Model-based evaluation of circularity efforts in the recycling of steels

Bernd Koch, Igor Alperovich and Uwe Diekmann
Matplus GmbH, Hofaue 55, 42103 Wuppertal, Germany

Summary

For structural applications, steel already has the best overall recycling rate of all materials - however, steel for structural components, automotive chassis and bodywork is today largely produced via the classic blast furnace route, which is still associated with high CO2 emissions for the foreseeable future. A key aspect in reducing the overall life cycle balance is the step towards the "circular economy", in which largely complete recycling is to be achieved. To this end, a holistic view of the production, usage and end-of-life processes is required.
For steelmaking this task is faced with a “scale” issue – the actual processes are highly sophisticated and detailed down to atomistic chemical reaction scale, but the overarching material and energy flows are in the kiloton / GWh regime. While for both extremes process and simulation tools are available – classical LCA for the macroscale for instance – a universal modelling tool is missing, which bridges between the detail of process simulation and measurement and the macroflows, allowing to balance all efforts and outputs in a mathematically sound and cohesive manner.
In this paper an innovative approach is presented, integrating well-established flow analysis methodology in a state-of-the-art materials knowledge system. Concrete approaches for mapping and modelling EAF steelmaking processes in terms of material and energy flows from input scraps to steel and recyclate output are presented, and concepts for bridging the scale gap are developed.
Finally, the vision of a universal communication platform based on this model and data structure for all concerned parties, from waste managers over steelmakers to producers, is established.

Key Words

EAF steelmaking; circular materials; flow analysis; digital twin; process modeling; embodied energy

Introduction

Ever growing awareness of greenhouse gas emissions of energy-intensive engineering material provision and its subsequent production processes as well as foreseeable shortages of critical raw material supply have led to major efforts in increasing the “circularity” of scraps to avoid waste of material and energy. The EAF furnace route for steel scraps is the current method of choice due to its basic robustness in handling contaminations and usage of electricity as main energy source, which is promised to be “climate neutral” in the near future. However, the process is highly complex and influences of upstream processes may have a significant impact even to far downstream products. Judging whether an improvement of one small process step is really beneficial to the process as a whole is not an easy task, as the sophisticated and delicate details and their influences can be overwhelming, and a holistic view may get out of focus. Macroscale LCA data are of no help here, as they usually are based on aggregated and normalized data of the past and are not thought to be used in detailed process enhancement; detail model approaches, on the other hand, are necessarily highly localized and often do not consider data exchange to adjacent steps. This is what we call the “scale issue” – the need to establish a holistic model representing a complex process as a whole with rather simple relations without compromising the predictability of sub-process influences.

Improvements to the EAF processes at hand are multiple – ranging from simple enhancements to disruptive changes in technology. In the European commissions' Best Available Technologies, many established and experimental practices for electric steelmaking are given [1]. When using zinced steel sheet as scraps, the resulting zinc and iron-rich dust is not regarded solely as landfill anymore, but gives way to new recycling options, even in the furnace itself [2]–[5]. Evaluating enhancements like this for benefits in efficiency, cost and environmental impact is the task at hand, including eventual innovative pre- and post-processing of scraps and recyclates.

In this paper, the usage of an extended flow analysis technique for addressing this issue is proposed. By establishing a cohesive and consistent representation of shopfloor material flows, enhancing these flows with parameters like enthalpy, physical and mechanical properties and environmental footprints, and connecting it all via processes with transfer coefficients, a powerful tool for evaluation of parameter and process variations will be created.

Flow Analysis and its Application to Steelmaking Processes

An area of key interest in steelmaking is the analysis of energy flows for efficiency evaluations, and multiple efforts in this area have been made [6]–[9]. To visualize these flows, a “Sankey” depiction is common, in which the width of the flow is proportional to its amount (Figure 1). It gives a quick overview of the flow relations, but is limited to the energy – no link to other flow properties like mass is given, and as it is just a depiction, not a model itself, it cannot predict changes. The underlying data is in nearly all cases static.

