ABSTRACT

Iron and steel making requires a wide range of different raw materials significantly influencing process performance which demands a continuous optimization of process routes also with respect to energy efficiency as well as environmental emissions. Steadily changing raw material prices and qualities, market situations and product variations are challenging integrated steel plant operators in production planning and cost optimization. Primetals decided to develop a comprehensive metallurgical flow sheet model library for simulation and optimization of integrated steel plants. Intensive development efforts were taken to migrate existing well-established calculation and engineering routines as well as integrate newly developed models. The generated model library enables the setup of mass and energy balances for integrated steel plants, development and evaluation of new process concepts as well as integrate newly developed models. By using this process integration platform, it is possible to compare different iron and steelmaking routes within one standardized environment. In this publication an insight will be given on the competence of the model library in depicting integrated steel plant operation, enhance raw material planning, show the effect of new raw materials and operation optimization.

Keywords: operation cost optimization, strategic planning, optimization, raw material procurement, life cycle assessment

1. INTRODUCTION

Iron and steel making requires a wide range of different raw materials which are significantly influencing process performance resulting in a demand for a continuous optimisation of process routes. This applies to economic efficiency and in recent times to an increasing extent also to energy efficiency and environmental emissions [1-2]. Additionally to this situation, integrated steel plant operators are more and more challenged by steadily changing market conditions – for raw materials as well as products – thus experiencing an increased demand for sophisticated strategic operation planning support.

With rising power of computer hardware, the enhanced analysis of operation data, condition monitoring and computational operation support gained ground in the metallurgical industries resulting in the digitalization initiative. As elaborated in [3] the vertical integration of systems (from sensors to enterprise resource planning – ERP – applications) is a major challenge and so far, there was no holistic solution found. Despite many available and proven in use level 2 systems, the supply of ERP systems for metallurgical process modelling to support offline operations planning in an industrial environment is limited. Facing this challenge, some operators have developed own software implementations, others work with standalone solutions focusing on specific equipment or sub-plants [4-10]. A wide usage of process simulation tools such as AspenPlus®, PRO/II®, IPSEpro®, ChemCad® amongst others like in the chemical, oil and gas, pharmaceutical industries or the power generation sectors could not be achieved in the iron and steel making industry due to limitations of these tools.
After a detailed state of the art evaluation on integrated steel plant optimization platforms, Primetals Technologies decided to develop a holistic metallurgical model library based on a fundamental scientific approach. This library – called m.simtop – strategic operation planning for integrated steel plants is now enhanced to a new level and thus providing a professional platform for a metallurgical ERP system. The content of this publication will provide an overview on the contents of m.simtop models, functionalities, its applications and results from simulation and optimization.

2. MODELLING

During the last years a comprehensive metallurgical model library was developed by Primetals Technologies and partners (voestalpine, TU Wien), combining modelling knowledge, operation expertise as well as process and equipment know how. The library covers all types of chemical engineering related metallurgical process equipment including side facilities to simulate conventional (BF-BOF) and alternative (DR-EAF, COREX®, FINEX®) iron and steel making process routes. In terms of side facilities all various kinds of gas treatment plants, material handling, heat recovery as well as water and steam cycle applications can are covered by the libraries models.

The models are suitable for operation planning and optimization as well as technological investigations. It was found that for all applications about 30 chemical elements resulting in more than 220 essential chemical species/molecules are sufficient. Currently about 250 models are implemented in a well-established equation-oriented solver. Thermodynamic properties were evaluated in literature and from various software packages and afterwards implemented directly in the model library, thus accelerating calculation times and avoiding additional interfaces.

As per the structure of the software and the models, extensions and changes can be easily applied which enables flexible modelling of any type of process route variation of interest. For a user-friendly human-machine interaction a MS Excel graphical user interface can be implemented.

An integrated steel plant model being set up with m.simtop models enables various functionalities, such as the execution of simulations, optimizations, goal seek routines as well as the opportunity to include or exclude parts of the model from an execution. Due to the equation oriented system it is easily possible to include regression models for the calculation of eg. mechanical or metallurgical properties of coke.

2.1 Simulations

Precondition for a simulation activity is the availability of all raw materials analyses, the underlying process route set up including gas network and material handling – covering all relevant recycling streams. With know how about specific operation practices related models can be adjusted accordingly to reach optimal fit to operation data for a m.simtop implementation. Based on given inputs (raw materials, operation parameters, etc) a discrete solution for the implemented integrated steel plant system or sub-systems thereof can be obtained. This application may be seen like an experiment with a digital twin, or in other words some kind of “what-if”/sensitivity analysis for a given set of inputs and operation philosophy idea performed offline from real operation.

