METALLURGICAL PLANT OPTIMIZATION THROUGH THE USE OF FLOWSHEET SIMULATION MODELLING

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Abstract

Modern metallurgical plants typically have complex flowsheets and operate on a continuous basis. Real time interactions within such processes can be complex and the impacts of streams such as recycles on process efficiency and stability can be highly unexpected prior to actual operation. Current desktop computing power, combined with state-of-the-art flowsheet simulation software like Metsim, allow for thorough analysis of designs to explore the interaction between operating rate, heat and mass balances and in particular the potential negative impact of recycles. Using plant information systems, it is possible to combine real plant data with simple steady state models, using dynamic data exchange links to allow for near real time de-bottlenecking of operations. Accurate analytical results can also be combined with detailed unit operations models to allow for feed-forward model-based-control. This paper will explore some examples of the application of Metsim to real world engineering and plant operational issues.

Introduction

Modern metallurgical plants are increasingly complex; often incorporating closely coupled 'high intensity' unit operations, interacting with complicated pollution control systems. It is difficult for the designers of such systems to predict all of the interactions, particularly when combined with single or multiple recycle streams. When such a system is also associated with multiple, complex or impure feed stocks, the result during operations can be a constant hunt for 'steady state', reduced operating rate, energy efficiency, product quality and/or recovery.

Flowsheet modeling is a powerful tool to improve metallurgical plant performance at different project stages, including: (i) research and development, (ii) design, and (iii) plant start-up/ramp-up/operation and continuous improvement. The focus of this paper will be on: When, Why, and What can be usefully modeled at different project stages. How to model is specific to the chosen software and will therefore be discussed only to a limited extent.

Many different flowsheet simulators are commercially available. Some simulators are of a more 'general' nature and intended for application to many types of processes, e.g.: Aspen HYSYS or Aspen Plus [1], CHEMCAD [2], Cycad process [3], HSC Sim [4, 5], IDEAS [6, 7], Metsim [8], Pro/II [9], SysCAD [10], etc., while others are more specific, e.g. for mining/mineral processing: JKSimMet, JKSimfloat, USIMPAC, AggFlow, etc. Metsim is used as an example in this article, due to the direct experience of the author and this is not intended to imply that Metsim is the best or only choice for any particular application.

Various project stages are listed in Table I and related to the possible applications of flowsheet models and the quality of data that is typically available (given on a scale of 1-10) during each project stage. The scale of data quality is explained in Table II.

Table I. Some Applications of Flowsheet Modeling at Different Project Stages, Related to Available Data 'Quality'

Project Stage	Idea	Lab Scale	Pilot Plant	Scoping Study	Demonstration Plant	Pre-feasibility Study	Basic Engineering	Detailled Engineering	Commissioning	Ramp-up	Early Operation	Continuous Improvement
Quality of Data	1	2	3	4	5	5	6	7	7	8	9	10
Applications of Flowsheet Models												
Technical feasibility of ideas	X	X	X	X	X	X	X	X	X	X	X	X
Economic analysis of concepts	X	X	X	X	X	X	X	X				X
Equipment sizing			X	X	X	X	X	X				X
Trade-off studies	X			X		X	X					X
Process control strategy testing			X	X	X	X	X	X		X	X	X
Emergency scenario planning			X		X		X	X				
Commissioning scenarios					X		X	X				
Ramp-up check					X		X	X				
Feed forward control			X		X					X	X	X
Process improvements			X		X					X	X	X

Table II. Description of Data 'Quality', Types and Relation to Project Status

Quality of Data	Description of Data Types and Project Status
1	Guesses (hypotheses), theory, literature, order of magnitude 'models' or estimates.
2	Basic calculations, conceptual models, beaker scale measurements.
3	Advanced calculations, semi-valid mathematical models, real data at signficant 'scale'.
4	Conceptual engineering and flowsheet design, selection of final technology and scale of unit operations.
5	Real operating data of the conceptual flowsheet at a semi-industrial scale, validated mathematical models and equipment concepts, observations of operating stability and reliability, initial estimates of equipment life and maintenance costs.
6	Industrial benchmarks, engineering calculations, basic: (i) flowsheet specification, (ii) materials of construction and (iii) design criteria, initial equipment specification and vendor selection.
7	Detailled engineering calculations, material specifications, equipment designs and final vendor packages. Execution plan including: Construction, Commissioning, Ramp-up, Emergency Scenarios, e.g. power and equipment failure. How to bring plant to a safe state under all scenarios?
8	Initial operating data, first modelling of real plant data, observation of cause and effect, observations of process instability/recycle feed back loops.
9	Approach to the real bottlenecks (undersized unit operations), rapid process changes to improve stability, operability and reliability.
10	Significant historical plant data, and error-minimized mass-energy balances. Status: Debottlenecking, identification of cause and effect, search for solutions to real world problems with a corresponding return to guesses, theory and literature.

