Fulfilling Evolving End-Users Expectations for Site-Wide Emission Monitoring: the Role of PEMS

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Abstract

Environmental regulation evolution in mature countries and the expected leapfrog in emerging countries guidelines are contributing to substantial changes in the emission monitoring techniques. Predictive Emission Monitoring Systems (PEMS) have been around for almost 20 years starting as a niche technology for fond engineers and practitioners and slowly gaining acceptance as an alternative to HW-based Continuous Emission Monitoring Systems (CEMS). Assisted and reassured by rigorous regulations and procedures, issued and revised by the main environmental Authorities, customers and end-users have progressively learned to consider and use them as a smart option for a number of stationary emission sources rather than a one-fit-all solution.

This trend is becoming even more apparent recently, when a growing number of large end-users, especially in the Oil & Gas sector, are starting to adopt a systemic approach for their environmental sustainability policies cleverly selecting the most suited technology, among a pool of available ones, according to different units characteristics and operations. Market requirements are much influenced by these changes in regulating framework and in end-user orientation; PEMS technology is becoming a key pillar in the emission monitoring strategies at plant level.

The paper will describe how designing, developing, deploying and maintaining the optimal site-wide emission monitoring strategy, is quite an engineering and operational challenge, which requires a wide span of competencies, expertise, engineering tools and service capabilities in order to identify the most performing and cost effective solution for each process unit.

The increased complexity requires systems suppliers to evolve their role so to be able to master very different technologies and provide the needed consultancy and assistance to the end users from the early design stages up to the system commissioning, deployment and maintenance.

1 Introduction

Environmental sustainability and pollution control are nowadays crucial matters, which have a significant impact on everyday life. Air quality is becoming a major concern not only in mature countries but also in emerging nations, as India and China, which are experiencing ambitious initiatives to abate the pollution levels. On a global scale, this new perception led to the development of stringent constraints on the release of emissions, which are among the key factors affecting industrial production: limit exceeding, in fact, can result in severe economic penalties and failure to provide emission data to environmental authorities may lead to plant shutdown.
Uncompromising regulations have been developed and are continuously updated in order to properly define and certify solutions and technologies for emission monitoring at stacks.

In Europe, several directives and technical standards have been enacted on this theme (e.g. the Large Combustion Plant Directive, the Incineration of Waste Directive, EN14181, etc.). In the US, Environmental Protection Agency (EPA) issued regulations 40CFR Part 60 and 75 which provide the reference framework for emission monitoring requirements [1].

The core of both legislations is the adoption of monitoring technologies, used to acquire reliable and timely information about real emission levels and to identify and put in place dedicated control actions to keep pollutant releases within the limits. In both regulating frameworks, great emphasis is given to hardware-based technologies, defined as the total equipment used to acquire, process, store and report data (i.e. sample probe, heated line for sample transport, analyzer, data recording and processing hardware and related software). They actually represent the most common approach for emission monitoring and are broadly referred as Continuous Emission Monitoring Systems (CEMS).

On the other hand, it should be noted that EPA stretches its definition of CEMS, so to include also Predictive Emission Monitoring Systems (PEMS), as shown in Figure 1.

For the sake of clarity, hereafter in this paper the term CEMS will be used referring only to the technologies based on hardware analyzers, while PEMS will represent predictive ones.

Predictive technologies are software based (see [3], [4] and the Appendix for a more detailed introduction): they exploit a model in order to estimate emission values on the ground of the actual operating conditions (i.e. from process variables like pressure, temperature, flowrate, etc.).

Being based on mathematical modeling techniques, PEMS can be developed using two different approaches:
First principle (fundamental) modeling – where the descriptive equations are derived from the basic chemical and thermodynamics laws.

Empirical (or data-driven) modeling – where the models are built through a fitting-like procedure over plant data.

It has to be taken into account that PEMS lifecycle cost is typically around 50% [5] of hardware based instrumentation: while benefitting from a lower initial CapEx, the cost for ongoing maintenance, recalibration and quality assurance for PEMS is almost negligible compared to hardware instrumentation.

