RECONCILIATION: MAKE YOUR DATA RELIABLE AND ENABLE ROBUST PLANT OPTIMIZATION THROUGH ADVANCED AUTOMATION TOOLS

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A few years ago we had the honor and the opportunity to meet Professor Sauro Pierucci and to know him as a Professor and Tutor of our Theses degree. The celebration of his 65th birthday is for us the best way to pay him our tribute and demonstrate him our deepest gratitude. We are very glad to have collaborated with him in one of his main research area: Data Reconciliation and On-line Optimization. In those decades 80s and 90s he was a pioneer in this development activity. He spent a considerable amount of time at different sites, in the DCS rooms, close to the plants, to implement and test his software applications: theory became practice to help and support the operators. Today, after several years, we want to document and share with a wider audience what he did, since we were with him in those occasions. He gave us, young Chemical Engineers mainly dedicated to process and plant modeling and simulation, the exciting opportunity to operate on the real plant, reconciling data and optimizing their performance, thanks to the implementation of its SW packages.

1. INTRODUCTION

The simulation of chemical processes using the so called “flow-sheeting programs” has become a readily accepted practice and an effective tool for process design and analysis. Still today in the commercial environments the general-purpose simulators are based on:

- the sequential modular approach, where the model equations are solved along the flow-sheet of the plant unit by unit as the topology of the plant itself
- the equation oriented approach, where the model equations describing the process are globally and simultaneously solved.

In those years there has been a large debate in literature in order to assess what would have been the best approach between the above quoted. Professor Pierucci decided to choose the former approach and on that basis he developed the ORO (On-line Reconciliation and Optimization) package. Advantages of this approach over competitive alternatives have been described by Pierucci et al., 1991: where package availability, quality of the models, solidity, hardware improvement and human factors are explained. The most important lesson learnt was about the value of the data reconciliation, it was and it also now remains necessary and fundamental.

2. ON-LINE RECONCILIATION AND OPTIMIZATION

As already mentioned ORO package was structurally based on a sequential modular approach. One of the main features of the proposed solution strategy was the close relationship existing between the simulation package “PRISMA”, also authored by Pierucci, and the black box model of the plant included into the ORO package.
ORO Package performed the complete set of calculation ranging from the pure simulation of the plants, through data reconciliation up to the complete on-line optimization. Special attention was addressed to the application in an on-line environment: so that a user interface and low computing times could be taken into account accordingly. Both reconciliation and optimization problems were solved with a feasible black box method by successive quadratic programming SQP method (Powell M.J.D., 1977); inequality constraints were treated by a modification of the penalty function method.

The simulation package PRISMA was used to define the topology of the plant and to set the design parameters of each unit, including the operating conditions data, necessary to satisfy all the degrees of freedom of the problem. PRISMA included specific rigorous models of the plant units and is capable to simulate very accurately the plants behavior. The simulation results had to be verified and compared with the plant measurement in order to match the data values and to obtain a reliable picture of the plant process.

Three examples of existing implementation on industrial plants will be illustrated to show the successful results achieved.

3. PLANT APPLICATIONS

3.1 Olefin Plant

The package ORO was the result of an intense development activity in the area of olefin plants process simulation (Dente and Ranzi, 1989), combined with the area of on-line reconciliation and optimization problems (Pierucci et al. 1991a/b, Pierucci et al. 1995); these development topics were both well established for the chemical engineering research team led by Prof. Dente et alter at the Politecnico di Milano, where Prof Pierucci was also working as a fellow Professor.
An Olefin Plant consists in its main elements of a set of furnaces arranged in parallel, which crack hydrocarbon feedstocks. This process is followed by a quench system, a cracked gas compressor system and an integrated and highly complex separation section, including cold box, refrigeration cycles and distillation columns, that outputs the olefins (ethylene, propylene, butenes, etc.) and side products. Olefins are key intermediates compounds used for a plenty of different final products like gums, plastics, etc. The olefins market, as for any products so widely used, is highly sensitive to the worldwide demand variation. The olefins plant is a typical example of a ‘ market driven Plant’ in which the price of the products may vary very widely in a short time period. Due to the fact that the plant capacities are high in terms of absolute values (typical range of several Tons per hours), it becomes imperative to manage them with tools, that warrant the prediction of the optimal set-points which operate the plant at the optimum conditions, following the external economic scenario.
Olefin plants are simulated by a generalized model linking the rigorous models for the description of the furnaces section (SPYRO, TES etc…) and the typical design models for the down-stream sections.