Note that incremental changes in data quality are listed in the table. Guesses, theory, and literature values will continue to be used until replaced by high quality engineering calculations, validated models or real process information from benchmarks or pilot/demo/industrial operation, e.g. overall plant operating reliability.

Modeling During Research and Development

During research and development 'unknowns' often outnumber 'knowns'. When so little information is available one may reasonably ask, "How can flowsheet modeling be usefully applied at such an early project stage?" The answer can be found by exploring two additional questions:

1. "What process option will theoretically give the best results for the project?"
2. "What data must the research program find or develop to realize the 'best' process option?"

The answers to these two questions can be usefully evaluated using flowsheet simulations at very early stages.

The way forward in a research program is often unclear at early stages, particularly when beginning with a 'blank page' on a green field project and using new technology. Many options are possible and little data exists to allow different options to be compared accurately. Flowsheet simulation can be usefully applied to explore the various processes or combinations of processes to determine which are possible (but not necessarily economically feasible) by making reasonable assumptions and applying data from standard thermo-chemical databases. Of those which are possible, basic flowsheet modeling can give 'best-case' operating cost (Op-ex) results using theoretically optimal process performance. Processes or options which give a negative or insufficient cash flow even under ideal conditions, can then be quickly eliminated, and the total number of cases reduced to a reasonable number for further consideration in the next project stage.

In order to determine the scope of a development program for new technology flowsheets, an efficient modeling approach is to ‘scale-up’ using the flowsheet simulator at a very early stage. A flowsheet simulator can be used to ‘design’ the next project scale equipment in order to determine: “What data must the research program find or develop to realize the preferred process option?” If you are at the lab scale, begin to design your pilot scale, if at the pilot scale begin to design your demonstration scale, etc.

A simple example of a single unit operation (electric smelting furnace) is shown in Figure 1. High accuracy modeling of such a unit operation would require the following information:

- Feed rate of each component (e.g. reductant, flux and ore), including uncontrolled streams like “infiltration air” and electrode usage.
- Temperature and composition of each stream totaling 100% including: mineralogy, free moisture and size distributions for solid streams (the latter two being somewhat related to dust in the off-gas).
- Complete thermodynamic data for the solid, gas, slag, metal, aqueous, and organic phases.
- All of the chemical reactions, their extents and correlation with temperature (kinetics and/or equilibria).
- Temperatures of all output streams.
- Physical properties such as density.
- Efficiencies of the phase separations between metal, slag, solid and gas.
- Heat transfer coefficients between slag and charge, slag and wall, gas and wall/roof, etc.
- Dimensions of the equipment to determine overall thermal efficiency and required power input.

As the simulation is built, many of the key data listed above will be found to be missing, e.g. the composition (totaling 100%!), mineralogy and size distribution of the natural solid raw materials, i.e. reductant, flux and ore. Most of the process data required for modeling may be also be lacking, e.g. the amount of infiltration air into the freeboard, fraction of dust carry over, heat transfer coefficients to the charge and walls, phase temperatures, efficiency of phase separations, extents of reactions, etc.

Assumptions must be used in place of actual process data and ‘dummy’ chemical data such as ‘unknown’ species (with some thermodynamic data typical of the average feed composition) added to feed streams to allow them to total 100%. Quantification of each unknown and assumption then becomes an objective/deliverable of the development program. Several project/engineering stages will likely be required to replace all guesses or assumptions with real data. Once a flowsheet model can be created with all of the key design parameters being ‘known’ rather than assumed, the project is clearly ready to pass through the final Stage-Gate and proceed to execution.

