

Inferential Sensors for Emission Monitoring: an Industrial Perspective

Nunzio Bonavita¹, Gregorio Ciarlo²

ABB S.p.A., Italy, Via Albareto, 35 – 16153 Genoa, Italy

*nunzio.bonavita@it.abb.com; gregorio.ciarlo@it.abb.com

Abstract

Industrial plants, to comply with environmental regulation, have to monitor, store and report emission data. The traditional and most performing approach, and therefore the most applied one, is represented by the Continuous Emission Monitoring Systems (CEMS), where a continuous stream of data is acquired by rapid-response instruments, displayed in real-time and stored for archiving and reporting purposes. However in the last years, advanced modeling technologies have made available a powerful complement to the hardware based analyzers which are the heart of most CEMS.

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 through any hardware device, but use computer models to predict emission concentrations on the ground of process data (e.g. fuel flow, load, and ambient air temperature). They actually represent a relevant application arena for the so-called Inferential Sensor technology which has quickly proved to be invaluable in modern process automation and optimization strategies.

While lots of applications prove that software systems provide accuracy comparable to that of hardware-based CEMS, virtual analyzers are able to offer additional features and capabilities which are often not properly considered by end-users. Depending on local regulations and constraints, PEMS can be exploited either as primary source of emission monitoring or as an enhancement to hardware-based CEMS.

The present paper aims at providing feedback from industrial field experience related to both the approaches. Lessons learnt at two large projects in O&G Production and Refinery will be used as examples which justify the quickly growing confidence on this modern and efficient technology.

Keywords

Inferential Sensor; PEMS; Emission Monitoring; Virtual Analyzers; Non-invasive Monitoring

Introduction

According to ISO 14001, the goal of Environmental Management Systems (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” [ISO]. In accordance with this, a typical EMS is designed to provide a number of functions, including:

- Collecting and processing environmental-related data
- Providing key environmental performance indicators
- Providing environmental performance evaluation planning
- Emission calculation and reporting
- Record keeping and audit trail functionalities.

Within any EMS, a major role is played by air pollution control and prevention. In order to monitor the pollutant released into the atmosphere, the industry typically relies on Continuous Emission Monitoring System (CEMS). A CEMS is defined as the total equipment used to acquire reliable data on air emission levels, including sample extraction, treatment and transportation hardware, analyser, data recording and processing hardware and software [Arioni].

CEMS can broadly be broken into three types of methods (Fig. 1, see also [EPA Handbook]):

- Extractive Methods
- In-situ Instrumental Methods
- Parameter-based Methods.

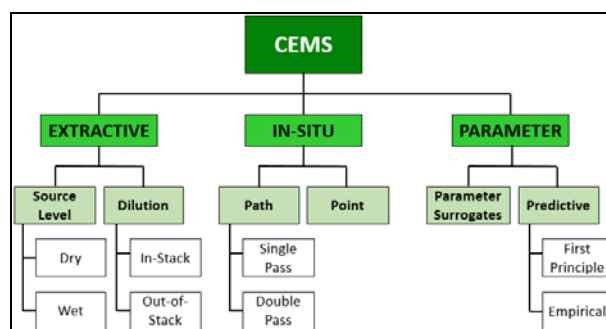


FIG. 1 TYPICAL CEMS CONFIGURATIONS

There are two classes of parameter-based methods: surrogate and predictive.

Surrogates may be used to determine the compliance of a source with the emission standard. Predictive parameters are applied in cases where a functional relationship between process conditions and emission levels is such that it cannot be properly described by a single parameter. This is where the inferential sensor technology applies under the name of predictive emission monitoring system (PEMS).

PEMS are software-based systems that exploit advanced mathematical models in order to estimate emission values. Typically PEMS models are built on process data, such as fuel flow, load, operating pressure and temperature. PEMS provide an effective way in order to obtain a continuous stream of (estimated) emission values in process units where CEMS are not present. According to a growing number of environmental regulations, plants are allowed to lease a portable CEMS to gather sufficient emissions data to build and validate mathematical models.

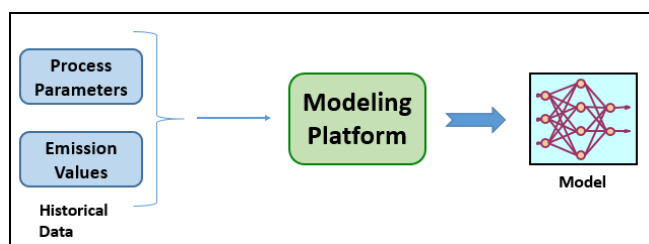


FIG.2 INFERRENTIAL MODELING FOR EMISSION MONITORING

Once the models have been qualified, temporary CEMS is removed and replaced by the inferential-type system. PEMS can also be used as a back-up if a CEMS is in place, and irrespective of which role it plays, it provides numerous benefits in different applications [Samdami].

