Improving resource efficiency through a general-purpose methodological approach combining standard techniques, modelling and simulation

1. Introduction

A better management of resources reducing waste materials and minimizing raw material intake is the aim of the REFFIPLANT project and according to the "Zero Waste" European directive this is a common objective of several steelmaking industries.

To this aim, SSSA developed the present document in order to give guidelines and advices to the staff of steelworks outside the REFFIPLANT consortium related to the overall methodological approach elaborated, formalised and pursued within the REFFIPLANT project.

The documents is organized as follow: Section 2 introduces the overall methodology, while Section 3 deepens each phase it is composed of. Furthermore, deep information about main used simulation software are given in the description of the Modelling & Simulation step.

2. Overall methodological approach for improving efficiency in resource management

Several can be the issues to address when process modifications or plant revamping have to be done in order to improve the efficiency of the resource management. The combination of simulation and on-site investigations can simplify the problem and can reduce man-hours spent to find the best solution. In addition, a strict collaboration between researches and plant managers and engineers is fundamental because know-how can be shared and different skills and expertise can be combined.

Based on these presuppositions, the methodological approach can be represented in the onion diagram depicted in the **Figure 1**

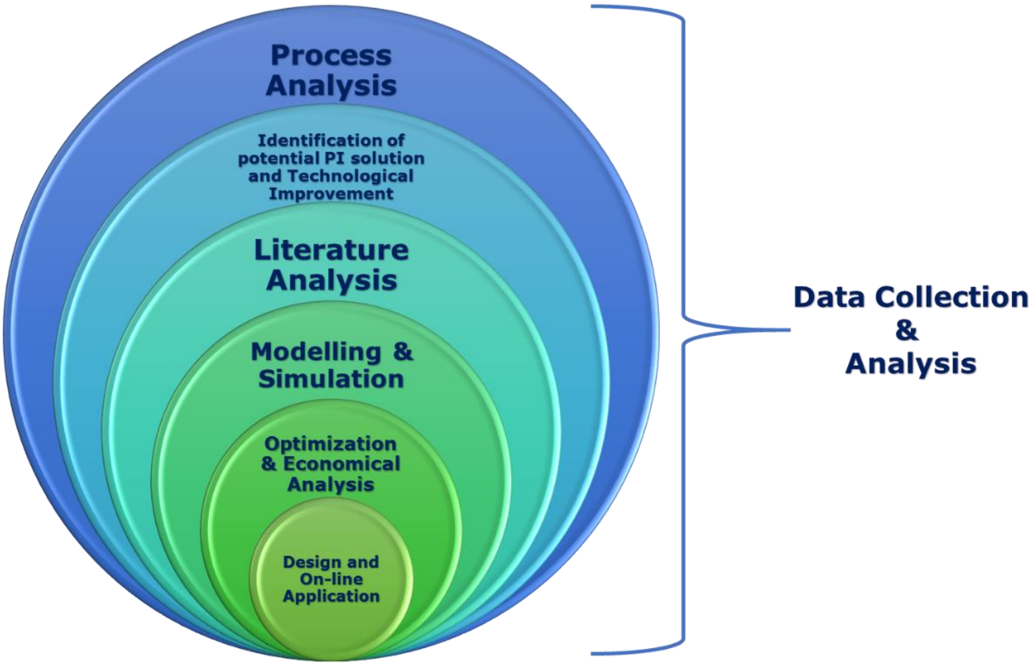

Figure1 Methodological approach diagram.

The methodology is composed by a series of steps which forego the goal of the on-line application but only in this way is possible to acquire a deep knowledge of the process to analyse and to avoid costly investigations related to non viable or non convenient solutions. The diagram highlights that data collection and analyses is a fundamental step to be carried out in the whole investigation study, as only a deep data collection allow avoiding the neglecting of important process parameters.

3. Steps of the methodological approach

3.1. Process Analysis

The first and main step is the process analysis. The process know how has to be acquired and the collaboration between researcher and steelworkers is of utmost importance. The process analysis have to be carried out through a deep examination of process route, Piping and Instrumentation Diagrams (P&IDs) related to main production process and to auxiliary treatments and equipment datasheet. In this way, a deep knowledge of the current industrial practices can be acquired.

3.2. Identification of potential PI solution and Technological Improvement

A detailed process analysis allows identifying possible improvement margins or bottlenecks. In this phase, common and well-established techniques can be used in order to obtain a list of potential PI alternatives or plant improvement.

In the case of water system, water pinch analysis is a systematic technique, usually carried out by plant managers: the starting point is the identification of similarity of water properties, contamination and process constraints in order to identify potential water sources and water sinks. Clearly data collection is fundamental in order to acquire the following information for the pinch analysis: streams flowrates, chemical compositions, equipment and pipes sizes and capabilities, treatments and process efficiencies, plant layout for water sources and sinks allocations, process constraints (e.g. in terms of contaminant amount). The development of source and sink composite curves or the water cascade analysis is the following phase. The first approach is widely adopted: it considers each water-using operation focusing on the mass transfer of one or more contaminants from the process to the water streams and the limiting composite water profile is the results of the pinch analysis. However, in the case of a single contaminant this kind of investigation has a high accuracy. On the other hand, when multiple contaminants must be considered, some simplifications are required and deeper assessment have to be done in order to avoid neglecting important parameters that lead to unfeasible solutions. Furthermore, water pinch analyses does not consider the interactions between contaminants, the contaminants variation and the possibilities that ad-hoc treatments can be required to obtain suitable water to be reused.