The difficulties that may be encountered when aiming at such an objective may be summarized here below:

- Significant plant size and complexity, up to more than 1500 streams and 500 equipment strictly linked each other by means of several recycles;
- Need of robust and rigorous models, for equipment description, to ensure accurate results and adequate model performances even when drastic conditions may occur;
- Possible presence of multiple solutions detected in optimization phase when oversimplified models are used (Pierucci et al, 1994).
- Effective and fast computing program to ensure continuous, under all conditions, interfacing with plant control system in order to enable seamless implementation of optimization result (i.e. new set-points) in the plant control system.

In spite of the above difficulties, Prof. Pierucci with his team successfully implemented the application of data reconciliation and optimization package ORO to one olefin plant located in the USA in the early 90’s (Pierucci et. al. 1995).
Due to the complexity of the kinetics in the reaction sections (furnaces), of the plant process’s lay-out and operations in the downstream compressing and separation sections, an accurate selection and tailoring of the dependent and independent variables was required in order to ensure the successful package implementation; the

same attention was required to define the set of constraints needed to guarantee the feasibility of the implementation of the optimized solution. The set of decision (independent) variables included feed flow, steam dilution ratio, cracking severity (i.e. coil outlet temperature), purities of distillation columns effluents, strokes of valves which direct streams from one separation section to alternative ones.

To summarize the problem size the following key parameter are worth to be pointed out:

- 124 chemical components have been used for effective description of the furnace sections
- 35 components have been used for effective description of the separation sections
- 500 equipment have been modeled
- 600 plant measures are field input for the data reconciliation and optimization package
- 60 different decision variables have been considered for optimization
- 85 different constraints have been considered for optimization

The sequential modular approach and the experience in kinetic modeling developed by Prof. Pierucci has allowed the easy integration of rigorous models used for furnaces section simulation (i.e. SPYRO®, TES) in the data reconciliation and optimization package ORO. The results reported in the following pictures, shown in a generic format for confidentiality reasons, are sufficient to demonstrate the good performance of the ORO application in this specific on-line environment.
Figure 1 reports behavior of a severity parameter (ethylene over propylene ratio) for one furnace in a 2 day time. Within this time period, ORO provided the plant operation manager with 15 consecutive predictions which are compared with plant measures. This figure simply shows both that the plant has been moved to fit new set-point value and that further ORO predictions were consistent and stable with the new operating conditions.
A similar behavior is reported in Figure 2, where the rate of the feedstock to the above mentioned furnace is plotted in comparison with the plant data. Also in this case the results demonstrate that the ORO package is capable to predict for all time stable and consistent data.
Figure 3 reports for the same period of time of the previous figures the difference between the initial and final values of the objective function, which is the "delta value for operating at the Optimum". It is evident that this value decreases with the plant approaching the optimum identified by ORO package.
All the figures and results achieved demonstrated that the pioneering approach developed by Prof. Pierucci in the ORO package implementation to the olefin plant provided good results and therefore that it was possible to think, even for large scale industrial problems such as the olefin one, to pursue even more accurate and successful optimization applications, that have been indeed achieved, by deploying further robust research efforts, in the following years.