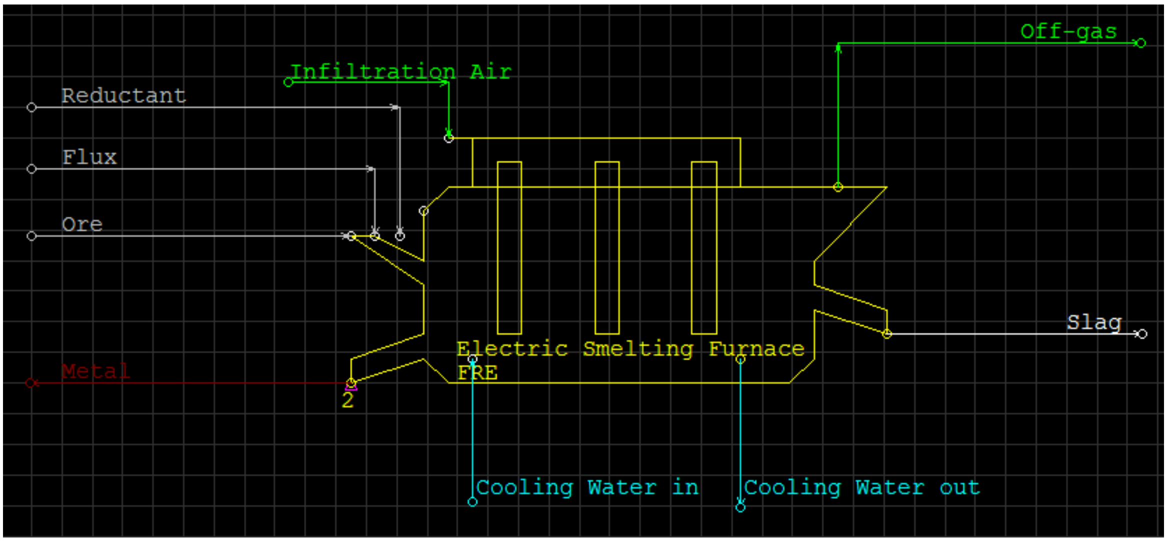

Figure 1. Electric Smelting Furnace Example using Metsim.

Modeling During the Design Stage

The design stage of most large projects usually consists of several sub-stages associated with increasing levels of engineering completion and greater precision in the operating cost (Op-ex) and capital cost (Cap-ex) estimates [20]:

- Scoping studies, including Trade-offs,
- Prefeasibility,
- Basic Engineering, including the Bankable feasibility and finishing with the Budget authorization,
- Detailed Engineering, with the associated Control and Final estimates.

Scoping Studies

Flowsheet modeling has a role to play at every engineering stage. At early stages such as during Scoping studies, flowsheets are created and modified with ‘gross’ changes. Due to the early stage of engineering, typical or assumed data often continue to be used even for key design parameters.

Important project issues are evaluated during the scoping stage, such as:

1. Economics of using different raw materials or energy sources.
2. Economics of producing process reagents (like acid) vs. purchasing.
3. Impact of plant scale on overall project return.
4. Integration of energy recovery on total consumption, project cost and reliability.
5. Open vs. closed water balances.

Many (perhaps hundreds) of mass-energy balances are typically calculated using the flowsheet simulator exploring the above factors. Sensitivity analyses are performed examining the impact of different parameters, such as raw material purity vs. production rate and quality. Entire sections or process unit operations are added and removed from the flowsheet model as decisions are made whether reagents like acid should be bought or produced on-site. At this stage of a project, it will become apparent to those working with spreadsheet models that this approach is not sufficiently flexible to allow for major flowsheet changes without considerable risk of programming errors and/or delays in delivering accurate results.

Prefeasibility and Feasibility

After many trade-off studies and one or more scoping studies, many of the key flowsheet decisions have been determined and one concept (now much more concrete) moves forward to prefeasibility. During prefeasibility and bankable feasibility, most of the assumed data used in the flowsheet simulator are replaced with validated values from sources such as demonstration scale test results, geological model or pilot mining results, industrial benchmarks, design studies and so on. The uncertainties in the calculations are thus reduced in proportion to the required accuracy of the estimates, e.g. typically -5 to +15% at Budget authorization [20].