Within 40 CFR 60 and 75, EPA defined the clear procedure in order to install PEMS as an alternative technology to conventional CEMS. In particular, Performance Specification 16 (PS-16) includes the tests that have to be performed in order to certify that model accuracy is equivalent to an HW-based reference method.

In Europe PEMS, while being generally accepted as back-up of traditional CEMS, lack of a complete framework for the adoption as an alternative monitoring method: presently a standard providing the requirements for the applicability is under development by Working Group 37 within the European Committee for Standardization (CEN) Technical Committee 264 “Air Quality” [6]. Working Group 37 is moving from the standard issued in the Netherlands [7], the first European country approving PEMS application. Netherlands technical agreement NTA 7379 provides the general guidelines for the usage of PEMS, identifying the key requirements, a preliminary list of processes not suited for PEMS and the general steps to be performed for model building and validation. Finally, NTA 7379 recalls the requirements of EN 14181 about quality assurance (QA), which addresses QA requirements for conventional CEMS.

Nowadays, PEMS are mainly applied in countries following US-EPA regulations, since these standards have been consistent and in place for some years; together with North America, Middle East is the most active region. However, also in a few Asian countries (e.g. Malaysia, Singapore, Korea), new releases of local environmental regulations start to include PEMS, opening the door to giants like China and India, which are expected to become the most relevant markets for emission monitoring solutions. Therefore, it is reasonable to expect that the new regulating framework that will be developed in these countries will benefit from the existing legislations and that a leapfrog in emission monitoring technology adoption can be foreseen.

2 End-users Evolving Approach to Emission Monitoring

The evolving regulating framework is having a major impact on end-users behaviors and approach to emission monitoring programs.

Together with the tighter standard requested, there is also a significant thrust for the end-users to be perceived as “green” companies, very sensitive to environmental and sustainability matters.
This renovated approach is leading several companies to develop its own internal guidelines and requirement for emission monitoring, sometimes driven by Country legislation, sometimes even anticipating or hardening law-enforced limitations.

Emission monitoring suppliers are witnessing a very interesting change of attitude in end-users, based on a top-down approach aimed at designating the most appropriate technology for each process. The most advanced corporations are in fact using a very pragmatic strategy, planning to use a well-balanced mix of HW-based and predictive technologies, according to the nature of the stationary emission sources, that can be classified in two broad categories:

- Units that are not subject to large sources of variations and where the combustion process is pretty stable (“class 1 units”);
- Units that, because of the feed processed or their position in the production chain, may experience a wide range of chemical and physical conditions resulting in very different emission levels (“class 2 units”).

Typically, the first group includes units such as gas turbines, boilers (especially gas-fired), heaters, furnaces, combustion engines. Units like waste incinerators or where feed can vary in unpredictable way – because just an intermediate product of other upstream units – should be included in the second group.

As a general practice, PEMS are well suited for the first class of units, while conventional CEMS should remain the solution of choice on the most complex applications (sulfur recovery units, catalytic cracking units, etc.).

A sensible selection of the most appropriate technology allows end-user to develop site-wide (or even company-wide) strategies aimed at monitoring all the stationary sources, drastically reducing the overall investment: as seen, PEMS represent in fact a very cost-effective alternative to conventional CEMS that are, hence, installed only on a precise boundary of applications.

In the next sections, further details about this strategy and the role of predictive systems will be presented.

### 2.1 An Oil and Gas Example of New Guidelines/Requirements

A remarkable example of what described above is represented by a major Middle East Oil and Gas Corporation, which has developed its own guidelines and is now in the process of implementing an Air Quality Monitoring and Management System (AQMS) in line with its HSE policies.

This is a very ambitious and comprehensive program, which involves all company subsidiaries, imposing the adoption of monitoring technologies at each site for every source emitting more than a predefined threshold of selected pollutants (e.g. NOₓ, SO₂, CO, etc.).

