Chemical Product and Process Modeling

From Reacting to Predicting Technologies: A Novel Performance Monitoring Technique Based on Detailed Dynamic Models

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Abstract

Performance monitoring has the main aim to analyze operating process unit efficiencies especially to lower variable costs, increase profitability, and improve the supply chain optimization in terms of enterprise resource planning (ERP), production accounting, and optimal scheduling of maintenances. Nevertheless, the industrial state of the art is based on approximated techniques for data reconciliation and performance monitoring, which make use of the plant historical database and adopt regressive methods to predict trends of future efficiencies, whereas more reliable performance monitoring techniques are needed to obtain an effective ERP. On this subject, the paper shows how the process performance monitoring is fast moving from reacting towards predicting methodologies and proposes a novel promising technique based on unsteady detailed models to tackle this issue.

KEYWORDS: performance monitoring, predicting techniques, robust ERP, process uncertainties

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1. INTRODUCTION

The renewed interest in process data reconciliation and real-time performance monitoring by both the academic world and the process industries is mainly due to the introduction of new process control technologies and the increasing number of advanced control applications, i.e. nonlinear model predictive control, dynamic optimization, and enterprise resource planning (ERP).

It is worth noting that, after feedstock supplies and energy consumptions, process maintenances represent the largest portion of operative costs for crude oil refineries and natural gas plants. Moreover, failure maintenances that are due to accidents or malfunctions can occur without any advice to reduce further the enterprise profit margins. Actually, unexpected failures can strongly influence the overall production and, consequently, both the long-term operational planning and the production accounting.

On this subject, the main aim of the present work is to investigate the performance monitoring techniques and approaches that manage to predict the future behavior of unit operations, in order to reduce the number and, at the same time, the duration of maintenance shutdowns by means of a detailed prediction of the unit efficiencies. Such an approach is more and more necessary in process industries especially if we think that it is not possible to obtain a reliable production scheduling through the existing techniques.

Actually, by means of the existing techniques, either several units fail before the expected stop or the maintenance is erroneously predicted in advance. These two scenarios are both characterized by economic losses and they require an instantaneous production scheduling redefinition.

Recently, some authors (White, 2003; Grottoli et al., 2008) described the importance of some detailed mathematical models to plan both future production and programmed maintenances in a more accurate way, even though a lot of them are still conceived as steady state tools, which are usually incapable to follow the process dynamics, especially on the long-term scale. Several studies try to extend the use of complex mathematical models to achieve a robust ERP (White, 2001; White, 2003; Kim and Joo, 2005; Manenti, 2007).

The stiff hierarchy that constitutes the ERP is explained (see section 2). A survey of existing techniques for raw data reconciliation is given in section 3. Performance monitoring and the novel predictive technique are discussed in section 4. At last, the predictive performance monitoring is implemented to estimate the future key performance indicator (KPI) trajectories for some critical process units. A detailed model of natural gas plant, which is already discussed elsewhere (Manenti, 2009), is adopted as a case study.
2. ERP ARCHITECTURE

Data reconciliation and performance monitoring systems are strictly related since the former allows transforming real-time process data into consistent and reliable information for business, whereas the latter uses this filtered information to produce accurate KPIs of plant/unit performances. It is not a coincidence that capital investments on data reconciliation feasibility studies as well as practical on-line implementations are recently increased in the industrialized countries during these last years (Narasimhan and Jordache, 2000; Grottoli et al., 2008).

Specifically, the reconciliation of raw data coming from the field may be seen as a comprehensive solution for:

− outlier detection;
− data validation;
− instrument analysis.

On the other hand, the performance monitoring can be considered as the necessary tool for:

− daily/weekly/monthly/yearly production accounting;
− supporting the model predictive control and the real time optimization;
− process design and operating/tactical optimization;
− supporting the scheduling of programmed maintenances;
− obtaining a robust ERP.