During prefeasibility it is important to begin to explore the role of recycles and controls on process stability. As preliminary functional descriptions and Process and Instrumentation Diagrams (P&ID's) are developed, it becomes possible to program realistic controllers into flowsheet simulators like Metsim. Each recycle stream and Feed Back Controller (FBC) creates a 'loop' in the mathematical model and will also do so in the real plant. Cascaded controllers and multiple recycles create nested loops, and may result in mathematical instability in Metsim due to its Sequential Modular solution algorithm. In the Sequential Modular algorithm, each unit operation is solved in sequence, and the system is 'looped' until overall convergence is achieved. While this algorithm can result in mathematical instability, it does tend to: (i) behave in a highly analogous fashion to real plant systems and (ii) lend itself very well to dynamic simulation using discrete time steps. Control strategies which fail to converge rapidly in steady-state simulations using Metsim, will also fail to rapidly achieve steady-state in the real world; therefore, rather counter-intuitively, Metsim steady-state simulations can be used to determine the dynamic suitability of real-world control strategies on a qualitative basis.

The use of Feed Forward Control (FFC) in Metsim allows for the use of fixed ratios, e.g. fuel-to-air on a burner and avoids the creation of feedback loops. FFCs can therefore be used to increase real world process stability, as well as model computational efficiency. FFC can also be used to control recipes, e.g. slag basicity and thereby avoid nesting the entire flowsheet in a loop. In the real world this has implications for analysis of raw materials, blending and plant procedures.

Basic and Detailed Engineering

During basic and detailed engineering, a flowsheet simulator can be used as a 'warehouse' of process design criteria. No calculation anywhere within the project should be allowed to use data which is not compatible with the data used in the process flowsheet simulation. Ideally a single set of: (i) minimum, (ii) nominal and (iii) maximum values should define all valid process conditions for use both in flowsheet simulations and off-line calculations. Metsim FBC controllers allow the definition of minimum and maximum controlled variable values, as well as set point targets.

Some specific activities for which a flowsheet simulator can be used during basic and detailed engineering have been listed in Table I and will be examined in further detail in this section.

Emergency Scenarios are sometimes not thoroughly explored during engineering of metallurgical processes. Emergency scenarios include, but are not limited to failure of:

- Power,
- Major mechanical equipment,
- Total unit operations, and the
- Control system.

Using Metsim, controllers can be manually frozen at the last value (hold-last-position), set to maximum (fail-open), or set to minimum (fail-closed) in order to simulate the appropriate failure states. Heat or other energy additions can be interrupted. Cooling water can set to 'failure' values to simulate the use of back up systems or stopped altogether to simulate worst case scenarios. Such testing can explore the control and safety system interaction with the process equipment using simple steady-state simulations in order to determine if the plant achieves a safe state under each failure scenario.

Using a flowsheet simulator like Metsim, unit operations can be 'turned off' to simulate total failure and the rest of the flow sheet operated independently to observe the consequences. Observation of the mathematical instabilities created can allow an experienced Metsim modeler an initial indication of the dynamic response, even using only steady state simulations. Changes can subsequently be made to the flowsheet to ensure that the plant can always achieve a safe state, for example by installing emergency venting or flares for dangerous process gases or 'pits' for the molten contents of smelting furnaces.

Commissioning should be considered early in a project design. A plant should be divided up into sub-'Systems' that allow it to be commissioned and started-up in realistically sized portions. A plant 'System' can be defined as the equipment capable of relatively independent operation for significant periods; typically located between a sizable source and sink. Temporary vents, bleeds, back-up heating and cooling systems may be necessary in order to allow for completely independent commissioning. Plant 'Sections' as they are defined in Metsim can be operated individually. This can be used to determine if they are capable of independent operation and to establish what temporary auxiliary systems or product sinks might be required, e.g. diesel supply for nominally coal fired equipment prior to coal pulverizing plant commissioning, or a coal fired/water spray cooled 'flare' to allow for commissioning of precision coal pulverizing equipment prior to process plant start-up.

Reliability modeling of 'Systems' should be performed to ensure that individual systems each contain sufficient internal redundancy to achieve their required reliabilities. Systems should be separated by temporary sinks/supplies (e.g. surge bins, drains, vents and tanks) of sufficient size to avoid downtime in one system unduly influencing the availability of the next. Flowsheet simulators can be used to determine the likely sizes of such isolation equipment and their most effective location in the flowsheet. This represents an attractive objective for a dynamic flowsheet simulation.