Inferential Sensors and PEMS

Highly complex processes mostly characterize modern industrial plants. The complexity stems from the number of inputs and outputs, the frequent occurrence of delays, the inherent process non-linearity and the high degree of interconnection between the various process units (heat regeneration, recirculation, etc.), indispensable to make production more energy efficient.

Complexity management strategies need to access accurate, timely and reliable information on process conditions in order to properly select the set of actions

which can assure safety, mitigate environmental impact and optimize economic performances.

Modelling techniques have become a key pillar for control and monitoring strategies for its capability to provide compact and efficient descriptions of the behaviour of a process or event. Essentially models are based on equations which are able to compute values of unmeasured variables using other process variables as input values. Depending on the nature of the model, this may or may not represent a causal relationship.

One of the main application of modelling in process control aims at inferring hard-to-measure variables from other measurable process variables. Paradoxically hard-to measure variables are often among the most important ones for plant economic performances, as they include final or intermediate product qualities. Because of their relevance they are traditionally measured through devoted and expensive laboratory tests. However meaningful results are affected by two kinds of problems related to their limited availability (analysis are performed infrequently, usually 1-4 times a day) and the unavoidable delays (one or more hours) due to sample extraction and processing times. These problems have heavy impact on overall performances often preventing any possibility for process optimization. A possible solution is represented by including more and more process analysers in the process, but this could result expensive (both as Capex and Opex, due to disposables and calibration costs) and difficult to be implemented in harsh environment or when available room is an issue.

Inferential sensors have been designed, developed and deployed mainly to provide a practical and affordable alternative to process analysers. They are in fact able to deliver reliable, real-time and continuous estimation of critical quality variables with a non-invasive technology requiring much less initial investment and only a fraction of the maintenance costs.

The fundamental principle behind inferential sensors is that there is a functional relationship between the variables to be predicted and process operating conditions [Qin]. Since 1978 when the Kalman filter approach was proposed, once a state space model is available [Joseph and Brosilow], several different technologies have been exploited to the scope. Nowadays there are two poles in modelling technology, the theoretical and the empirical [Bonavita and Matsko]. 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. The empirical model may just imply that the same driving forces move both the input and output variables, and that they are related by the underlying theoretical model. So the user must insure that the underlying process does not change behaviour if an empirical model is used.

In practice, full theoretical models, although in principle very powerful, require such an effort so as to make them very expensive to derive and only used in full scale optimization projects.

On the other side the massive presence of computers and IT technology in control room has made process plants become actual “data-manufacturers”, where hundreds of thousands data are collected and stored each day [Bonavita and Martini]. With such an abundance of “raw data” the problem moves from how to write and solve complex theoretical equations to how to manage process data in order to distillate a reduced amount of valuable key information. A number of data processing and modelling techniques come to help the end-user and are included in several software packages that are commercially available in user-friendly formats, reducing the entry barrier to the scope.

The merging of the reduced developer effort (and competence needed), the abundance of data and the growing power and ease of use of data mining techniques, makes quite a case in favour of the empirical modelling approach.

While real-time product quality prediction was the original reason for developing inferential sensors, starting from mid-90s air emission monitoring became a relevant application field as well [Keeler]. The extension is pretty straightforward: like Inferentials are a convenient alternative to process analysers, so PEMS can be the same for hardware-based CEMS. Although there are relevant differences mainly due to regulations and implementation (for example PEMS outputs are very seldom used for closing control loops), the two applications share most of the technical challenges.

In the last fifteen years, many projects have proven that software systems are practically just as accurate as the hardware-based CEMS. In addition, virtual analysers offer other exclusive functionalities that can:

- Identify the key variables that cause emissions

- Automatically validate sensors
- Reconstruct emission levels from historical data when the hardware device fails
- Complement and enhance process optimization strategies.

However PEMS penetration has been slower than expected and seems ready to accelerate just now [Shoker]. A reasonable explanation is that not enough attention has been paid to practical implementation issues. As a matter of fact, PEMS technology is at the crossroad among different technical disciplines, combining knowledge and expertise from process automation, process analytics and Information Technology.