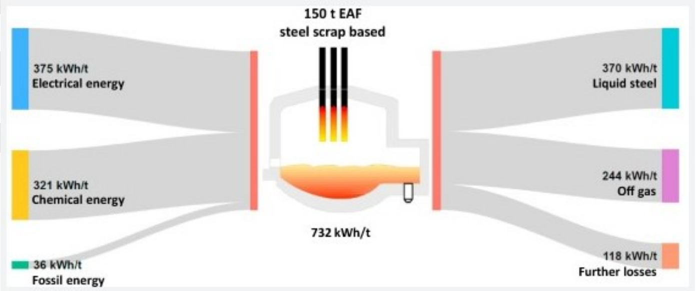


Figure 1: Sankey flow diagram of EAF energies, acc. to [10]

In contrast, classical flow analysis establishes a mathematical model to ensure consistency of all flows and to calculate unknown ones. Flows are connected with processes and can be split and joined with transfer coefficients. Each flow can have several layers of properties, which can be interconnected with the master, being usually the material / goods / mass layer. A basic setup is shown in Figure 2. An input flow is separated by transfer coefficients (TC) into an output flow and a loss flow. Several example property layers are given; naturally, the transfer coefficient may be different for each layer. Please note that some of the properties like strength may not be part of the basic flow analysis, but attributed to certain flows only.

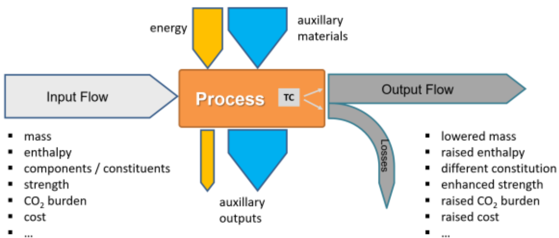
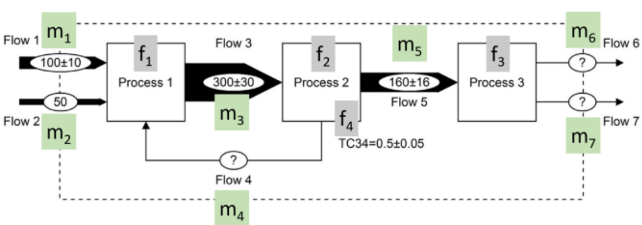


Figure 2: Principal flow analysis structure with added flow properties (layers)

Besides the main material input-output-loss flow there can be several auxiliary flows to join the process – additional energy input and miscellaneous material, for instance cooling fluid. Their transfer coefficients are not shown here, but naturally they interact the same way – the aux energy can heat up the output flow, for instance.
Flow analysis setups can also use the Sankey depiction to visualize the flow amounts per layer. A popular and well-established tool for such an approach, and allowing uncertainty propagation calculation of flow values, is the free software STAN® by TU Vienna [11], [12].
From the flow and process setups a mathematical equation matrix is generated, balancing all input and output flows, transfers and relations between flows. As long as there are (n-1) unknown variables for n equations, the matrix can be solved by regression analysis. Figure 3 shows a simple example for one (mass) layer only. For the calculation it is irrelevant if the unknown values are flows or transfer coefficients, or if they are input or output flows, so the analysis can even run "backwards", calculating needed inputs for given output flows.



$$f_1 = m_1 + m_2 + m_4 - m_3 = 0,$$

$$f_2 = m_3 - m_4 - m_5 = 0,$$

$$f_3 = m_5 - m_6 - m_7 = 0,$$

$$f_4 = m_4 - m_3 \cdot tc_{34} = 0.$$

Figure 3: Equation matrix for mass balance on a simple STAN example, acc. to [11]

Crucial for usage of flow analysis on shopfloor modeling is the interconnection of layers by mass concentration or specific energy values. An energy value can be

calculated from the mass flow by using specific energy, or an enthalpy at a given temperature. The same would apply for an elementary flow as percentage of a mass flow, for instance 1% manganese in a steel material flow, or for CO_2 burden on a certain amount of primary aluminium. By this, flow values in dependent layers cannot only be static attributes, but dynamically follow the mass flow.
On the energy layer, this even allows for a “creative” usage of the energy content of a mass flow – on the one hand, the already mentioned enthalpy, on the other hand something that Ashby called the “embodied energy” – the energy that was needed for the production of the material flow [13]. In Figure 4 a simple example of those options is illustrated.