Stability of operation should be studied in conjunction with the definition and modeling of 'Systems', and the determination of commissioning and reliability requirements. The size of system 'separators' or surges, may need to be increased in flowsheets containing large numbers of recycle loops in order to ensure that individual systems do not interact too closely. Strong interaction caused by recycles result in unstable simulations and poor operation in the real world. Recycles may create positive feed back loops leading to catastrophic failures in the worst case.

Overflows, vents, or auxiliary ‘make-up’ supplies may need to be added to the flowsheet to stabilize the volume, mass or quality of recycle streams. The impact of such unit operations, (SUBs as they are called in Metsim), on process stability can be observed easily during steady state simulations, i.e. by faster mathematical convergence.

Ramp-up is sometimes completely forgotten, even during detailed engineering. A typical error is the specification of valves which are either too large or of the wrong type to control at the low range often required during ‘ramp-up’. Flowsheet simulators can be used to solve for a number of mass-energy balances from low, e.g. 10%, to high, e.g. 125% of the nominal design throughputs. Having performed such calculations, it may then be observed that some unit operations dramatically change requirements at low throughput. For example, high temperature metal vapor condensers require heating at low and cooling at high throughputs, in order to maintain a liquid discharge at all times.

Start-up (after the initial plant start-up) is a special type of ‘ramp-up’ encountered after every maintenance stop. Equipment designed for smooth ramp-up, will subsequently start-up well during later operating phases of the project.

Plant Operation

Flowsheet models developed early in a project cycle can ‘live’ and ‘grow’, and ultimately be used during production stages. Steady-state models developed during engineering can be converted to dynamic (at least using Metsim) and utilized during operator training. Using Dynamic Data Exchange (DDE), a Metsim model can simulate the process responses to changes in operator set points, chemical compositions or equipment conditions, e.g. heat loss. If provided with suitable interfacing, such a model can sit behind a Human Machine Interface (HMI) and act like the real process during operator training sessions. Often training models are not started early enough during engineering to be available when required. A continuously evolving model is much more likely to have reached the required stage of development prior to the commencement of operator training.

Near real time data from Plant Information Management Systems (PIMS), Laboratory Information Management Systems (LIMS), data warehouses or process historians like PI, can also be interfaced with flowsheet simulation software. This enables the flowsheet simulation to provide forewarning to operators of the consequences of changing feed grades on product quality or of the future impact of operator set-point changes on the process heat balance, before the changes have fully occurred. The model can act as a sort of ‘crystal ball’ on the process. This allows the plant operators to take active steps to avoid economically unfavorable or unsafe future ‘steady-states’ from occurring. With correct programming of steady-state simulators, even large changes occurring in complex flowsheets can be solved in seconds or at most a few minutes, using standard portables or desktop computers.

Flowsheet models can be used for feed forward recipe setting. Such models can help set feed blends, which simultaneously achieve multiple constraints or objectives, such as economically optimal product quality and recovery.

Advanced Modeling Techniques

In Metsim complex and unique unit operations can be modeled either for steady-state or dynamically using custom APL (A Programming Language) code. Functions can be defined by the user and executed within standard unit operations such as the electric smelting furnace shown in Figure 1, or in custom unit operations built from multiple simple ‘blocks’ of mixers (MIX), splitters (phase-SPP, stream-SPS, component-SPC), stream distributors (SUB) and free energy minimizers (FEM). Complex chemistry in many separate phases can be modeled using either the built in database, external databases such as FactSage, or manually entered data. The author has often used information from the HSC database to expand the already considerable data found in Metsim or used pre-defined look-up tables to relate complex FactSage equilibria to Metsim operating conditions. The use of pre-calculated look-up tables avoids the need to execute external software and greatly reduces convergence times.

Examples of advanced Metsim models used in academic research can be found in the literature [11-19]. These often represent a ‘special’ class of early stage modeling, where the focus is on technology rather than project development. The application of dynamic Metsim modeling in such academic work is particularly noteworthy [12, 14, 19] and potentially of industrial interest to those wishing to extend the scope of traditional steady-state models used during most large scale metallurgical plant engineering in the last 20 years.

Conclusions

Flowsheet simulators have a place in nearly any process research, engineering or technology development project.

Effective application at each project stage can:

- Streamline development,
- Eliminate wasted effort/improve engineering productivity,
- Increase plant operability, reliability and safety, and
- Ultimately help to ensure a financially successful project outcome.

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