In performing simulations the feasibility of the combination of raw materials and a specific operation philosophy can be proven or shown to be impossible. Thus, simulations can serve for:

- Quick conceptual operations planning experiments
- Operation data controlling – feasibility/consistency checking of sub plants departments operation reports consumption figures
- Cost and KPI upfront simulation in the form of case studies
- Supporting life cycle assessment applications
- CO₂ emission evaluations
- Trace material investigations (alkalines, sulphur, etc.)
As special feature and helpful functionality “goal-seek” calculations can be performed on an optional basis. Examples therefore are:

- Required additive amount to reach a desired product/by-product basicity set point – applicable for pellet/sinter plant, blast furnace, basic oxygen furnace and electric arc furnace
- Required ore amount to reach a desired production rate set point (eg for sinter, pellet or blast furnace operation planning). This is also applicable for coal and produced coke at the coking plant
- Required hot blast amount to reach a desired blast furnace top gas temperature set point
- Required coke amount to reach RIST equilibrium condition set points at the blast furnace

Additionally - as in reality sometimes sub plants of integrated steel plants are in shut down the option to exclude sub plants from calculations is provided. This enables in strategic operations planning also the consideration of part shutdown and maintenance scenarios.

For each defined sub plant group, the option to exclude the same from calculations by switching it “off” is available – this furthermore enables the calculation of sub plants in stand-alone operation. If a sub plant group is switched off, then this setting is active for simulation and optimization – same applies to goal seek calculations – if active, they are so for simulation and optimization.

2.2 Optimizations

In extension of the simulation capability also mathematical optimization calculations can be performed, the importance of the same is proven due to its wide presence in literature [11, 12]. Based on given inputs (raw materials, operation parameters, etc.) – depicting a feasible operation case – the optimum value of the target variable is obtained by an automated algorithm/sensitivity analysis under consideration of additional boundary conditions. The boundary conditions are of utmost importance and embrace control variables and constraint variables.

Control variables are predefined variables by the user, being assumed to have significant influence on the value of the target variable. During the automated algorithm process these variables are varied (in certain predefined ranges – defined by the user) acting on the target variable. Based on convergence criteria the solver will find new values for the control variables values which result in the desired minimization/maximization of the target variable.

Constraint variables are boundary conditions for important key performance indicators beside the target variable, which shall stay in certain ranges which are specified by the user, despite of the minimization/maximization of the target variable.

Here it is worth mentioning that control and constraint parameters are core chemical/metallurgical parameters and that during the entire optimization all process related calculations are performed in full extent.

Performing optimizations is a key functionality of m.simtop and enables the user to:

- Optimize production costs for given plants availability and input parameters
- Finding the optimum raw material mixture for an envisaged operation philosophy
- Keeping key performance indicators in desired ranges despite adapted raw material mixture
- Ranges for control and constraint variables are editable by the user

2.3 Global variables

Having a holistic integrated steel plant model implemented enables the usage of global variables of special interest to the user. As such important variables production costs based on summed up raw material costs and CO₂ emissions are seen.
m.simtop provides a holistic cost function calculating the overall production costs including all involved equipment. This holds also for the simulation/optimization of shut down scenarios or single plant investigations.

As CO₂ emissions are of increasing importance, m.simtop models also provide detailed CO₂ emission figures for all involved sub plants as well as for the holistic integrated steel plant. These figures are also available if parts of the steel plant are being switched off. Apart from these variables, any other type of variable – depicting eg. special trace materials of interest (e.g. sulphur, alkalines, …) can be made available.

3. RESULTS AND DISCUSSION

All models for core metallurgical processes such as sinter and coke production, hot blast stoves, blast furnace, hot metal desulphurisation, basic oxygen furnace etc. were validated against operation data. In the next section an overview on model results compared to operation data as well as applications on integrated steel plant optimizations are shown.

3.1 Coking and agglomeration plants models

In the coking plant model coal mixtures are converted to coke, coke oven gas and by-products such as ammonia, hydrogen sulphide, tar and benzene, toluene and xlenes (BTX). For firing purposes produced coke oven gas can be utilized in a mixture with any other type of combustion gas like eg. blast furnace gas, natural gas, etc. All related products parameters such as coke-, coke oven gas and by-products parameters (flow, analyses) as well as flue gas details from under-firing are received as results.

Additionally to the simulation of coke production regression models for the estimation of mechanical and metallurgical parameters of coke are implemented [13-16]. An overview on models results compared to operation data is given in Table 1. Plant A corresponds to a central European and plant B to an eastern European production site, both plants operate recovery type coking ovens.