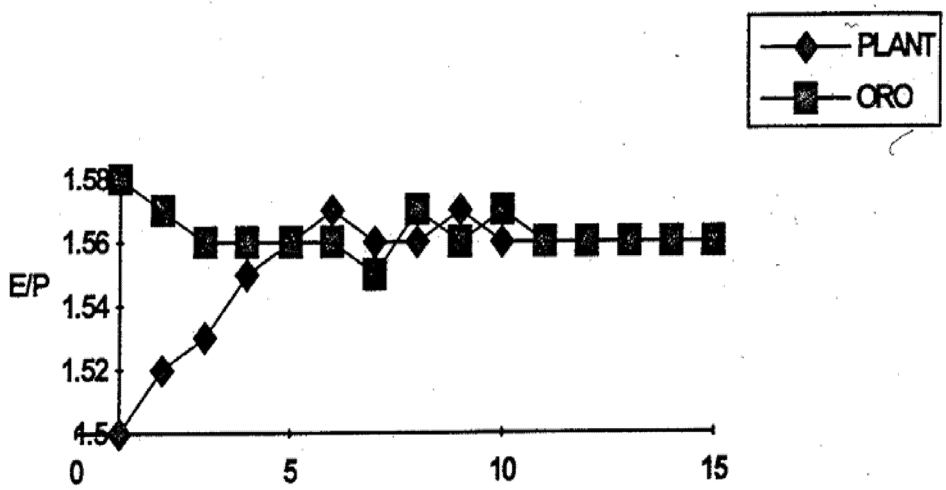


Figure 1: Predicted ORO vs. Plant Data for E/P severity parameters

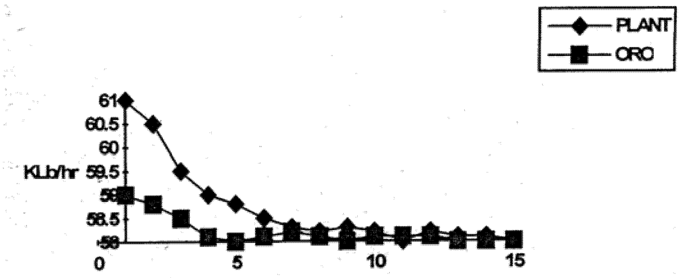


Figure 2: Predicted vs. Plant data for a feedstock rate

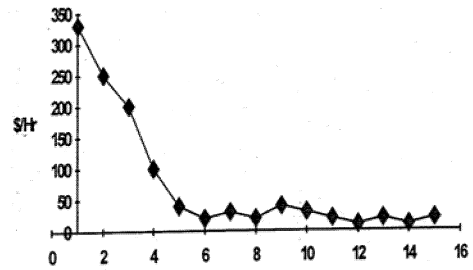


Figure 3: Delta $ for operating at optimum

3.2 Hydrogen Plant

The target of project was the implementation of an on-line open loop optimizer for the Hydrogen plant in the AGIP refinery of Sannazzaro de' Burgondi, Italy. Expected results were the reduction of the operating costs and a major flexibility, through a better knowledge of the operations. The plant was built to produce high purity hydrogen for make-up of the downstream hydrocracking unit. As a consequence any limitation in the hydrogen plant operability might have had higher impact on the hydrocracker operability which would have eventually yielded negative results on the overall refinery economics. Fig.1 reports the process flow diagram of the plant which had a nameplate capacity of 40,000 Nm3/hr of hydrogen (99% purity). The plant was designed for operation ranging from 40 to 100% of nameplate capacity with a feed gas composition ranging from refinery gas to LPG. The plant was working with a mixed feed of refinery gas and propane stream.

The initial hurdle was the availability of reliable and accurate plant data that were required to match the overall refinery material balances and to baseline the simulation of the unit to further enable the desired optimization. The reconciliation phase ran the error minimization of about 60 measures by moving 20 independent variables and was based on the above mentioned SQP method.

In practical terms the result of the reconciliation phase was to reach an overall plant scenario where each reconciled variable deviated from the corresponding plant measurement less than the instrument accuracy. This result was achieved by minimizing an error function based on the squared deviation between each variable and the corresponding plant measurement. For most of the cases this approach allowed the identification of a reliable and coherent picture for all the measured variables and, in some cases, allowed the identification of gross errors due to likely instruments malfunctioning requiring specific maintenance intervention.

The optimization phase had the scope to maximize an operational objective function and it was constrained by the plant in several sections such as bridge-wall temperature, feed gas flow, steam dilution ratio, minimum hydrogen production. Decision variables (optimization degrees of freedom) were the standard set points for the key plant variables such as: feed flow, steam dilution ratio, coil outlet temperature, etc. The next figures show how the plant had been operated as a response of the prediction of new set points after the optimization phase. It is worth remarking that 2 different objective functions had been installed and they were optionally optimized in accordance with general strategies defined by the refinery operational manager. They were the maximization of hydrogen production (function 1) and maximization of plant profit (function 2). The Figure 4 finally demonstrates how the target of hydrogen maximization had been successfully met and the Figure 7 confirms that operating plant costs had been minimized. From the Figure 4 we can also observe that the offset between measured and reconciled values was always maintained within the instrument accuracy.