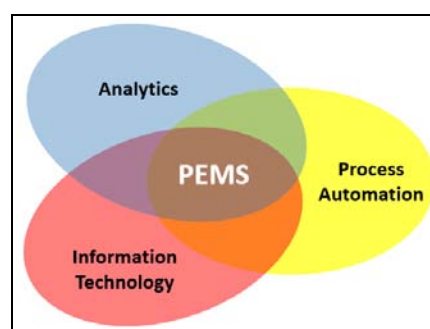


FIG.3 PEMS KEY TOPICS

To fulfil the requirements from the industry and deliver an effective solution, PEMS providers must be able to condensate their know-how in process and analytics and integrate it within the complexity of plant infrastructure and network.

In the following a number of lessons learnt and experience-driven considerations will be shared complemented by two actual case studies related to the use of PEMS in industrial applications.

Industrial Applications Fields

Inferential analysers are nowadays a widely accepted technology for emission monitoring purposes, although their usage is quite different depending on the provisions of the local environmental regulations. Essentially PEMS can play two main roles:

- As the primary source for emission monitoring; this option is accepted by several US states and by a growing number of countries especially in Middle East [Shoker].
- As a back-up of traditional CEMS to provide a redundant measurement which increases the availability of emission data. This option is acknowledged especially in Europe and Far East because of the possibility to extend the

service factor of CEMS, covering periods when the hardware-based devices are not available because of failures or maintenance activities.

There is also a third possibility for PEMS usage, which is somehow an intermediate between the back-up and the primary source approach: predictive systems allows the extension of emission monitoring programs from campaign-based to continuous ones.

In the last section of this paper two industrial applications where authors have been involved will be briefly described in order to outline the different approaches and the peculiarities of each one.

PEMS Project Workflow

No matter the final applications, implementing a PEMS systems encompasses three main activities:

- Data-collection
- Model building and off-line validation
- System commissioning.

The data-collection phase is aimed at gathering a baseline of process and emission data to be used for model development. This phase is quite different if PEMS is designed to back-up an existing CEMS or to act as the primary emission monitoring tool. In the first case the data-collection can be easily performed extracting emission and process data from plant data acquisition systems (e.g. historian, EMS). Otherwise, a temporary analyser has to be installed at plant-site for a period in order to collect pollutant concentration values, while in parallel real-time values are gathered from the control system.

The data-collection phase has to be accurately designed and executed in order to cover all the normal operating conditions and to ensure the maximum reliability and robustness to the final models. The key requirement is related to the characteristics of the data: emission and process data must be in raw format with minimal or no time-compression factor in order not to lose relevant information concerning variability of the different operating and emission parameters. It is in this phase that analytical competences have an invaluable role: choosing the best technologies for the temporary analysers to be installed at site and validating the provided emission measurements (allowing, for example, a pre-identification of bad-quality data) will have a tremendous impact on system final performances.

Model building and validation are “the heart” of any PEMS project: it includes all the tasks from pre-processing of raw data to the final testing of the

inferentials and requires the usage of advanced statistical, mathematical and modeling techniques. The amount of mathematics and statistics to be used here is not trivial and could represent an entrance barrier to this solution (and actually it did in the past). However technology comes to help the developer with advanced software packages which provide powerful algorithms in easy-to-use formats and environments

Several years of experience allow to specify at least three critical phases where IT and data management tools are essential for PEMS successful implementation:

- Data Pre-processing, which includes the removal of outliers and other bad-quality data, the definition of the proper sampling time and the identification of the most representative variables to be used for model development. An easy to use interface is crucial to exploit advanced statistical methods, like Principal Component Analysis (PCA), that support the developer in creating much better performing models.
- Model Building itself, where a number of modelling techniques, such as Artificial Neural Networks (ANN), Genetic Algorithms, Partial Least Squares (PLS), could be selected and used depending on goals and constraints. In particular neural networks have proved to ensure the needed flexibility and robustness to the models and are commonly used for emission monitoring purposes.
- Model Validation, where models have to be carefully validated off-line in order to ensure their performances and reliability is suitable for on-field application.

Several commercial packages are nowadays available in order to assist PEMS engineers in the phases above. No wide spread of PEMS is and will be possible without their presence and further progress.