Figure 4: Usage of the energy flow layer for different mass-related energy types

In STAN, only one layer of energy can be used in a flow system, so the simultaneous use of “embodied energy” and enthalpy is a bit tricky (yet not impossible). Future versions of flow analysis software, like in the EDA® system presented later, will overcome this limitation.

Example EAF Flow Model

To illustrate the possibilities of a flow analysis-based shopfloor model, an exemplary EAF setup was constructed in STAN, Figure 5 (material flow layer depicted only). Goal of this model was to illustrate the consequences of varying scrap inputs, namely the addition of highly Zn-bearing coated steel sheets on the reaction energies and the dust output of the EAF process.
A “charging” process is fed by four different types of scraps, pig iron and coal surcharge. Adhesions and contaminants are summarized by a “dirt” flow. In the “charger”, the transfer coefficients divide all input flows in their elementary constituents and a sorting loss. The constituents are forwarded to a “reaction splitter”, allowing to determine the contributions of each element to the final alloy or to oxidation reactions (if the alloy composition is known, the reaction elements are calculated accordingly). In the reaction process, per oxide an additional oxygen flow is fed, which is coupled to the respective input reaction element with the stochiometric amount needed by a flow relation (not shown here). Those “reactions” result in the output flows of the created oxides. The transfer coefficients of the “EAF melt” process determine the distribution of the inputs to raw steel, slag, dust and exhaust gases. As a downstream process, a simplified aspiration of the EAF and the factory hall is added – EAF primary aspiration is cooled, mixed with secondary aspiration. EAF dust is filtered out, and two additional recyclate outputs of Fe-rich resp. Zn-rich dust are generated.
From the cooler, a return flow is led back to the charger, representing a simple scrap pre-heat device. As this flow is “energy only”, it is zero on the material layer, but has

a value on the energy layer. This allows for otherwise wasted exhaust energy to be fed back in the process and thus save energy.

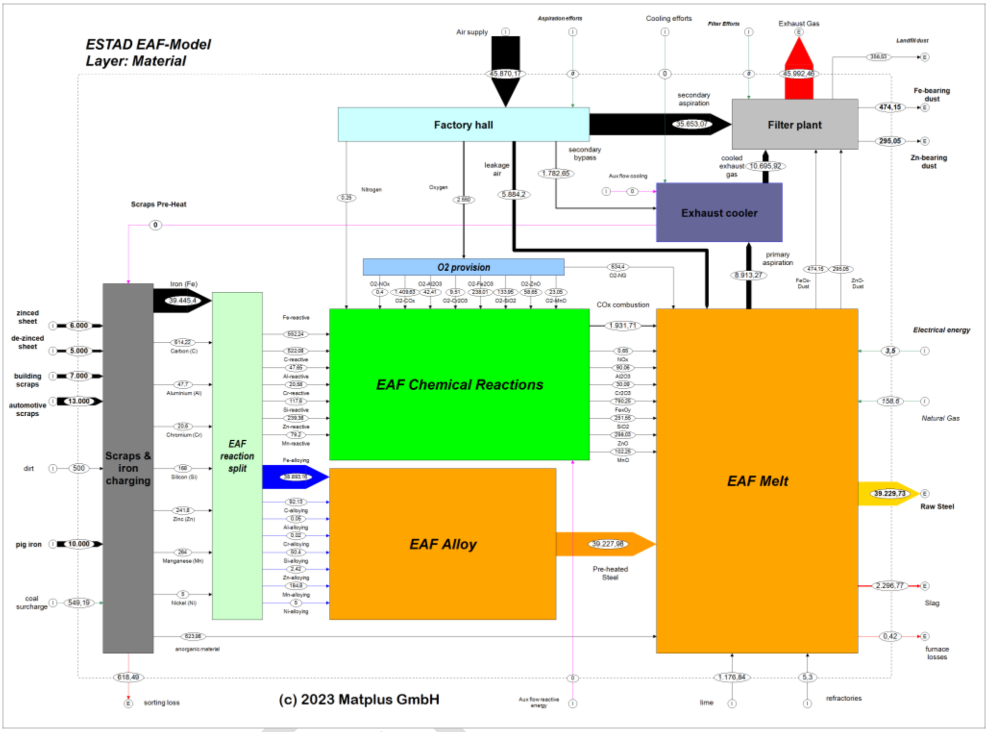


Figure 5: EAF furnace flow model example, material layer. For full detail, see the presentation file.