In the case of by-product and waste management, preliminary experimental investigations are needed. Indeed, deep analyses of by-products and waste features through conventional techniques (e.g. XRF, XRD, SEM analyses, leaching test, etc.) are fundamental to identify potential possibility of internal or external recovery after or without treatments. It is possible that a by-product in the current situation is contaminated (e.g. mill scale from oil) or need to be separated in its main fractions (e.g. magnetic and non-magnetic); for this reason the possibility to develop a new treatment or to apply well know technologies can be identified in this step.

In conclusion, this step is of primary importance to outline the scope of the subsequent deep analyses.

3.3. Literature Analysis

This step aims at the following objectives:

- Achieving a deep theoretical insight of the considered problem
- Searching if similar problems were addressed
- making a benchmarking of existing technologies suitable to treat for example a kind of by-products or water coming from a production area
- filling eventual missing data.

3.4. Modelling & Simulation

In order to make complete analyses of the identified potential PI solutions or technological improvements, Modelling and Simulation (M&S) can be exploited. Indeed, M&S allow obtaining information about the behaviour of a process, a treatment or a phenomenon in a wide range of conditions, also uncommon or that cannot be tested easily or safely.

Modelling is the first sub-step and consists in the conceptualization of the considered system and have the aim of representing industrial processes (existing or not) composed of some unit operations and linked by material and energy streams. Each phase of the real process have to be adequately represented and it is possible that a single operation have to be represented through different sub-units to consider each phenomena or that multiple real operations have to be aggregated in a single one because they characterise a single phenomenon. Simplifications can be necessary but it is important that the parameters fundamental for the final aim of the study are not neglected during the modelling. From this considerations, it is clear that the model have to be developed as similar as possible to the real system (if it is exists also in a pilot scale) and its results have to be similar to the real case. For this reason, data collection is fundamental: if data are not available, an ad-hoc experimental campaign is needed. In the case of new processes, parallel experimental studies (e.g. laboratory tests) are fundamental in order to represent each involved phenomenon in a way that is the as close as possible to experimental results, literature and experience information.

The model developed and tuned in this way represents a sort of virtual plant that can be used to make scenarios and sensitivity analyses changing operating conditions or configurations (e.g. the addition of a new water stream or the analyses of different physical treatment arrangement). Indeed, the model can be used in the simulation phase. In this phase the model is run in order to assess complex or unexplored scenarios filling the approximations made in the preliminary phase of the proposed methodology and giving useful indications for the next final steps: simulation answer to the "what if" question.

In this phase, a selection of the correct simulation software is essential. A software can be chosen according to the level of detail and the complexity required. The choice can be also guided by licencing costs.

This aspect is well depicted by the REFFIPLANT project, in which four different software were used:

- Microsoft Excel®
- Water-Int™
- reMIND
- Aspen Plus®

3.4.1. Microsoft Excel®

Microsoft Excel® can be used to develop theoretical, holistic or empirical models of a unit operations, resource users or process treatments. The model have to be based on algorithm in which only main parameters are considered. The simplified developed models can be used stand-alone or linked together for preliminary and less accurate investigations or can be included as a part of more complex models developed with commercial simulation software. Microsoft Excel was used within REFFIPLANT to develop holistic/heuristic models of water and by-products treatments. Some of them were included in the Water-int™ software. Other ones were used in the evaluation of the best arrangement of treatment units to separate BOF slag in its main fractions in order to allow the complete reuse or to generate scenarios data to be used in reMIND software.

3.4.2. Water-Int

This software was developed by Process Integration Ltd (PIL); some holistic models of water treatments developed during the REFFIPLANT project were included in Water-int™. It is based on linear optimisation framework and does not consider complex ionic interactions between different chemical species. It works on the basis of fixed or linearly varying separation factors based on theoretical laws and it can be used for preliminary studies of simulation and optimization of the structure of an industrial water network minimizing for example economic and environmental impacts. More information about its use are given by PIL in the Water-Int User Guide.

3.4.3. reMIND®

reMIND is a Java-based software based on the Method for analysis of INDustrial energy system which is based on Mixed Integer Linear Programming. The software allows the development of a complex superstructure of nodes and branches in which several aspect of a process are considered. The user can insert the data obtained by Excel models, other simulations or real situations and the software is able to create a list of equations that can be used by optimization software to pursue a multi-objective optimization of the developed system according also to the defined constraints. In the REFFIPLANT project, reMIND proved to be a powerful tool to analyse and optimize solutions for management of solid streams of by-products and wastes.

