CHEMICAL ENGINEERING TRANSACTIONS
VOL. 70, 2018
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet
Guest Editors: Timothy G. Walmsley, Petar S. Varbanov, Rongxin Su, Jiří J. Klemeš

ISBN 978-88-95608-67-9; **ISSN** 2283-9216
DOI: 10.3303/CET1870137

Trace Species Investigations for Integrated Steel Plants in m.simtop

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Iron and steel making requires a wide range of different raw materials which are significantly influencing process performance and demands a continuous optimisation 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. To successfully counter this global market situation by the use of a simulation platform, the effort was taken to develop a holistic model library for optimization of integrated steel plants. This simulation platform – "m.simtop" is capable of a sophisticated depiction of any integrated steel plant setup and a wide range of calculation functionalities including optimization routines. In a detailed process analysis with m.simtop of a central European iron making route – consisting of a sinter plant, two blast furnaces including hot blast stoves and a hot metal desulphurisation ladle – simulation results were compared to operation data and showed highly accurate accordance. The special task of this process analysis was to specifically trace sulphur in the iron making production route – an environmentally and operationally crucial element. Due to this study generated simulation results delivered more insight on the sulphur distribution throughout the production process and robust figures which can be used for strategic operation planning are thus now available. In this summary the process chain, its depiction in m.simtop and related results are described.

1. Introduction

In recent years simulation, analysis of operation data, condition monitoring and computational operation support gain more and more ground in metallurgical plant operation. Fields of application for these techniques range from strategic planning, research and development as well as online operation consulting in many areas of every day´s life of integrated steel plant operation. Applied techniques are computational fluid dynamics, online operation data analysis and advice deduction for provision of operation consulting and first approaches of process simulation. Especially the challenge of strategic operation planning was found to be still suffering from a lack of robust scientifically based simulation platforms for holistic integrated steel plant optimization.
During an evaluation on the state of the art in chemical and metallurgical modelling platforms, it was found that there is no tool available for comprehensive technologically based plant calculations. The wide usage of process simulation tools such as AspenPlus®, PRO/II®, IPSEpro®, ChemCad®, etc. 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. Problems found during the evaluation on the state of the art showed incomplete raw material implementation in the simulation systems, a lack in scientifically based models or insufficient process/chemistry depiction. There have been some approaches for using flow sheeting tools for balancing selected steel making aggregates (Petersen et al., 2007), limited integrated process depictions like described by (Renz et al., 2006) or production site specific implementations (Grip et al., 2013), but a widespread usage of these related specific platforms wasn´t reached either.

Please cite this article as: Weiss B., Haibock F., Spanlang A., Wukovits W., 2018, Trace species investigations for integrated steel plants in m.simtop , Chemical Engineering Transactions, 70, 817-822 DOI:10.3303/CET1870137

These findings led to the decision of a joint development of a holistic scientifically based model library, covering all areas of iron and steel making to be used in a flow sheeting environment enabling flexible combination of the models for depiction of integrated steel plants.

1.1 m.simtop model library and simulation platform

During the last years a comprehensive metallurgical model library was developed – to be used in a well-established equation-oriented flow sheeting platform, covering all processes of integrated steel plants. The flow sheeting environment enhances flexible setups of each type of iron and steel making process route – including the blast furnace route as well as alternative routes. According to the process simulation mode of operation, production sites are depicted specifically as a flow sheet in the desired degree of detail. Special plants or equipment can be easily implemented as a new model and included in the flow sheet. More than 250 models are available for customized flow sheet modelling of existing plants as well as development of new processes (Weiss et al., 2016). Table 1 gives an overview of process modelling capabilities of m.simtop.

Table 1: Process modelling capabilities of m.simtop

Raw material preparation	Iron + steel making routes	Heat + waste heat integration	Gas treatment plants
• Beneficiation plant	• Hot blast stoves	• Directly/indirectly fired heaters	• Pressure swing adsorption
• Pelletizing plant	• Blast furnace	• Heat exchangers	• Reformer
• Sinter plant	• Corex ®, Finex®	• Off gas heat recovery	• Electrostatic precipitator
• Coking plant	• Midrex ®	• Combined steam cycles	• Cyclone
	• Basic oxygen furnace		• Baghouse filter
	• Electric arc furnace		• Top gas recovery turbine