The core components of the energy layer are presented in Figure 6. On the left, chemical reaction energies are calculated by their reaction enthalpies and fed into the EAF melt process. The raw steel and slag leave the process with the enthalpy representing their mass and temperature, same for hot gas of primary aspiration. Natural gas consumption can be measured as volume flow – the model calculates the resulting energy input by density, mass and reaction enthalpy. Finally, from all those given flows, the resulting electrical energy of the arc is calculated.
It is important to notice that the model is consistent and fully dynamic, for instance:

- Increasing zinc bearing inputs give higher amounts of Zn-bearing dust, but also higher inputs of reaction energy - thus lowering the need for external EAF energy input, but raising the energy consumption of dust processing
- Decreasing natural gas flow lowers energy input, primary aspiration output and raises electrical energy demand
- Increasing scrap pre-heat lowers overall energy demand
- Lowering coal surcharge lowers combustion reaction energy
- Raising dirt input raises slag amount, which has to be heated and increases energy demand

The model can easily be enhanced in many ways, for instance by detailing the EAF melt processes and the filter plant by sub-models. A CO_2-layer could be added, in which the CO_2-contribution of coal, gas and electricity energy carriers can be considered etc.

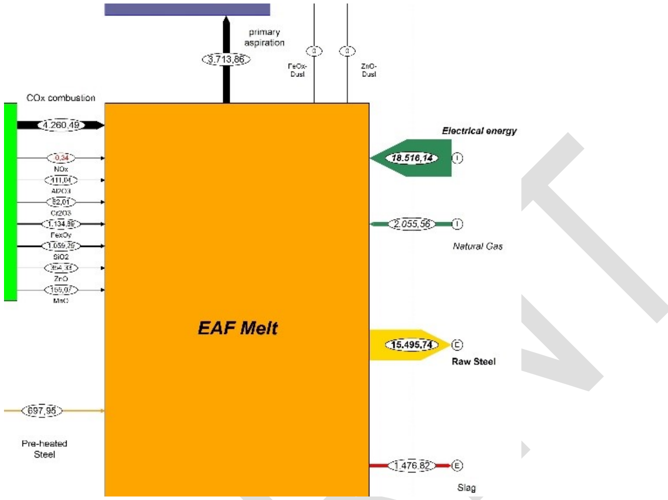


Figure 6: EAF furnace flow model, excerpt of energy layer showing reaction enthalpies and energy usage

Future work: a universal communication platform for circular materials

As shown, the complex issue of evaluating the effects of zinc contents of the EAF process can be encountered by flow modeling, allowing to simplify the relevant effects without being oversimplistic and plotting it in an easy-to-understand Sankey visualization. Detail and complexity level can easily be raised or lowered according to the task requested. Overall process benefits and eventual trade-offs can be evaluated using different scenarios of parametrization.

Furthermore, the possibilities of flow analysis can be greatly enhanced by integration of this technology into a full-featured Materials Information System. Not only can each flow be represented with a virtually unlimited number of interconnected layers, but enriched with material and ERP data, like strength, cost, chemical composition and ROHS information about hazardous substance content. With the system Matplus EDA® e.g., enthalpies of the exact alloy composition can be provided by integration of JMatPro® material simulation capabilities instead of using average estimations.

As this is integrated as a whole in a dynamic flow model on multiple layers, with each layer fed by EDA® database content or simulation data when needed, each process variation has repercussions on the other steps, so enhancements (or errors) directly influence the attributes of the final product leaving the shopfloor.

Complete real-world setups can easily be replicated and virtually modified to simulate the impact before introduction of new technology in the process.

The integration of this extended mass & energy flow analysis including mathematical optimization is subject of current activities within the scope of an extended EDA®.