3.4.4. Aspen Plus®

Aspen Plus® is a commercial simulation software part of the AspenONE® Engineering suite, focused on process engineering and optimization. It allows the development of rigorous models with a high accuracy and the monitoring of almost all the features that in a real plant are normally monitored.

It has been intensively used within REFFIPLANT in complex scenario and sensitivity analyses, as it is a very flexible software that allow the modelling and the analyses of very different chemical species and processes (e.g. electrolytes, water and solids systems, etc.) considering the interactions between the considered species. This is possible thanks to a significant number of databanks of chemical compounds and libraries of several kind of unit operations, which are included in the software, as well as to the possibility to include customized blocks.

The translation of a process into an Aspen Plus model follows five main steps:

- Specify the chemical components in the process (they can be defined if not presents in databanks)
- Specify thermodynamic models to represent the physical properties of the components and mixtures in the process
- Define the process flowsheet (unit operations, streams to and from the unit operations, …)
- Specify the component flow rates and the thermodynamic conditions (temperature, pressure, etc.) of feed stream
- Specify the operating conditions for the unit operation models

Before the modelling in Aspen Plus very important is the full understanding of the process to be modelled and of the issue to be focused. In this way is possible to choose the best property method that is fundamental for the property calculation and so for the calculation of results: for example a water network in which electrolytes are presents need the "ELECNRTL" property method. Some indications are given in **Figure 2**

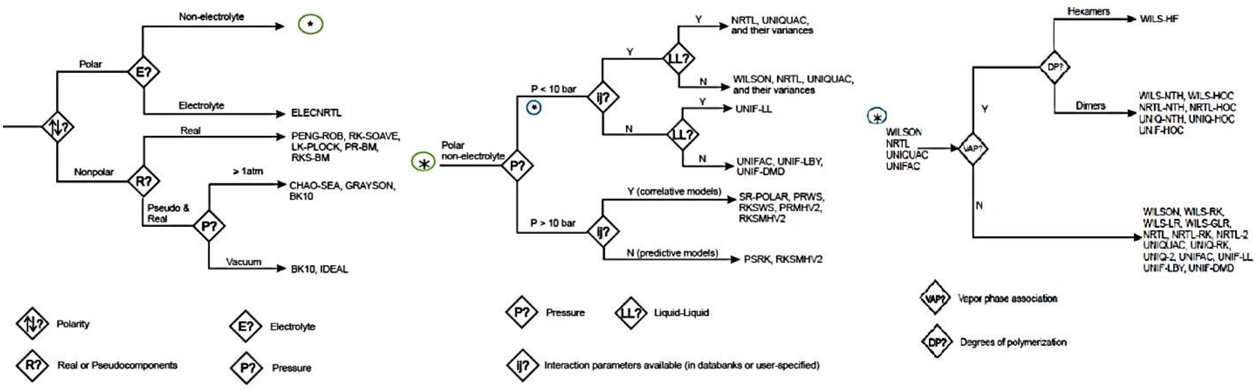

Figure 2 Indications to choose the best property method in Aspen Plus®

Furthermore, the understanding of the problem to model allows focusing only on the most relevant aspects, by neglecting those issues and aspects that do not affect the considered phenomena. In this way, a global process is divided into its main conceptual aspects, which have to be represented in the simplest possible way in order to save valuable time and developed a fast model implying low computational costs.

As previously mentioned, Aspen Plus® can be customized: for instance, it is possible to create new compounds or complex mixtures, new unit operations as well as to customize calculator blocks in order to compute some parameters. Within REFFIPLANT, this feature has been widely adopted and some examples of customization are here listed: oil in oily mill scale has been modelled as a mixture of pseudo-components created by Aspen Plus® starting from some oil parameters, electrical conductivity in water solution has been calculated through an ad-hoc written FORTRAN-based calculator block. The software allows also the integration of previously developed Excel models. It is clear that the user has many degrees of freedom in such customization.

Depending to the aim of the investigations, the simulations can be carried in steady state or in dynamic environment: steady state simulations were suitable to the aims of REFFIPLANT.

Finally Aspen Plus® allows a simplified management of complex model with Aspen Simulation Workbook that connects the model with Excel spreadsheet and allow controlling it from a more familiar software.

3.5. Optimization and Economical Analyses

Simulations can provide useful indications on the behaviour of an existing plant changing the operating conditions or the current configurations in the analyses of different solutions related to the resource management. Moreover, indications on the efficiency of a treatment to provide potentially reusable material can also be obtained by simulations. However, it is possible that the best solution identified analysing the simulation results is not the best in terms of economic and environmental impact. To this aim, a parallel economic analysis (costs and barriers) and multi-objective optimization studies to minimize the costs and the environmental impact are fundamental in order to find the best solution to the analysed problem between the most promising simulation solutions.

Furthermore, the optimization of some process parameters can be carried out through on-site trials and experiments exploiting pilot plants.

3.6. Design and On-line Application

The deep analyses carried out in the previously described steps allow identifying and designing the best solution to improve resource management without risks in terms of safety, environmental impact and costs. The application of unfeasible solutions are avoided.