Unfortunately, facing their relevant impact on the process industry, the aforementioned systems are also strongly interconnected to other process control and optimization applications in a stiff hierarchical structure (see Figure 1), which makes the problem multifaceted and hard to solve. Actually, all the measures coming from the plant are sent to the DCS, where the most significant pieces of information are visualized and at the control-room operators’ disposal.

The information system allows reconciling the stored raw industrial data and transferring it to off- and on-line applications associated to the plant.

Besides the reconciliation of raw data (and, sometimes, besides the quadratic optimization dictated by the nonlinear model predictive control level), KPIs are evaluated for the critical process units. KPIs allow defining both the medium term optimization (schedule of maintenances) and the long-term optimization (ERP).

It is worth considering that a good scheduling gives a relevant support to the ERP; in turn, an adequate performance monitoring allows defining a more reliable scheduling of maintenances; an appropriate tool for data reconciliation provides an accurate performance monitoring. Therefore, data reconciliation and performance monitoring tools unavoidably are the key-components for a robust ERP, which allows enterprises reducing risks in the capital investments.
3. DATA RECONCILIATION TECHNIQUES

The data reconciliation is a useful tool to reconcile measures in order to satisfy material and energy balances of every process unit and plant sub-section that is characterized by an adequate measurement redundancy.

The idea of reconciling measures is quite old and can be brought back to the early 50s of the previous century. Nevertheless, the recent implementation of the advanced process control and optimization techniques (see Figure 1) as well as the advances in the information technology, which is the fundamental support to ERP and decision-making process, are forcing process industries to be interested in performing and robust tools for the process data analysis and reconciliation (Romagnoli and Sanchez, 1999).

On this subject, to provide a coherent picture of plant performances, the objective is to minimize a function \( F \), which is usually the weighed sum of square residuals between measured and reconciled variable values:

\[
\min_{x_i} F = \sum_i \omega_i (m_i - x_i)^2
\]

subject to:

\[
\begin{align*}
g(x) &= 0 \\
h(x) &\leq 0
\end{align*}
\]

subject to equality \( g(x) = 0 \) and inequality \( h(x) \leq 0 \) constraints. \( \omega_i \) is the weight vector, usually the variance or the standard deviation. \( x_i \) and \( m_i \) are the
reconciled and measured values, respectively. This sum accounts for all the relevant measures.

3.1. Linear Reconciliation

The linear technique is usually employed in facilities and utilities for steam generation, where the only component is water (other components are negligible). As a consequence, these processes do not require any in-line analyzer to measure molar compositions. Again, they are often characterized by small redundancies in measures, especially for the reduced interest to place some instrumentation on all the condensed water lines. By chance, the overall mass and energy balances are enough to characterize the process.

In this context, apart from a stream compensation that has the aim to equalize the vapor flow rates to the liquid ones, the material reconciliation problem can be easily defined as follows:

\[
\min F = \sum_{i} \omega_{i} \left( w_{i} - w_{i,\text{rec}} \right)^{2}
\]

subject to:

\[
\begin{align*}
    g(w) &= 0 \\
    h(w) &\leq 0
\end{align*}
\]

where \( w_{i} \) is the mass flow rate. Depending on redundancy (or the degree of redundancy, DOR):

\[
DOR = \text{equations} + \text{measures} - \text{reconciled}
\]

four different situations can occur:

1. the total amount of measures and equations is slightly larger than the number of process flow rates. In such a condition of reduced redundancy, the data reconciliation can be regularly carried out, even if it may be difficult to detect possible outliers (Buzzi-Ferraris and Manenti, 2009a; Buzzi-Ferraris and Manenti, 2009c; Manenti and Buzzi-Ferraris, 2009), which commonly affect measures coming from the field;

2. the total amount of measures and equations is equal to the number of process flow rates. The reconciliation becomes critical since the presence of one outlier makes the reconciliation infeasible and may lead to the so-called masking effect (Buzzi-Ferraris and Manenti, 2009b). However, the data reconciliation can be still carried out;
3. the total amount of measures and equations is equal to the number of process flow rates minus one. The reconciliation problem is transformed into a coaptation problem. Under the assumption of total absence of outliers (in order to make the problem feasible), missing data can be evaluated;

4. the total amount of measures and equations is smaller than the number of process flow rates minus one. No actions are possible in this case, except for the data reconciliation of some specific sub-sections that agree with one of the previous points.