This is a major upgrade in emission monitoring practice since, probably for the first time provides a common framework based on the criteria described above, with a further category represented by flaring units:

- Traditional CEMS are prescribed for units such as Sulfur Recovery Units (SRU) incinerator stacks in order to monitor at least SO₂ and O₂. For other compounds (VOCs, NOₓ, CO, CO₂, etc.), further
than conventional analyzers, it is allowed to use estimations based on approved emission factors or stoichiometric calculations.

- PEMS are required in order to provide emission values of units such as boilers, gas turbines, heaters and engines.
- A simplified PEMS approach is suggested for flares: here it is requested to use calculations based on flared gas flow rate and composition.

These guidelines reveal the great commitment of the parent company towards environmental practices and show how end-user competences and knowledge are becoming extensive and focused.

Executing such high level, far-reaching programs is often quite a challenge at plant site, due to a reduced level of awareness about technologies, and to everyday operating constraints. In order to facilitate the on-site implementation a two-step approach is often advisable:

- A Front-End Engineering Design (FEED) stage, where key requirements for the implementation are defined;
- An execution stage where the emission monitoring program is implemented.

3 PEMS Growing Role

The scenario introduced in section 2 shows the increasing role PEMS is gaining on international market. Although the concept and first applications appeared in literature, more than 20 years ago [8], only in the last years they have been progressively accepted because of the documented economic savings [5] and of the thousands of successful implementations.

In such regulating setup, PEMS characteristics perfectly fit with the requirements and represent an optimal solution in order to protect the investments of the end users:

- On the “class 1” units, PEMS performances are more than adequate to the scope (and regulations). The following table reports an example of the relative accuracy (RA) obtained in a PEMS application at turbines driving compressors used for gas injection.

<table>
<thead>
<tr>
<th>Property</th>
<th>RA (Load 95%)</th>
<th>RA (Load 100%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂</td>
<td>&lt; 10%</td>
<td>&lt; 10%</td>
</tr>
<tr>
<td>NOx</td>
<td>&lt; 10%</td>
<td>≈ 15%</td>
</tr>
<tr>
<td>SO₂</td>
<td>Undetected (below 1ppm)</td>
<td>Undetected (below 1ppm)</td>
</tr>
<tr>
<td>CO</td>
<td>&lt; 10%</td>
<td>&lt; 15%</td>
</tr>
<tr>
<td>CO₂</td>
<td>&lt; 10%</td>
<td>&lt; 10%</td>
</tr>
</tbody>
</table>

![Figure 2 – PEMS performance at RATA test required for certification [3]](image_url)

- When PEMS are requested to upgrade and substitute existing CEMS, it is possible to resort to them in order to retrieve historical data, removing the need for temporary analyzers and slashing development cost. Here PEMS could act as back-up in the first stage and then remain the only monitoring technology once hardware analyzers become obsolete and have to be dismantled.
Alternatively PEMS can also be implemented as back-up of CEMS for complex, “class 2” units (even for SRUs in certain cases) in order to provide a redundant measurement when maintenance/off-service periods are encountered and extend the overall service factor. While the first approach is and will be the most typical – in literature there are a number of applications of PEMS as unique source for emission monitoring in simple units as gas turbines [9] – the second one represents a very interesting extension of PEMS usage.

Units to be equipped with CEMS are typically characterized by very harsh environment and severe process conditions that may cause issues and malfunctioning to conventional analyzers. In this case, the safest approach, in order to guarantee the availability of emission data would be to have a redundant measurement able to cover the off-service periods. However installing a second conventional CEMS would result in doubling the initial investment and largely increase also the operational expenses, while introducing predictive systems as back-up can be done at a marginal incremental price and provide the user with a sound model capable of substituting the hardware instrumentation in an accurate way [10].

The following picture provides an example of PEMS implementation as a back-up to CEMS at a catalytic cracking unit: in particular, it shows how the technology is able to provide an accurate measurement of the NO and that it can be a valuable alternative during any maintenance activity on the analyzers.