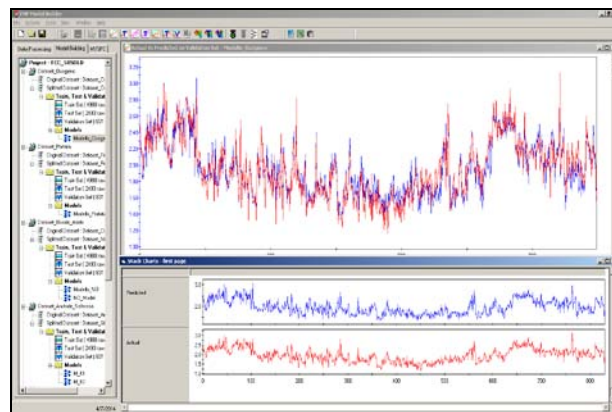


FIG.4 EXAMPLE OF A SOFTWARE FOR PEMS DEVELOPMENT

The final stage of PEMS projects is the implementation of the models at plant side: here they must be properly installed in computing platforms connected to the basic automation layers so to be fed with the real-time process values in order to generate the required predictions (see Fig.5).

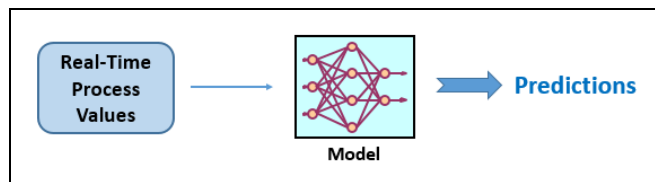


FIG.5 ON-LINE MODEL DEPLOYMENT

Putting the models on-line is not enough. A number of possible additional schemes could be added to improve PEMS performances. For example, when a physical measurement is available (e.g. from infrequent lab analysis or from CEMS if PEMS acts as back-up), models are typically accompanied with a periodic recalibration procedure able to improve their accuracy over the time. These strategies compute the discrepancies between model prediction and physical measurement. The difference is statistically treated (in order to mitigate possible errors from noise or outliers and provide bumpless adjustment) and, if exceeds predefined thresholds, a recalibration factor is calculated and added to the model output, enhancing its accuracy and avoiding drift in case of failure in input sensors.

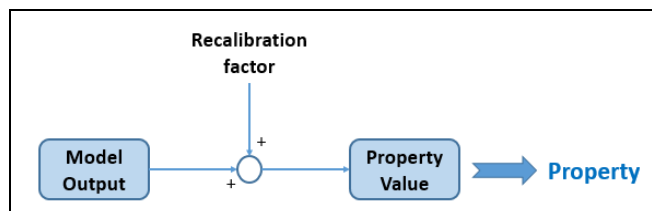


FIG.6 RECALIBRATION FACTOR CONCEPT

From an operative point of view it is very important that the recalibration strategies are implemented in order to update models only when a statistically significant change in the process is detected.

Practical Issues

From an industrial perspective, the development of an effective PEMS solution is much more than the simple creation of the models, but it is a combination of several ingredients that have to be put properly together.

As seen, process and automation know-how has a major role. PEMS developers need an extensive and sound understanding of process dynamics and control

strategy in order to check and validate the inputs from mathematical and statistical tools. Another fundamental element to be considered concerns final PEMS implementation at plant. Developing reliable and accurate models is not enough to fulfil end-users requirements: successful applications necessitate to overcome the gap between the advanced modeling techniques and the implementation in the control room. The seamless integration with the existing infrastructure is crucial in order to provide an effective solution. Predictive systems have to be able to dialog and interface with other automation layers through standard communication protocols, minimizing times and efforts for the commissioning phase.

When installing PEMS on site, providers shall take into account also that plant personnel is often not familiar nor comfortable with advanced mathematical and modeling techniques. Software platform shall be fully transparent to the operators regarding the technology background but must provide them all the relevant information concerning emission values in a clear and manageable way. This point is clearly of paramount importance since it makes the solution truly effective once at site: otherwise, the risk is to develop a very powerful application which operators are not confident in because of its “complexity”.

A final and often neglected issue to be considered is related to application maintenance. Generally process units operate under time-varying conditions. Different market requirements, feed or raw material quality variations, normal component aging slowly may drive unit conditions outside the ‘window’ which has been explored (and modelled) during project execution. Because empirical models, and neural networks in particular, are not specifically good in extrapolating [Qin], it is recommended and good engineering practice to foresee a periodic data collection campaign (usually 1 week per year) which will be used to retune and refine the models. Further than improving the overall PEMS performances (“Neural networks learn from experience”) this practice will also allow to increase detailed process know-how and personnel awareness on what’s going on and how the plant is behaving. Because of the impact on long-term performances, logistics and cost of yearly maintenance should be taken into consideration in the life-cycle cost assessment. From a practical perspective periodic recalibrations highlight the benefit of wide-spread service networks which can efficiently perform the after-commissioning activities with minimal intervention time and reduced cost.