Table 1. Comparison of coking plant models results with operation data in % relative deviation

<table>
<thead>
<tr>
<th></th>
<th>Coke production</th>
<th>CSR</th>
<th>CRI</th>
<th>I10/I40</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plant A</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Plant B</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Deviation</td>
<td>0,02</td>
<td>1,8</td>
<td>0,14</td>
<td>0,74</td>
</tr>
<tr>
<td>Plant A</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0,56/0,43</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The figures presented in table 1 show good agreement with operation data, also for the estimation of mechanical and metallurgical parameters of coke, which were derived by literature models.

The sinter plant model produces sinter from sinter feed ores and concentrates, sinter plant internal and external recycle material (BF fines, sludges, dusts, residuals etc.) and coke breeze. Sinter plant internal hot and cold recycles are modelled as well as ignition gas conversion in the ignition hood. As a technological extension, functionalities for selective/non-selective waste gas recirculation as well as fuel gas injection can be provided as well. Table 2 depicts results obtained from sinter plant model calculations compared to operation data.

Table 2. Comparison of sinter plant models results with operation data in % relative deviation

<table>
<thead>
<tr>
<th>Sinter production</th>
<th>Plant A</th>
<th>Plant B</th>
<th>Plant C</th>
<th>Plant D1</th>
<th>Plant D2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deviation</td>
<td>0,06</td>
<td>7,5</td>
<td>0,85</td>
<td>0,13</td>
<td>1,34</td>
</tr>
</tbody>
</table>
Data included in table 2 shows the data of one further eastern European plant “C” and a central European plant with two cases “D1” and “D2”. The result for plant B was significantly affected by uncertainties of measurement data, which results in the relative deviation of 7.5%.

Outputs of the sinter plant model are sinter production amount including flow rate, temperature and analysis, waste gas composition including flow rate, temperature and dust content. Calculations are based on raw materials analyses, flow rates and operation philosophy specific model settings embracing e.g. sinter properties and chemical reactions.

3.2 Hot metal and DRI production models

Related models here are embracing the blast furnace, stoves, COREX®, FINEX®, DR-shaft and side facilities models. As a showcase the blast furnace model will be briefly described. The blast furnace model consists of three calculation layers. The task of the main layer is the depiction of the material flows of the blast furnace process. The chemical and physical conversions which are responsible for the transformation of burden, coke, hot blast and injectants into hot metal, slag and blast furnace gas including dust are implemented using sub models. In recent years, multiphase equilibrium calculation routines have already been developed for the comparable melter gasifier model [17]. However, due to observed deviations regarding manganese and silicon contents in hot metal and slag, this approach was rejected for the blast furnace model. Hence, empiric elemental assignments, distribution coefficients or regression models are used for conversions and reactions of affected elements.

The second calculation layer is used to investigate the gasification conditions at the blast furnace tuyeres, more precisely delivering the raceway adiabatic flame temperature (RAFT). The third calculation layer is used to determine the overall thermodynamic conditions of the blast furnace process by making use of a specifically developed Rist sub model. Due to this combined modelling approach, the results of the adiabatic flame temperature sub model and the Rist sub model are indirectly exerting influence on the mass and energy balance of the overall model. Therefore, the interdependencies between blast furnace process, RAFT and thermodynamic conditions can be described within this single mathematical model of the blast furnace. Table 3 compares results of the blast furnace model with operation data.

<table>
<thead>
<tr>
<th></th>
<th>Melting rate</th>
<th>BFG temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plant A</td>
<td>0,43</td>
<td>8</td>
</tr>
<tr>
<td>Plant B</td>
<td>2,5</td>
<td>7</td>
</tr>
<tr>
<td>Plant C</td>
<td>0,58</td>
<td>25</td>
</tr>
<tr>
<td>Plant D1</td>
<td>0,36</td>
<td>9</td>
</tr>
<tr>
<td>Plant D2</td>
<td>0,4</td>
<td>5</td>
</tr>
</tbody>
</table>

The results regarding mass balance – for melting rate figures in table 3 show good accordance to operation data. The comparison of blast furnace gas temperatures shows deviations which were investigated in a detailed analysis. Significant potential for minimizing these deviations was found for raw materials moisture contents, slightly adapted hot blast flow rates and heat losses. Especially moisture contents may vary from the time of measurement to furnace charging and heat losses can never be determined exactly.

The remaining figure of the hot blast flow rate was found to have a standard deviation of about 10% for its flow rate measurement which is significantly higher than the sensitivity of the model found for this parameter. Considering the robustness of the measured data and sensitivity of the model its successful applicability can be concluded.