![Figure 3 - NO PEMS estimation versus traditional CEMS](image-url)
3.1 Impact on PEMS projects

The implementation of comprehensive and site-wide strategies determines also some changes in typical PEMS project, providing additional advantages that further contribute to its cost-effectiveness.

PEMS implementation includes a number of different phases (Figure 4, for further details about PEMS project development refer to Appendix). Approaching entire plants and identifying preliminarily the major requirements provides clear advantages in most of the different steps:

- Data collection duration can be optimized. Large sites often include several identical units (e.g. furnaces, gas turbines, boilers): in this case, data collection could be performed only on one unit, limiting scope and duration on the other identical ones.
- For the same reason, the engineering phases (data-processing, model building and validation) are shorter and simpler since they should be only replicated on several twin units. Predefined templates could therefore be created and simply tailored to the specific units. Similarly, also the costs for developing the documentation could be largely cut down.
- Commissioning time and cost can be drastically reduced, as well, since in a single session it is possible to implement predictive models on multiple sources.
- Integration with existing software and automation infrastructure becomes straightforward since typically, the main issues have been already analyzed during previous FEED and the interfaces between the automation layers at plant with the new PEM system are clearly defined.
- At last, personnel training and after-sales services can benefit from this approach: dealing with a large number of different units to be monitored at the same time allows arranging onsite resources training alongside commissioning activities in a single mobilization to site.
Finally, the comprehensive top-down approach affects the choice between the data-driven and the first principles modeling, giving the former a significant edge over theoretical ones: in fact, when dealing with a large number of units, empirical algorithms provide more flexibility and possibility to be applied to very different units at limited costs.

Developing a first principle model requires a substantial knowledge about the combustion process and large initial investments from the suppliers; therefore they are normally built only for a specific equipment (sometimes even for single manufacturer).

On the other end, data-driven models, as neural networks, which do not imply any cause-effect relationship, are much easier to be developed [4] and can be easily adopted for same units from different OEMs and for different ranges of applications (boilers, turbines, etc.).

4 Technology Providers Enhanced Challenges

Recognizing PEMS as an alternative to CEMS places new challenges to emission monitoring solution providers, which are requested to enhance their product portfolio and to extend their competences if they want to be accepted as reliable and knowledgeable partners since the early phases. Clearly only suppliers able to equally master and provide both technologies will be perceived sufficiently not-biased and independent to advice, design, implement and maintain such an integrated corporate strategy.

The ideal technology provider should offer solutions and services able to blend the following three fundamental ingredients:

- **Technology**: hardware analyzers as well as user-friendly software environments for both model development and model deployment. Whatever the solution of choice, an additional software layer shall also guarantee the flexibility to dialogue and interface with plant automation infrastructure by means of standard protocols, and – possibly – web browser connectivity for remote maintenance.

- **Know-how**: PEMS development requires to complement analytical, process and instrumentation skills (crucial for CEMS) with information technology and modeling capabilities. This means to extend substantially the set of internal competences required to successfully develop and deploy both PEMS and CEMS and make them available to the market.

- **Local Presence**: Offering a brilliant solution is not enough if it is not supported by timely and effective engineering services, both during project deployment and for regular maintenance and assistance. In particular, it is crucial to have skilled resources that can be quickly mobilized to perform upgrades, recalibration and first-level services, both on traditional analyzers (for CEMS or temporary set-up during PEMS data collection and certification) and on models and software infrastructure.
5 Conclusions
Emission monitoring needs and perspectives are evolving under the combined effects of increasingly tight regulations, technology advances and growing need for social and environmental reputation. Predictive Emission Monitoring Systems, although available in a few regions since more than 15 years, are gaining momentum and consideration and are becoming quite a standard option for well-defined stationary sources in corporate-wide strategies. The paper has focused on some of the consequences that this shift will bring to both end-users and technology suppliers, highlighting the need for flexible approaches, extended solution portfolio and availability of resources skilled in multiple disciplines. The reward for the plant owner will be better performances at a reduced capital cost, easier and cheaper maintenance and an overall standardization of environmental practices, which will help in reducing and managing the inherent complexity.