Case Study I: PEMS as a Primary Monitoring Source

PEMS have been successfully implemented as the primary emission monitoring source at a gas injection unit in a major O&G production facility in the Gulf Region.

The injection plant is made of two parallel compression trains: before injection, gas undergoes two compression stages each driven by a gas turbine, as depicted in figure 7.

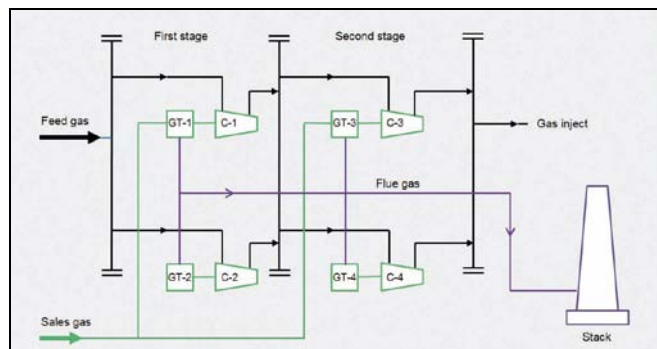


FIG. 7 GAS INJECTION PLANT LAYOUT

PEMS solution was developed in order to monitor the following pollutant emissions from each gas turbines:

- NO_x;
- SO₂
- O₂;
- CO;
- CO₂.

In order to acquire the emission values needed from models creation, a temporary CEMS was used at each stack, while a simultaneous set of data was collected directly from the plant control system through a standard OPC protocol. This data-collection phase lasted about six weeks in order to cover the widest range of operating conditions, providing an adequate baseline for an effective predictive solution.

Following the data gathering, plant and emission data were processed in order to remove bad-quality data and outliers and to identify the relevant variables to be used as input for the models. Each model was developed using a set of 6-8 input identified among most relevant process (e.g. fuel gas flow, exhaust gas temperature, compressor gas flow) and ambient parameters (e.g. air humidity). Feedforward neural networks were chosen as model architecture since they proved to be the most accurate and robust.

Inferential models were implemented at site and integrated with the existing IT infrastructure: a standard OPC protocol was used to gather real-time data from plant DCS and to write back the predictions. After the commissioning, an Environmental Protection Agency (EPA) assessment was performed in order to verify system performances and compliance to the applicable regulations [EPA]. PEMS estimations were compared with the measurements of a certified temporary CEMS: 18 test runs lasting 30 minutes each at different operating conditions were performed in order to calculate PEMS relative accuracy:

Pollutant	RA (95% Load)	RA (100% Load)
O ₂	< 10%	< 10%
NO _x	< 10%	< 15%
SO ₂	Undetected (< 1 ppm)	Undetected (< 1 ppm)
CO	< 10%	< 15%
CO ₂	< 10%	< 10%

FIG. 8 FINAL PERFORMANCES OF THE SYSTEM

PEMS performances proved to be comparable with the temporary CEMS, allowing to obtain the final certification.

Case Study II: PEMS as an Enhancement and Back-up to Hardware-based CEMS

A major European refinery had the necessity to increase the up-time of its Emission Monitoring System in order to fully comply with local regulation in terms of emission data availability. Environmental authorities may impose plant shutdown in case pollutant concentration data are not available for extended periods. The end user chose to install PEMS to back-up traditional CEMS installed at two relevant units: Fluid Catalytic Cracking and Sulphur Recovery Units.

PEMS system was designed to provide an estimation of the following pollutant parameters from each plant:

- NO;
- SO₂
- O₂;
- CO;
- Flue gas flow;
- Particulate.

SRU and FCC processes determined additional challenges to the development of an effective inferential solution: their operations (and consequently the final emission output) are strictly related to the characteristics of the processed feeds and to the performances of the upstream units which are obviously subjected to wide and unforeseeable variations.

Historical process data and emission values were extracted, respectively, from the plant historian and the emission data acquisition system in order to gather a significant set of information suitable for model creation: a six month baseline of synchronized data were necessary to assess properly the model building and validation phases.