In a detailed review thermodynamic properties of all necessary chemical species for metallurgical systems were collected and implemented directly – without any interface to 3rd party software – into m.simtop. Gibbs minimization, calculations according to the RIST method (Rist A. and Bonnivard G., 1962) and Baur Glaessner diagrams (Weiss et al., 2009) are available directly in the platform. It was found, that the introduction of raw materials chemistry is of utmost importance for highly accurate calculation results. Therefore for solids also LOI (loss on ignition) and for coals/coke ultimate, elemental and ash analysis are necessary as input figures.
Model development was done based on existing well-established routines – for complex models following hierarchical approaches. Apart from material exchange, also signal exchange is possible in between models. Global aim of the model implementation was the correct introduction of raw materials into the simulation environment, implementation of a holistic basis of models covering all parts of the process related equipment in the integrated steel plant and the possibility to combine these models for any type of integrated steel plant set up in the flow sheeting environment.

1.2 m.simtop capabilities

The above described model library in combination with a robust equation-oriented flow sheeting platform enables a wide range of calculation applications as well as solution options. Besides feed-forward calculations (e.g. raw materials defined, product amount/quality calculated), also backward calculations (e.g. product amount/quality defined, raw material demand calculated) are possible, even across large sophisticated flow sheets (Weiss et al., 2017). Apart from the simulation functionality, also optimization routines can be executed for user defined objective functions.
Due to flow sheet modelling of the real integrated plant installation, all relevant materials recycles and intermediate products are considered in the simulations/optimizations. As the simulation system is equation oriented, it is also possible to implement statistical models for e.g. mechanical or metallurgic coke parameters. Having generated this powerful optimization environment, the user is capable of sophisticated technology-based investigations for operation analysis and investment case studies. As per the chemistry based consideration of raw materials, raw material consumption figures can be calculated with an accuracy of below 1% (relative deviation). Furthermore also material costs are embedded and in combination with optimization functions – for e.g. minimization of operation costs, strategic operation planning is easily possible – with consideration of the overall plant setup and all materials involved. So far the following core features of m.simtop can be presented:

- Integrated plant calculations – considering the real plant installation in the specific desired modelling detail
- Due to the realistic depiction of the real plant setup, also recycles and by-product streams are included in simulations/optimizations
- Simulations show directly the influence of changed raw material on product and by-product qualities and quantities
- The flow sheeting environment enables the investigation of the consequences of new/changed material recycles
- Performance of forward and backward calculations, even across large flow sheets
- Simulation and optimization in the same simulation environment
- Strategic operation planning for the overall integrated steel plant set up in real time simulation time
- Investment case studies for modifications of production routes – easy exchange of equipment in the simulation due to flow sheeting environment
- Trace materials investigations – the sophisticated implementation of metallurgic chemistry enables technological operation investigations on problematic trace materials like e.g. sulphur, alkalines, halides.

As one of the milestones in m.simtop development was the implementation of trace materials chemistry, the authors want to show the capabilities of the simulation environment in a sulphur material cycle of a real plant installation.

2. Sulphur material cycle investigation

During the production of steel, various elements are removed from the initial raw material – iron bearing ores – or added in the form of alloy elements to reach the finally desired composition of steel. Besides of oxygen being the most important element which is removed in the production route of steel from oxidic ores, sulphur is one of the major undesired and problematic trace elements (Scharma et al., 2017). Sulphur increases the brittleness of steel and decreases the weldability and corrosion resistance (Visser H. J., 2016) as well as being environmentally relevant as emission in the form of SO_2 after combustion. Therefore, sulphur needs to be removed, typically below a limit of 0,015% - while being introduced in the production route by nearly all solid raw materials. In this study the iron making route of a central European integrated steel plant operator was investigated and detailed results of the sulphur distribution in the production route were generated.

2.1 Underlying plant system and operation basis

The investigated process is consisting of the major process steps of a sinter plant, two blast furnaces with hot blast stoves systems and a hot metal desulphurisation ladle. The oxidic ore is charged together with additives and coke breeze after mixing to the sinter plant. In the sinter process, the mixture is agglomerated by ignition of the coke and resulting partial melting and sintering of metal oxides – thus producing “sinter” product. After crushing and sieving the sinter is charged together with pellets and lump ore alternating with lump coke to the blast furnaces. From the blast furnaces molten hot metal (liquid iron) and slag are tapped and the hot metal is charged to a hot metal desulphurisation ladle. In Figure 1 a simplified block diagram of the process is shown.