In terms of raw material usage the blast furnace model is satisfying all state of the art demands – thus all types of substitute reducing agents such as PCI, natural gas, coke oven gas, plastics, biomass, hydrogen and also charging of HBI can be successfully applied. Blast furnace gas is processed in dedusting models – here wet and dry systems are available as well as a top gas recovery turbine model for the calculation of electric power generation resulting from residual top gas pressure.

3.3 Steel production models
For further processing of hot metal, models for hot metal desulphurisation, the basic oxygen and electric arc furnace were implemented. Exemplary the basic oxygen furnace model implementation is briefly explained.

The basic oxygen furnace (BOF) model produces steel, slag and off gas based on hot metal, scrap, additives and oxygen inputs. The model is split into zones for dust generation, bath-metallurgy, steel/slag losses and off gas post combustion including dust oxidation. Dust from input materials as well as steel and slag spitting droplets are implemented as losses to the off gas. Off gas is formed by conversion of oxygen with carbon before being partly combusted with air entering the system via the skirt. Oxygen conversion, off gas post combustion and various other settings can be adjusted by the user.

<table>
<thead>
<tr>
<th></th>
<th>Steel production</th>
<th>Steel Fe content</th>
<th>Steel Si content</th>
<th>CO production</th>
<th>CO₂ production</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel grade A</td>
<td>0,3</td>
<td>0,53</td>
<td>0,43</td>
<td>13,1</td>
<td>13,06</td>
</tr>
<tr>
<td>Steel grade B</td>
<td>1,15</td>
<td>0,57</td>
<td>2,1</td>
<td>8,7</td>
<td>8,8</td>
</tr>
</tbody>
</table>

The results presented in table 4 have been found to be significantly affected by the transient characteristics and measurement uncertainties especially in the gas phase. While robust values for steel and slag analysis figures were available, gas phase data accuracy was not satisfying. Nevertheless, models’ results are in good accordance with operation data and remaining deviations limited to figures generally known to be imprecise.

3.4 Material handling, gas facilities and power plant models

Essential for the competent depiction of integrated steel plants, strategic planning and optimization procedures is the detailed consideration of chemical characteristics of input materials, material distribution streams networks and side facilities. Thus, in all implementations detailed characterization of raw materials must be specified in the form of chemical analyses including humidity and LOI for solid oxidic materials and proximate, ultimate and ash analysis for fuel/carbonaceous materials. In terms of material distribution networks all relevant streams are considered including various recycle materials and internal reusage of gases and solids.

Furthermore, side facilities of metallurgical aggregates such as gas treatment plants, power plants, heating facilities etc are included in integrated steel plant modelling as they supply added value in terms of economic or environmental point of view.

4. FULL PRODUCTION SITE CONSIDERATIONS

According to the holistic model set up and the full process depiction of all involved sub-plants the application of global variables of deeper interest is inviting and highly beneficial as well as the extraction of special information. As mentioned in above chapters, applications of this kind are:

- Combined cost calculations and optimizations
- Evaluations on global emissions of eg CO₂
- Investigations on special trace materials cycles, such as for example alkalines besides of others

Due to the complexity of integrated steel plant setups and models derived therefore – implementations in m.simtop enable far more insight on effects of changes to the overall system – compared to smaller sub plant models or simplified global approaches. An example for such an application was already given in [19] – showing the elaboration of the sulphur cycle of an integrated steel plant. Based on a model set up embracing the iron making route of the respective site, special attention in post processing steps was drawn to the sulphur species in various raw materials, intermediate and final products. The result – as
shown in figure 1 – is a comprehensive overview on the sulphur distribution in the overall iron making process route.

![Sankey diagram of the integrated sulphur cycle](image)

Figure 1. Sankey diagram of the integrated sulphur cycle [19]

Having global variables implemented, it is also possible to apply special routines such as optimizations – benefiting from powerful software functionalities in enabling more complex mathematical operations to be applied on large models. As shown in literature [11, 12], significant efforts are undertaken for such implementations proving the industrial demand of such solutions. Additionally – considering that especially in Europe steel producing companies are driven to supply CO₂ balances and environmental reports by federal regulations, the need of sophisticated holistic integrated steel plant simulation platforms is obvious and applications are already found in literature in terms of life cycle assessments [20].

5. CONCLUSIONS

The work presented here enables holistic mass and energy balancing for integrated steel plants and links to enhanced strategic operation planning in terms of costs and CO₂ – full based on and ensuring chemical and metallurgical back grounds. This additionally allows a variety of possible applications including verification and benchmarking of existing as well as predictive simulation of new production route set ups. The results presented in this work demonstrate the considerable potential of such approaches to reduce costs and CO₂ emissions in parallel to process investigations.

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