During the model building phase a close interaction with plant personnel was instrumental to support PEMS developing team in identifying model input variables, validating simulations and tests performed through PCA and other advanced mathematical techniques. Once the design and validation phases were completed, the predictive system was commissioned and integrated with the existing IT data acquisition system, allowing the usage of predicted measures for the refinery bubble limit when CEMS are out of service.

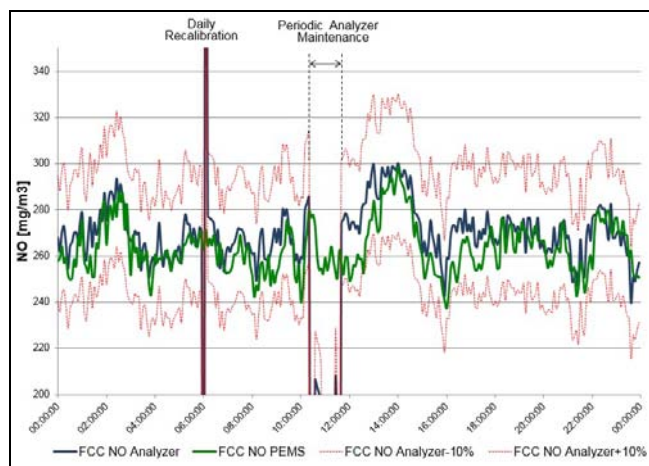


FIG. 9 PEMS SUBSTITUING OFF-SERVICE ANALYZERS

The adoption of PEMS as a complement to the traditional HW-based system provided the plant with a very accurate alternative to traditional HW-based analysers, allowing to comply with the provisions of the environmental regulation and to extend the operating availability of the emission monitoring system well above 97.5%. Fig. 9 shows the excellent agreement between CEMS and PEMS, and the reliability of the latter during the period when CEMS had to be shut-off for Periodic Maintenance.

Conclusions

Industry focus on emission monitoring is growing significantly due to the ever increasing public perception and interest on environmental matters and to regulating frameworks that are becoming more and more stringent. PEMS have shown the capability to provide a valuable alternative to traditional HW-based analysers, offering comparable level of performances and reliability. Plant owners are becoming more and more aware of PEMS potentialities and are focusing their interests on this technology. However as this paper has described, the development of effective data-driven solutions for emission monitoring is not so straightforward.

Basing on the experience acquired on several years applying inferential technologies for both quality and emission monitoring, PEMS implementation at production sites is bounded to the fulfilment of these three fundamental requirements:

- **Technology:** since the model creation phase involves the usage of complex mathematical and statistical routines, it is required an easy-to-use software environment to enable the user to perform all the engineering steps in an easy and effective way. In addition PEMS require to be integrated within the plant network and automation infrastructure: this means that standard interfaces and communication protocols shall be provided in order to dialog with every system present at site.
- **Know-how:** to develop an effective solution, engineers should have an extensive background encompassing from process knowledge to automation and control strategies skills, from base instrumentation expertise to advanced analytics competences.
- **Local presence:** a wide-spread network of technicians and engineers is crucial to provide support to the users during the different phases of a project. In addition, local resources can be easily contacted and, if needed, mobilized in order to perform upgrades and first level services on the system.

PEMS successful diffusion is mainly conditioned by the acknowledgement and the overcoming of these potential issues. Some companies structured to overcome the hurdles and are now able to deal with PEMS challenge on a global scale.

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Nunzio Bonavita is the Business Development Manager for ABB Measurement Products Business Unit Italy. He graduated in Particle Physics from the University of Pisa working at the CDF experiment for the Top Quark quest at Fermi National Laboratory (Batavia - Illinois). He has over 25 years' experience in process automation with particular emphasis on advanced applications. For six years he led an international team who designed, realized and maintained a commercial advanced process control product suite. Recently he has been responsible for Technology Management in the Mediterranean Region, focusing on topics ranging from oil & gas, energy efficiency, water management in industrial plants and advanced instrumentation.

He is author or co-author of about 60 papers published on technical magazines or presented at international conferences.

Since 2009 he is Contract Professor at the Chemical Engineering Dept. of University of Genoa.



Gregorio Ciarlo was born in Genoa in 1984; he graduated in Environmental Engineering from the University of Genoa, Italy in 2009, focusing on modeling of hydraulics phenomena.

He is PEMS Product Manager for the ABB Measurement Products Business Unit in Genoa. He spent 3 years in the Technology Management Department focusing and developing specific experience in energy efficiency, advanced process control techniques and advanced instrumentation.