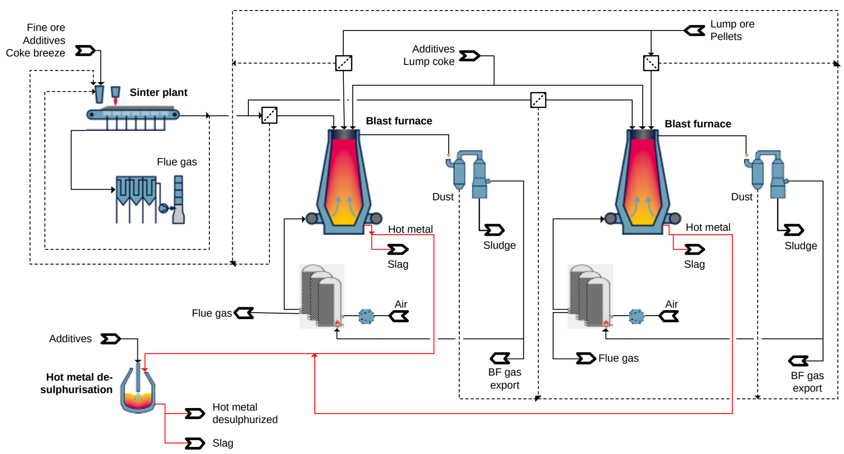

Figure 1: Simplified block diagram of the investigated blast furnace route process

The process includes various recycles, necessary for operation as well as for reintroduction of iron bearing waste materials – such as dusts – back in to the production route. During this process, sulphur enters the system with oxidic ores mainly in the form of SO_3, with coke and coal mainly as volatile elemental sulphur in complex organic compounds. In the sinter plant the sulphur is partly converted to SO_2 and leaving the system via the off gas to the atmosphere. During the blast furnace process, the major amount of the sulphur is discharged with the slag (CaS and various other phases), the residual amounts are found in the hot metal (dissolved elemental sulphur) and blast furnace gas in form of mainly H_2S and SO_2. Blast furnace gas is used for heating purposes via combustion in the hot blast stoves – heating of cold blast for the usage in the blast furnace to temperatures in the range of 1150°C – thus forming SO_2 and being exhausted to the atmosphere. In the last process step of this investigation – the hot metal desulphurisation – sulphur is removed from the hot metal via injection of an oxidic solid desulphurization powder and formation of a sulphur rich slag. Refined hot metal is then sent to the steel melt shop and there furthermore refined and alloyed to the finally desired quality.

2.2 Investigation methodology

Based on the use of the above described models from m.simtop, various other steps were necessary to gain robust results. These steps include the provision of accurate raw material mass analysis data, provision of operation data from a stable period of production, setting up the flow sheet in m.simtop and calibration of used models in m.simtop with operation data.
For all involved raw materials mass analysis were collected and averaged over one month of stable production, which also applies for any product or by-product of the process. Using this data basis, the process of interest was set up in m.simtop as an interactive flow sheet, connecting all relevant equipment of the hot metal production route of the real plant installation. To reach highest accuracy of simulation results, all recycles were included in the flow sheet, covering operational recycles like internal hearth layer usage in the sinter plant and raw materials return fines from blast furnaces as well as waste material recycles such as blast furnace dust. Following this procedure, simulation results with a deviation of below 1% (relative deviation) can be achieved and used for further analysis and comparison to operation data. Having a holistic set of simulation results of a real plant available, enables the user e.g. to specifically track measured plant data for doubtful or even erroneous values, critically investigate material streams across production departments, perform strategic planning or to research technological challenges.

3. Results and discussion

The investigated time period of one month of stable operation with an overall production of 139,000 tonnes of hot metal resulted from a total raw material flow (ores, pellets, coke, additives to sinter plant and blast furnaces) of 339,000 tonnes. For the calibration and benchmarking of the flow sheet a feed forward calculation of all raw materials was performed, delivering results for the sinter production amount and sinter product analysis, blast furnace hot metal production rates, blast furnace gas amount and analysis, just to name the most important materials. Table 2 gives an overview on simulation accuracies for the sinter plant, Table 3 gives an overview on the simulation accuracies of the blast furnaces.