It is important to highlight that a feasible reconciliation can be guaranteed by ensuring an adequate measurement distribution by the field and the development of an appropriate process control scheme. Actually, even though $DOR > 0$, some plant sub-sections might be not reconcilable; on the other hand, when $DOR < 0$ some plant sub-sections might be reconcilable.

3.2. Bi-linear Reconciliation

3.2.1. Component Balances

Contrarily to steam generation utilities and facilities, when the process flow rates are multi-components, the reconciliation problem has to be extended from the linear case to the bi-linear one. Actually, it is necessary to reconcile not only the overall material flow rate, but also the mass component rate. It unavoidably requires some in-line analyzers, besides the flow measures.

By doing so, the reconciliation problem assumes the following form:

\[
\min_{w_{i,rec}, n_{i,rec}} F = \sum_{i} a_i \left( n_i \cdot w_i - n_{i,rec} \cdot w_{i,rec} \right)^2
\]

subject to:

\[
\begin{align*}
g(n, w) &= 0 \\
h(n, w) &\leq 0
\end{align*}
\]

which makes the problem nonlinear. From a computational point of view, it is useful to keep the problem linear when possible. In this context, it is worth noting that, by introducing the overall component flow rate $N_i = n_i \cdot w_i$, it is possible to write the following bi-linear objective function (Crowe et al., 1983; Crowe, 1989):
\[
\min_{w_{i,rec}, N_{i,rec}} F = \sum_i \omega_i (w_i - w_{i,rec})^2 + \sum_i p_i (N_i - N_{i,rec})^2 \\
subject \ to: \quad \begin{cases}
g(N, w) = 0 \\
h(N, w) \leq 0
\end{cases}
\]

where \( p_i \) is a weight vector. Formulation (5) allows overcoming the initial nonlineairities of the objective function, by means of specific data pre- and post-processing.

### 3.2.2. Energy Balances

The same procedure can be followed in the simultaneous solution of mass and energy balances:

\[
\min_{w_{i,rec}, T_{i,rec}} F = \sum_i \omega_i (w_i \cdot c_p \cdot T_i - w_{i,rec} \cdot c_p \cdot T_{i,rec})^2 \\
subject \ to: \quad \begin{cases}
g(T, w) = 0 \\
h(T, w) \leq 0
\end{cases}
\]

by introducing \( H_i = w_i \cdot c_p \cdot T_i \) and, therefore, \( \tilde{H}_i = H_i / w_i \). The reconciliation problem becomes:

\[
\min_{w_{i,rec}, H_{i,rec}} F = \sum_i \omega_i (w_i - w_{i,rec})^2 + \sum_i p_i (\tilde{H}_i - \tilde{H}_{i,rec})^2 \\
subject \ to: \quad \begin{cases}
g(\tilde{H}) = 0 \\
h(w) = 0 \\
\hat{i}(\tilde{H}) \leq 0 \\
\hat{j}(w) \leq 0
\end{cases}
\]

Sometimes, specific problems require the simultaneous reconciliation of overall mass, component, and energy balances. Through the aforementioned
devices, it is possible to transform the nonlinear problem into the tri-linear data reconciliation. Theoretically, there are no limits to the number of linear terms.

3.3. Nonlinear Reconciliation

Contrarily to the aforementioned techniques, the nonlinear data reconciliation is fast acquiring interest in process industry, especially because the coupling of a reconciliation tool to an existing process simulation package, such as PRO/II™ developed by Simsci-Esscor, UNISIM™ by Honeywell, and HYSYS™ by Aspen Technology, may lead to several advantages.