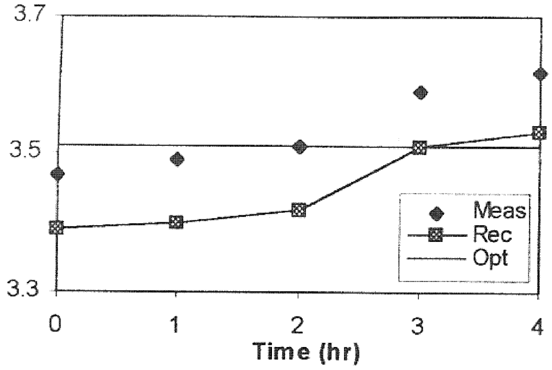


Figure 4 : Hydrogen Production (ton/hr) vs. time

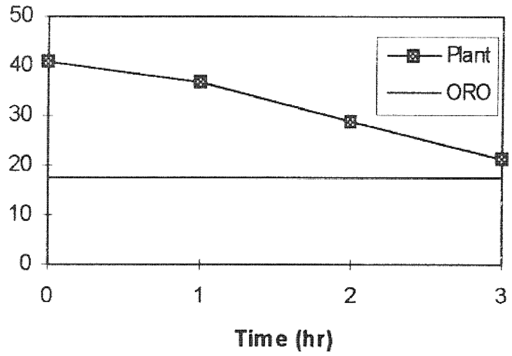
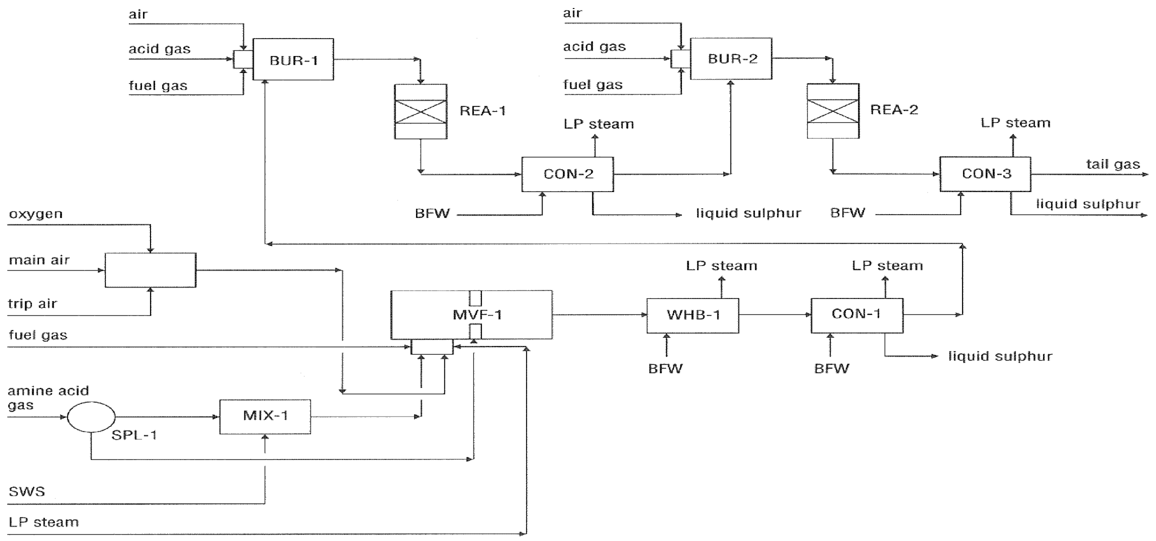


Figure 7 : Plant Operating Costs (USD/hr) vs. time

3.3 Sulphur Recovery Plant

ORO Package was also implemented at the Sulphur Recovery Unit (SRU) in the ENI Refinery of Sannazzaro de' Burgondi. The SRU was based on a Claus process that yields high purity, bright yellow, liquid sulphur and recovers high heat amount while meeting air quality requirements on discharge flue gas by reducing their hydrogen sulphide (H2S) content. The hydrogen sulphide feed gas came from regeneration of an amine solution absorbing H2S from product streams. The Claus process was also operated to treat sour water stripper (SWS) acid gas containing Ammonia, H2S and water. In this case the main objective of the application was the reconciliation of the plant measurements in order to have full understanding of the operation and a coherent picture of the plant performances. Effective monitoring of the plant performances in fact would have reduced the risk of possible infringement of the increasingly most stringent environmental regulations, which might have had a major impact on the whole refinery operations and economics. One the most important measure of the SRU is the H2S/SO2 ratio in the tail gas. The optimum ratio is "2" because, roughly speaking, it allows the full conversion into sulphur of all the sulphur compounds present in the feed gas, thus reducing to an absolute minimum the sulphur emissions.

Fig. 1: **Block diagram of the sulphur recovery unit**



The Figure 1 reports the block diagram of the Sulphur plant, here considered. The DCS adjusted the air flow rate to the thermal reactor on the basis of the H2S/SO2 ratio measured by the tail gas analyzer. In order to achieve an effective simulation and data reconciliation for the SRU unit specific models were developed and validated through the comparison with a considerable amount of plant data and the critical analysis coming from the consolidated Claus process technology know how available in the team led at that time by S. Villa at KTI SpA (now Tecnimont KT).

The main difficulties for the reconciliation phase were due both to the lack of key measures (i.e feed gas composition) and to the nature of the mathematical problem in terms of the sensitivity of the reconciliation function to H2S / SO2 ratio (Chiari et.al,1997).

