable data about emissions, allows to include them into standard plant control strategies as constraints. The cost deriving from the violation of these constraints can be included and weighed into the existing real-time economics-driven control strategies, based on modern, high-performance tools like multivariable process controllers. Figure 12 shows a possible scenario involving monitoring and controlling tools able to include environmental management issues into the overall process management policy. In this case the OptimizeIT Predict & Control MPC is used to control a process unit where emission levels are added as constraint-variables to the global control target.

Environmental constraints frequently enter process control problems in combustion processes. In a large utility power boiler, the NO\textsubscript{x} and CO constraints interact with the steam temperature control. As air flow increases or decreases, NO\textsubscript{x} and CO are affected, but the change in air flow also changes the energy balance resulting in more or less spray flows. Optimizing overall economic efficiency may require riding on an environmental constraint. In chemical plants and refineries, process heaters are used to preheat feed to chemical reactors or reboil liquid in the bottom of distillation columns. Frequently, waste fuels containing high sulfur are available as an alternate fuel at lower cost. A multivariable controller can manage SO\textsubscript{x} and CO constraints, while minimizing fuel cost while meeting process heating demands.
It is clear that such a configuration will be able to fully answer the requirements arising from the new scenario that the Emission Trading scheme will impose on the process industry.

**Conclusions and Potential Benefits**

Under the pressure of new stringent environmental regulations and the related opportunities which Emissions Trading regime will bring, Emission Monitoring Systems will become more and more crucial for day-by-day management of process industry installations.

The ability to correlate the actual operating conditions with the actual released amount of emissions, will deliver a number of important benefits:

- Availability of advanced and highly-reliable diagnostics on existing analyzers: this includes the complete measurement chain from sampling acquisition to electronics, from piping to instrument calibration;
- Availability of a software back-up for the actual instrument able to provide reliable emission estimates when the analyzer is out-of-service, in maintenance or needs calibration;
- Availability of a validation mechanism for the existing HW analyzer, which can be used in case of discrepancies with the certifying authority;
- Early identification of calibration/maintenance actions (allowing predictive maintenance instead of scheduled one);
- Increase of the duty time of the existing analysis system;
- Identification of possible inconsistencies among instrument readings which may suggest a complete check-out of the calibration procedures themselves (e.g. problems at the calibration cells and/or at the reference gas).
The model may be used off-line to perform both sensibility and what-if analysis able to correlate process parameters with emission levels and to provide insight on pollution creation mechanisms. This is particularly attractive for exploring emission trading scenarios and designing related actions.

The model allows also the customers to make predictions of the future state of emissions compliance by predicting the emissions profile of individual units and summarizing the predictions.

The bottom line return on investment for the process owner comes mainly from reducing the chances of litigation by and penalties from the regulatory authorities. Traditionally hardware analyzers have a service factor of 96-97%. The addition of a software back-up system can extend it up to 99 – 99,5%: in terms of days this implies an extension of 7-10 days per year. Additional savings comes from reduction in maintenance costs and in the environmental-related give-away. Although depending on case-by-case application details, a conservative estimate of the pay-back period for a PEMS extension to the existing CEM system, is between 4 and 8 months.

References:

4. ISO 14001
13. Decreto Ministeriale 21 Diecembre 1995, art. 2 (in Italian)