*Prima inter pares* there is the possibility to base the whole reconciliation on detailed mathematical models, which go beyond simple mass and energy balances. It may strongly increase the accuracy of data reconciliation and significantly support the detection of gross errors and masked outliers. Consequently, performance monitoring, scheduling, and ERP should be relevantly improved. Formulation of nonlinear data reconciliation problems corresponds to the aforementioned cases. The relevant difference is in constraints: physico-chemical properties, thermodynamic, equilibrium, hydraulic relations, etc., all deriving from a detailed process modeling, are introduced as additional (and nonlinear) constraints.

For example, let us consider a depropanizer column with three flow measures on feed, bottom, and distillate lines. To obtain an effective reconciliation, it is surely better to solve the mass reconciliation problem by implementing the whole model of the column rather than basing our results only on the overall mass balance. Of course, it requires a higher CPU time for solving the problem. Nevertheless, by considering industrial requirements (one data reconciliation per hour or per day), the current computational power ensures faster solutions of nonlinear reconciliation problems, making feasible their on-line implementability with extremely large CPU margins.

4. PREDICTIVE PERFORMANCE MONITORING

The monitoring of process unit performances is a useful tool in the definition of maintenance scheduling. Unfortunately, it is not an easy goal to achieve, since unit performances are subject to a combination of effects and their evaluation and prediction is a multifaceted problem and an open issue especially in computer-aided process engineering and process systems engineering communities.

Let us consider the qualitative trend that is reported in Figure 2. Supposing the production capacity constant, it shows two different kinds of unit performance losses:
1. *in primis*, it is worth noting that the clean nominal performance is not constant throughout the plant life-cycle. Actually, a falling clean performance characterizes each process unit and the gap with the initial performances (just the design condition) increases with the number of cleaning cycles. This situation suggests to operate programmed maintenances as late as possible, in order to reduce the derivative of the falling clean performance;

2. secondly, after each cleaning cycle, the current equipment performances decrease faster than the aforementioned falling clean performance. Moreover, the performance loss is strongly emphasized by increasing the number of cleaning cycles. This latter contribution leads to a rival solution if compared to the former one: since the highest performance is immediately after the cleaning cycle, the programmed maintenance should be carried out as soon as possible.

According to other previous works (Doymaz *et al.*, 2001; White, 2003), the performance monitoring procedure can be schematized in different steps. Figure 3 shows the five steps needed in the predictive approach:

- *measure*: process variables are measured by the field and values are sent to database, DCS and data storage;
- *data analysis*: raw data is reconciled to detect bad quality points (bad tags) and outliers. An optimizer is required to minimize the objective function and robust methods are needed in carrying out the gross error identification;
prediction: KPIs can be evaluated in an accurate way by adopting a
detailed mathematical model. Starting from the coherent picture of the
plant, which is obtained by means of the data reconciliation, the future
KPI trajectories can be predicted by adopting a dynamic model of the
plant. It requires either a first-principles differential and algebraic model
or a dynamic simulation by using ad hoc packages and an appropriate
solver to simulate the future evolution of the overall system and, therefore,
the potential KPI trajectories.
To improve this predictive performance monitoring technique, a moving
horizon methodology such as the one adopted in the model predictive
control and real-time dynamic optimization (Rawlings, 2000; Manenti and
Rovaglio, 2008), can be implemented, by allowing the on-line application;

decision: good KPI predictions lead to a more reliable scheduling of
programmed maintenances. Basing on the unit performance, the market
demand, and the storage capacity, the management decision-making
process) has more chances to define an appropriate schedule of
programmed plant shutdowns that allow satisfying completely the market
demand, without compromising process unit life-cycle (Manenti and
Manca, 2009);

implementation: decisions have to be implemented in the plant, usually
through control systems, field operators, and control-room operators
(Manenti and Manca, 2008). Then, the performance monitoring cycle can
be iterated.