Acronyms
CapEx Capital Expenditure
CEMS Continuous Emission Monitoring Systems
EPA Environmental Protection Agency
FEED Front-End Engineering Design
HSE Health Safety and Environment
PCA Principal Component Analysis
PEMS Predictive Emission Monitoring Systems
Technical Paper

PS Performance Specification
QA Quality Assurance
RA Relative Accuracy
SRU Sulfur Recovery Unit

References
Appendix – PEMS Generalities

Predictive Emission Monitoring Systems (PEMS) are an alternative technology for measuring emissions based on software. More in specific, PEMS use advanced mathematical and statistical models able to exploit the correlations existing between process parameters and the emission properties.

Predictive systems development and on-line deployment is performed in different stages; even if the core activity is represented by the model building itself, all other tasks are also essential in order to create accurate models:

- The data collection is performed in order to acquire a baseline dataset including both emission and process parameters suitable for developing the models. This dataset has two crucial requirements: a) it shall be representative of all the possible operating condition of the monitored unit/plant; b) it shall be able to describe properly process dynamics. Therefore, great care must be given to proper variable selection and to optimal sampling time. Data collection is substantially different if PEMS are used as back-up of existing CEMS or as a single source for emission monitoring: in the first case, emission and process data can be gathered from plant historians (or other platforms) available at site. In the latter, a temporary analyzer has to be installed at stack for a limited amount of time in order to acquire the emission values while simultaneously process data are extracted from the control system.

- Data processing is crucial in order to prepare the final refined dataset to be used for the model building phase: during this task, bad quality data and outliers are removed and the process variables are analyzed in order to identify the best candidate as model inputs. Here advanced statistical techniques – as the Principal Component Analysis (PCA) – are employed in order to support the engineer in this choice.

![Figure 6 - A typical software used for data processing, model development and validation](image)
Model Building and offline validation are the core parts of any PEMS project: here different models, using several algorithms and structures, are realized for each pollutant and finally tested on a fresh dataset in order to check their accuracy and robustness and to find out which is the most suited for being implemented on-line.

Deployment: once the final models have been validated offline, they are installed on-line and fed with real-time values acquired from the control system. PEMS software normally provides the facilities in order to read and validate on-line the data from the DCS and write back the emission estimation on the same system or other automation platform.

Certification phase is the final assessment performed on site and which is crucial in order to get the acceptance from the local authorities.
Typically, this is performed comparing the measurement from a physical analyzer and the values produced by PEMS and verifying that the accuracy of the models meets the requirements imposed by the regulations.

As PEMS are built on the ground of historical data, a crucial pre-requirements is that the plant has to be properly instrumented: the key process parameters shall be continuously measured and acquired by a control system with which the PEMS software shall interface.

The other important point is related to the quality of the fuels used in the process: this shall be quite stable or monitored in order to properly manage the fluctuations in some compounds, which directly affect emission values (e.g. H\textsubscript{2}S, CO\textsubscript{2}).

Provided that the above conditions are met, PEMS can be applied to any combustion process across the different industry sectors, from the oil and gas, petrochemical to power, cement. In particular, the technology is perfectly suited for the monitoring of some stationary sources as gas turbines, boilers, heaters.

PEMS solutions deliver some inherent advantages over the conventional hardware instrumentation. The main one is represented by their cost-effectiveness: typical lifecycle cost of predictive systems is around 50% of a conventional CEMS. This is due not only to the lower initial investment, but also to the lower requirements and costs of maintenance; being based on software, PEMS do not require any specific consumables or spare parts, allowing consistent savings in terms of material and warehouse costs.

Additionally, they are independent from the supplier of the control system: using standard communication protocols, PEMS are able to interface and to be integrated easily with the existing infrastructure available at site with limited engineering effort.

At last, also PEMS footprint is very compact (essentially, it is just a standard PC) and much less invasive than conventional CEMS, since they do not require any dedicated sampling line nor shelter and cabinets hosting the sensing elements.