Table 2: Simulation accuracies for the sinter plant

	Sinter production	Sinter mass analysis – species > 6%	Sinter mass analysis – species < 6%	Sinter plant off gas temperature
Deviation	0.13 % relative	0.19 % relative	4 % relative	9 °C

Major consumption figures of raw materials were found to be in good accordance with operation data – e.g. sinter production or melting rate mass balances. Deviations for e.g. blast furnace gas temperatures or blast furnace slag rates can be explained by the high sensitivity of the blast furnace model on the amount and oxygen content of the hot blast and in the steel industry in general neglected measurement accuracy of slag production rate respectively.
For the analysis of the sulphur material cycle in the process as depicted in Figure 1, standard operation data was extended for specific measurements of sulphur compounds in all involved raw materials, products and by-products. To establish a common basis for comparison, all measured values for sulphur components, such as H_2S, SO_2, elemental S in hot metal, various S compounds in the slag phase (e.g. CaS, FeS, S) were converted to elemental sulphur. This analysis resulted in a total amount of 400 tonnes of elemental sulphur being processed during the reference month. A detailed elaboration of the sulphur cycle contains Figure 2.

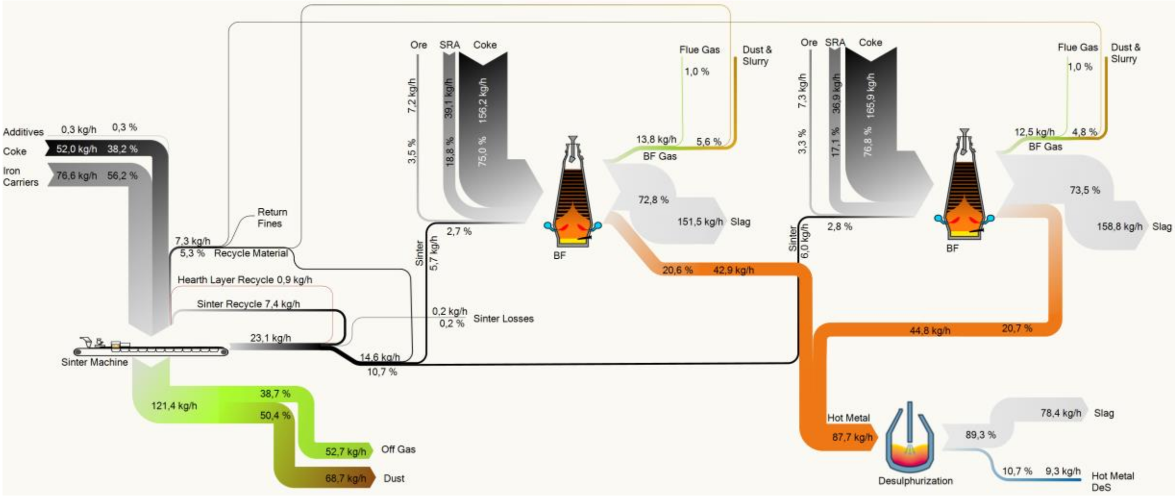

Figure 2: Detailed depiction of the elemental sulphur material cycle in the investigated iron making process

This analysis lays ground for deeper investigations, such as case studies with varying raw materials, different hot metal desulphurisation additives or even specific process variations. In the collection of the operation data on sulphur contents of by-products, especially the concentrations of H_2S and SO_2 in the blast furnace gas were rather imprecise, as they are not measured continuously during operation. To have a robust figure for comparison, values from measurement campaigns and literature data was used.

Table 3: Simulation accuracies for the blast furnace process

	Hot metal production	Slag production rate	Blast furnace gas amount	Blast furnace gas temperature
Deviation	0.35 % relative	0.19 % relative	0.19 % relative	15 °C // 12 % rel.

As the simulation results for sulphur contents in products and by-products are calculated partly from known adjusted values in the models and partly chemical reactions to close the mass balance, results for SO_2 in sinter plant off gas and sulphur content in blast furnace slag are received as result. A comparison of these values is shown in table 4.

Table 4: Simulation accuracies for the sulphur contents in sinter plant off gas and blast furnace slag

	Sinter plant off gas SO_2 - operation	Sinter plant off gas SO_2 - simulation	Slag S amount - operation	Slag S amount - simulation
Value	602 mg/Nm³	580 mg/Nm³	0.55 % mass	0.64 % mass

Related results show deviations of 3.6% relative for the content of SO_2 in the sinter plant off gas and 13% relative for sulphur in the blast furnace slag. Currently the standard deviation of the measured values is investigated – especially for the sulphur content of the slag, as it is commonly known that slag measurements are often imprecise. Future developments will include advanced model functionalities to get more insight on the formation and conversion of problematic trace materials in the iron and steel making process.