Figure 3: Predictive (or model-based) performance monitoring cycle.

Whereas all the other aforementioned points seem to be univocally
solvable, KPI prediction in the model based performance monitoring may require
different numerical techniques and tools. The employment of first-principles dynamic models seems to be the only way to obtain a reliable prediction of unit behavior and KPIs. The accuracy of the prediction is mainly related to the level of detail of the mathematical model.

5. PRELIMINARY SIMULATION RESULTS

This section consists of (i) the description of the complex information-technology structure that is adopted in the selected case study; (ii) a qualitative description of the selected plant; and (iii) some preliminary results, which are discussed and compared to the industrial practice.

5.1. Information Technology Architecture

As already discussed in Figure 1, the flow of decisions starts from management levels and goes down to the lowest levels and, finally, to the field. On the other hand, information flow starts from the field and goes up to the management.

Data reconciliation and performance monitoring have to filter the data coming from the field so to make reliable the pieces of information that are required by the management.

On this subject, Figure 4 shows the information flow from the plant up to the management. The data are continuously acquired by the field (every minute). Raw data are purified by possible outliers and reconciled every hour and the reconciled values are sent to a calculation engine to evaluate the current KPIs. Control-room operators, in order to detect immediately possible upset conditions and activate the real time alarm system, carry out a first check on KPIs. Every hour, both the reconciled values and KPIs are stored on a specific DCS hard disk to constitute a plant scenario. These plant scenarios are the initial condition of the dynamic simulation of the plant. Every three hours, the future behavior of the plant is simulated, accordingly to the management objective, which can vary from the daily production accounting up to the strategic planning. The prediction horizon may also vary in the range of few hours or some months. It is worth remarking that the CPU time that is required by the plant simulation has to be always smaller than three hours, which is the selected discretization time for KPIs re-evaluation (Manenti and Rovaglio, 2008). In this context, long-term predictions might require long CPU times, just in the order of some hours. In such a case, one can either enlarge the selected time discretization, if possible, or adopt different levels in the detail of the mathematical model of the plant (Dones et al., 2009). Through the dynamic simulation of the plant, it is possible to predict future KPIs. All the KPI predictions are then sent to the control room to predict possible upsets or emergencies, whereas some specific indexes, such as the daily production
accounting or the process efficiency, are sent to the management level. It is worth underlining that CPU times required by both the data reconciliation and the dynamic optimization to foresee KPIs are considerably smaller than the time discretization of the predictive monitoring (see also Figure 4).

5.2. Case Study: LNG Plant Sub-section

Refrigeration zone and propane-butane splitter, both belonging to an existing LNG process, are taken into consideration. A qualitative flow-sheet is proposed in Figure 5. The process flow is compressed up to the operating pressure of the distillation column (40 atm) and, subsequently, it is refrigerated to 260 K. KPIs are evaluated for the most important equipment and typical deteriorations (fouling, cleanliness factors, etc.) are introduced in the dynamic model through the support of DYNAMSIM™ (Simsci-Esscor, 2004). Main KPIs are listed in the following:

- for compression units: compression efficiency of the single stage and overall equipment; ratio between the actual compression and design conditions;
- for the splitter: overall separation efficiency in terms of distillate/feed ratio; head and bottom losses in key-components; cleanliness factor for each tray and the relative pressure drop;

Figure 4. Predictive monitoring flow-chart.
5.3. Model Based KPI Prediction

Some preliminary results are reported in Figure 6. They report trends related to heat exchangers of the refrigeration section, to the reflux pump at the top of column, and to the same distillation column. A normalized time-scale is adopted.