Conclusion

Circularity enhancements in steel production should lead to an optimized product footprint, but often the repercussions of single measures or variations are hard to estimate due to complexity of the processes and the process chains.
Flow analysis methods can be used to significantly improve the understanding of complex production systems like EAF steelmaking and its downstream processes. Enhancements of sub-processes and their repercussions across the whole production can be modeled and evaluated. Sophisticated information of deep single process understanding can be integrated in a simplified yet powerful overarching model.
Attribute-enriched flow analysis in a materials information system allows complete control of any production process with all up- and downstream processes and their contribution to the final footprint of the product.
The Matplus EDA® system integrates all aspects of material production, properties and knowledge.

Acknowledgements

We would like to thank O. Cencic and H. Rechberger from the Institute of Water Quality and Resource Management, TU Vienna, for fruitful collaboration in this project.

References

[1] O. Rentz, S. Hähre, R. Jochum, und T. Spengler, „Report on Best Available Techniques (BAT) in the Electric Steelmaking Industry". Deutsch-Französisches Institut für Umweltforschung (DFIU), Juni 1997.
[2] M. Auer und J. Antrekowitsch, „Alternative Solutions for the Recycling of Steel Mill Dust Using the 2sDR-process", in *Mineralische Nebenprodukte und Abfälle 7 – Aschen, Schlacken, Stäube und Baurestmassen* –, Neuruppin: Thomé-Kozmiensky Verlag GmbH, 2020, S. 223–231.
[3] M. Auer, „Innovative Lösung für das Recycling hoch-zinkhaltiger Stahlwerksstäube", University of Leoben, 2022. Zugegriffen: 6. Dezember 2022. [Online]. Verfügbar unter: https://pure.unileoben.ac.at/portal/de/publications/innovative-loesung-fur-das-recycling-hochzinkhaltiger-stahlwerksstaube(7da66e4b-13c5-4121-a2a4-7d68af1f8428).html?customType=theses
[4] J. Antrekowitsch, „Stahlwerksstaubrecycling im 21. Jahrhundert", in *Recycling und Rohstoffe*, Neuruppin: TK-Verlag, 2015, S. 363–370.
[5] F. Grillo, J. Coleti, D. Espinosa, J. Oliveira, und J. Ten^|^oacute;rio, „Zn and Fe Recovery from Electric Arc Furnace Dusts", *Mater. Trans.*, Bd. 55, S. 351–356, Feb. 2014, doi: 10.2320/matertrans.M2013385.
[6] K.-H. Heinen und Verein Deutscher Eisenhüttenleute, Hrsg., *Elektrostahl-Erzeugung*, 4., Völlig neu bearb. und erw. Aufl. Düsseldorf: Stahleisen, 1997.

[7] H. Pfeifer und M. Kirschen, „Thermodynamic analysis of EAF electrical energy demand“, gehalten auf der 8th European Electric Steelmaking Conference, Mai 2002.
[8] J. Wendelstorf und K.-H. Spitzer, „A process model for EAF steelmaking“, Bd. 2, Apr. 2006.
[9] V. Logar, „The Influence of Electric-Arc-Furnace Input Feeds on its Electrical Energy Consumption“, *J. Sustain. Metall.*, Bd. 7, S. 1–14, Juli 2021, doi: 10.1007/s40831-021-00390-y.
[10] T. Keplinger, M. Haider, T. Steinparzer, P. Trunner, A. Patrejko, und M. Haselgrübler, „Modeling, Simulation, and Validation with Measurements of a Heat Recovery Hot Gas Cooling Line for Electric Arc Furnaces“, *Steel Res. Int.*, Bd. 89, Nr. 6, S. 1800009, 2018, doi: 10.1002/srin.201800009.
[11] O. Cencic, „Nonlinear data reconciliation in material flow analysis with software STAN“, *Sustain. Environ. Res.*, Bd. 26, Nr. 6, S. 291–298, Nov. 2016, doi: 10.1016/j.serj.2016.06.002.
[12] O. Cencic und H. Rechberger, „Material flow analysis with Software STAN“, *J. Environ. Eng. Manag.*, Bd. 18, S. 3–7, Jan. 2008.
[13] M. F. Ashby, *Materials and the Environment - Eco-informed material choice*, 3rd Aufl. Elsevier, 2020. Zugegriffen: 3. Mai 2023. [Online]. Verfügbar unter: https://www.elsevier.com/books/materials-and-the-environment/ashby/978-0-12-821521-0