A total set of about 50 measurements was reconciled by moving a set of variables including: feed flow rate, H2S composition in the amine acid gas, heat losses in the thermal reactor, equilibrium approach in the catalytic reactors and in the in-line burners. A set of 14 data extracted at different plant capacity (from 40% to 100%) was used for the reconciliation validation and is reported in table below. In the table the initial and final values of the reconciliation objective function have been shown. The figures give a rough idea of the quality of the results, not being available the details of the reconciliation function (the weight of each single contribution to the overall reconciliation error function) for confidential restriction. These figures however indicated the capability of the reconciliation algorithm to manage the different plant capacities while predicting more consistent operating conditions. The next plots provide more details at least on the key measures of the plant. The first plot in Figure 12 reports the reconciled value versus the measured one of the total air flow to the plant. An average error of 4-4,3% was estimated, well inside the range of measuring instrument accuracy and existing dynamics of the process.

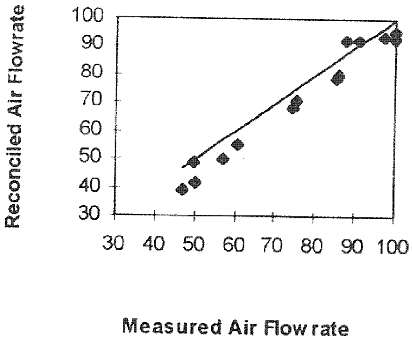


Figure 12 : Reconciled vs. Measured values of Combustion Air . Both scales are in % of Maximum Plant Capacity

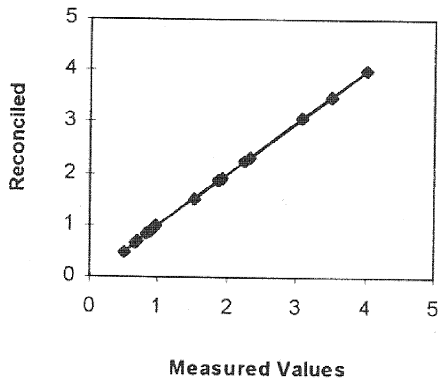


Figure 13 : Reconciled and Measured Values of H_2S/SO_2 ratio in Tail gas

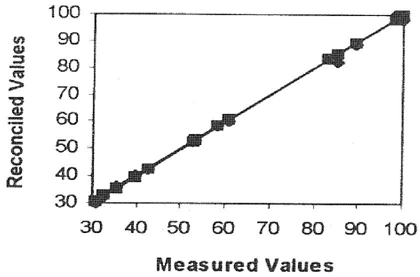


Figure 14 : Reconciled vs. Measured values of Export Steam . Both scales are in % of Maximum Plant Capacity

Next plot (see Figure 13) shows reconciled versus measured values of the H2S/SO2 ratio in the tail gas. The fitting between these 2 values is practically without error due to high weight and degree of accuracy attributed to this measurement. It is worth remembering that this measurement, as previously mentioned, must be considered as the key measure of the plant itself, affecting both the controllability of the plant itself and, above all, its environmental impact subject to the national legislation for environmental protection.
Finally a similar plot is reported in Figure 1 where the total production of low pressure steam is compared. The average error (less than 2%) demonstrates the accurate prediction of the model and of the overall reconciliation procedure. In fact this measure, even if associated to a side product, is strongly dependent on the main variables (flow rates, composition and temperature) of the whole process.

4. CONCLUSIONS

Three industrial applications of On-Line Data Reconciliation and Optimization package developed by Prof. Pierucci did show the potential benefits associated to the extensive implementation of such packages to the industrial environment. In this pioneeristic effort he had to face a number of challenges in his effort to establish an effective bridge between the academic and the industrial world. Despite the long hours and efforts spent so far in the programming and modeling as well as in the control rooms all around the world to ensure these applications could match the specifications of industrial requisitions, further effort has still to be spent by him and other enthusiastic followers to achieve the desired industrial robustness and operability.
In particular Sauro Pierucci had to face a number of typical industrial difficulties such as: lack or shortage of measurements; the need of robust gross error detection methodology; the consideration of the dynamic behavior of the units; the development and utilization of rigorous simulation tools capable to provide more detailed

information on the process and performing algorithms to reach reconciliation results in acceptable computing time.

These challenges did not allow to reach extensive utilization of reconciliation tecniques in on-line closed loop environment.

Since then new focus has been put on these research area's by Prof. Pierucci refining the data preprocessing methodologies needed to have a robust simulation baseline and therefore enabling an effective gross detection (coaptation of wrong or missing instrument measurements). New algorithms and calculation routines (Buzzi-Ferraris, 2009) more robust compared to what used in the past have enabled meaningful steps forward.

This evolution reopens the possibility to make industrially available tools for both off-line and on line applications.

5. REFERENCES

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