On each selected process units Figure 6 gives also a comparison between the predictive performance monitoring and the industrial practice. Results are organized as follows:

- **dashed lines**: linear extrapolations to predict the future behavior of process units starting from the historical database;
- **dotted lines**: nonlinear extrapolations that are based on the process data and empirical correlations;
- **solid lines**: predictive performance monitoring that is based on a detailed dynamic model, which is usually already available for large-scale plants that require an operator training simulator.

In the upper trend, two KPIs are shown: pressure drops and logarithmic mean temperature difference, both related to the chiller that is operating in the refrigeration section of the plant. It is worth noting how the future predictions are very different on both the KPIs to testify the current difficulties in their definitions.

However, some extrapolations are clearly erroneous and they are easily detectable. For example, the pressure losses in a heat exchanger (tube-side) generally increase rather than drop down as indicated by the nonlinear regression. It gives us immediately the (low) level of reliability of the predictions based on
the historical data. Hence, although the model-based approach is the single one that shows the achievement of pressure drop limit in the selected simulation time, its prediction is probably more reliable than the other solutions. As a consequence, the chiller will undergo to poor performance conditions just after 0.64 time units, whereas longer times were predicted by data extrapolations.

In the case of reflux pump, there is a similar prediction between the linear extrapolation and the model-based prediction. Unfortunately, this is only a coincidence, since the industrial data for the reflux pump were acquired by the field just a little time after its last maintenance shutdown. Therefore, the pump can operate close to its nominal point and a linear trend might be a good approximation in such a case. Nevertheless, at the end of the simulation, the gap between the two approaches is increasing faster. It unavoidably points out that, again, when the maintenance period is approaching, it is difficult to obtain a reliable solution by basing the KPI prediction only on the past process data.

The most significant trend is the lowest one, since it shows the real difference between the industrial best practice and the model-based approach. One of the most important KPIs on a distillation column is usually the separation efficiency. It is usually the ratio between the distillate flow rate and the feed flow rate, even though several alternatives exist. Once again, the nonlinear extrapolation has to be discarded, whereas the linear extrapolation and the model-based approach present a similar trend at the beginning of the prediction. Then, the model-based prediction has a sudden unexpected dynamics. To understand this behavior, it is worth remarking that the distillation column is usually subject to purity specifications that have to be continuously satisfied. In order to ensure these specifications, the control system (Stephanopoulos, 1984; Luyben et al., 1998) continuously adjusts manipulated variables. When some manipulated variable achieves its operating limit, the behavior of the distillation column can change more or less rapidly, depending on the column holdups. In the proposed case study, to keep the distillate at the required quality, the control system gradually increases the reflux ratio in order to bridging the gap in column separation that is decreasing in performance for the variation of cleanliness (fouling) factor on the column trays. Unfortunately, when the reflux ratio achieves its limits, there are no parameters to control the separation efficiency directly. As a consequence, the separation efficiency shows a fast dynamics since it cannot be controlled anymore by the reflux ratio.

No methods based on the historical database are able to predict a distillation column shutdown close to the one predicted by the model-based approach, on the condition that we measure every entity by the field, but this is not a feasible approach.
Figure 6. Predictive monitoring compared to the industrial best practice.
6. CONCLUSIONS

The paper shows a possible approach to obtain a more reliable enterprise resource planning. By doing so, it is necessary to define an accurate maintenance scheduling, which allows reducing downtimes and exploiting completely the process unit life-cycle. Unfortunately, this multifaceted problem is very hard to solve and several authors proposed different techniques in the literature. A promising approach is to define reliable tools for data reconciliation and performance monitoring as well.

Specifically, the paper gives a brief overview of mathematical methods to solve the data reconciliation problem and proposes a new technique in the KPI prediction. The main idea is based on the fact that the KPIs prediction could be done by means of detailed dynamic simulation packages, especially because they are more and more spreading in the process and gas&oil industry for the operator training simulation.

Some encouraging results related to a test run of an existing natural gas plant are proposed and discussed. By adopting a model predictive control methodology, it might be possible to implement on-line this predictive solution.

REFERENCES


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