4. Conclusions

The comparison of simulation results with given raw materials to operation data proved the competence of m.simtop to be used for integrated steel plant simulations. Remaining deviations can be clearly tracked and explained – indicating imprecise measurements or minor model functionalities to be improved.

The investigation of the sulphur material cycle lays ground for future investigations on alkalines, halides, Zn and other problematic trace materials in integrated steel plant processes. Focus of such investigations is the enhanced technological depth of integrated steel plant simulations and to provide robust operation advices to steel plant operators obtained by a technology based simulation environment. Advantage of the usage of m.simtop in trace material investigations are the now more detailed knowledge of quality and quantity of the appearance of trace material in the respective sub parts of large plant systems depending on different operation

philosophies and variation in raw material blends – gained by robustly and comfortable performed simulations – and not by high risk real plant operation trials. Based on such investigations operation problems and plant downtime can be significantly reduced and selection of raw materials optimized for untroubled production.
Over the last decades strategic planning has become essential for integrated steel plant operators – leading even to the setup of specific departments in steel plant operating enterprises for this task. With increased capabilities of computer hard- and software the simulation of overall integrated steel plants became feasible, but making it necessary to have a sophisticated modelling platform which was not available for a long time. With the development of m.simtop the component is now available to close this gap and enable strategic planning departments for specific investigations, such as:

- Raw material influence on operation performance and product qualities and quantities
- Detailed cost analyses and financial controlling activities globally beyond production departments interfaces
- Optimal raw material purchasing based on most recent material prices and consideration of all production costs, by-product credits and plant operator specific KPIs
- Performance of case studies to evaluate effects of different operation philosophies by simulations – not high risk operation trials
- Material distribution controlling across in-plant departments interfaces due to the simulation of the overall integrated steel plant set up, not just sub-parts of the production chain
- Calculation of optimization routines for production cost minimisation by variation of raw material blends with consideration of all constraints and KPIs
- Investigating production chain modifications in terms of changes equipment, process or operation philosophy and determination of the optimum solution

In summary, m.simtop is competent in creating added value to integrated steel plant operators, thus opening an extensive new field of simulation capabilities for cost reduction, process understanding, knowledge generation and KPI based production chain evaluations in one central process simulation platform.

References

Grip C.E., Larsson M., Harvey L., Nilson L., 2013, Process integration. Tests and application of different tools on an integrated steelmaking site, Applied Thermal Engineering, 53, 366-372.

Petersen S., Hack K., Monheim P., Pickartz U., 2007, SimuSage – the component library for rapid process modeling and its applications, Int. J. Mat. Res. (formerly Z. Metallkunde), 98, 10.

Renz O., Fröhling M., Nebel F., Schultmann F., Engels B., 2006, Integrierender Umweltschutz in der Metallerzeugung: Simulationsgestützte operative Produktionsplanung zur Optimierung metallurgischer Abfallverwertungsprozesse, Universitätsverlag Karlsruhe, 55.

Rist A., Bonnivard G., 1962, Etude Experimentale de la reduction d´agglomeres de Minerais de fer par un gaz a contre-courant, Revue de Métallurgie, 95, 401-415.

Scharma F. N. H., Beunder E. M., Van den Berg B., Yang Y., Boom R., 2017, Sulphur removal in ironmaking and steelmaking, Ironmaking and Steelmaking, 44(5), 333-343. DOI: 10.1080/03019233.2017.1303914.

Visser H. J.,j 2016, Modelling of injection processes in ladle metallurgy, Delft university of technology, Delft, Netherlands.

Weiss B., Sturn J., Winter F., Schenk J. L., 2009, Empirical reduction diagrams for reduction of iron oxides with H2 and CO gas mixtures considering non-stoichiometries of oxide phases, Ironmaking and Steelmaking, 36, 212-216

Weiss B., Spanlang A., Wukovits W., 2016, Flow sheet modelling of steel making routes in a process integration platform, 7th European coke and ironmaking congress – ECIC 2016, 8ff.

Weiss B., Spanlang A., Wukovits W., 2017, Integrated steel plant optimization in a flow sheeting process integration platform, European steel technology and application days 2017 – ESTAD 2017, 50.