

# Integrating CO<sub>2</sub> Reporting with Physically Consistent Material and Energy Flow Analysis to Improve Circularity of Steel Products

Uwe Diekmann\*, Marco Thomä\*, Yingyan Yu\*, Phillip Wallat\*\*

\*Matplus GmbH, Hofaue 55, 42103 Wuppertal, Germany

\*\* DfACE Strategy Systems, Gerhard-Rauschenbach-Straße 14, 38678 Clausthal-Zellerfeld, Germany

*The steel industry is responsible for a significant proportion of global CO<sub>2</sub> emissions and is therefore the focus of sustainable developments. The circular economy, which minimizes waste and uses resources efficiently, plays a central role in this. Physically consistent and comprehensible data based on mass and energy conservation is essential for sound sustainability decisions. However, combining CO<sub>2</sub> balancing with material and energy flows is challenging, for example due to incomplete data. This article presents a new method that combines physical consistency with current reporting standards such as ESRS, thereby improving environmental reporting and resource efficiency in the steel industry.*

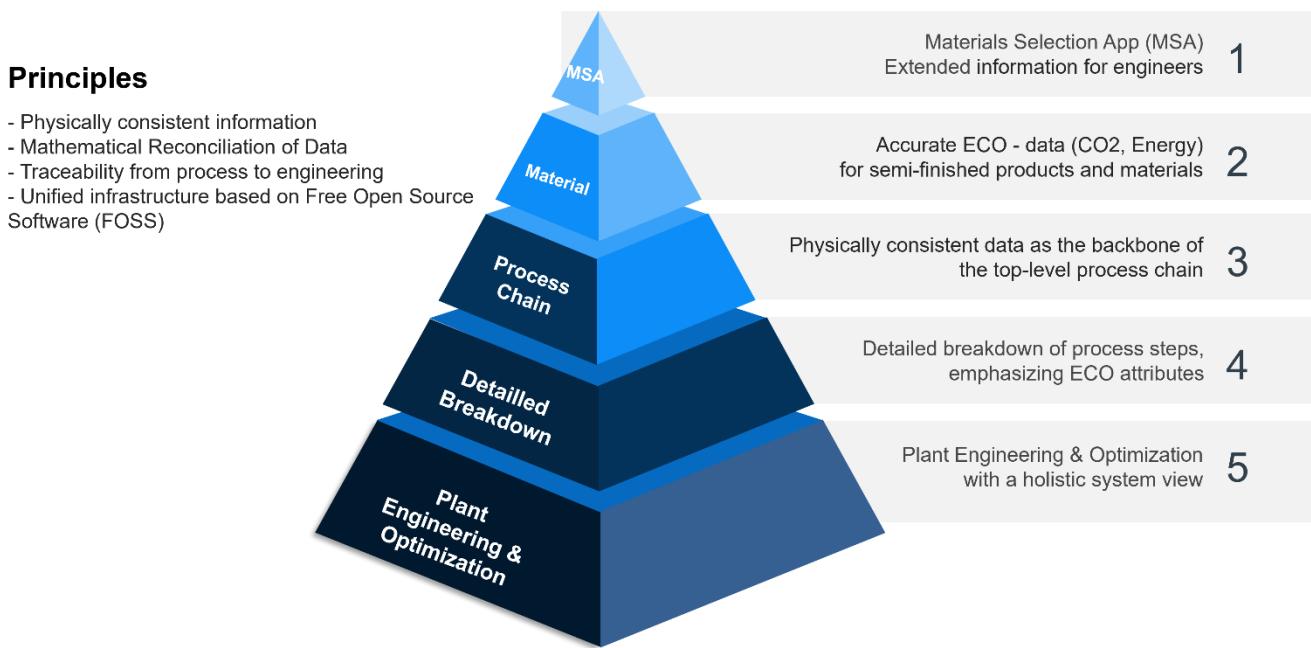
**KEYWORDS:** STEEL, DIGITALIZATION, CARBON FOOTPRINT, SUBSTANCE FLOW ANALYSIS, ENERGY FLOW ANALYSIS, PHYSICALLY CONSISTENT MODELLING, ESRS, ECO DESIGN

## INTRODUCTION

The steel industry is a major global CO<sub>2</sub> emitter and a key player in industrial development. With increasing environmental concerns, sustainable practices are crucial. A circular economy, focusing on waste minimization and resource efficiency, offers a promising solution (1). For the steel industry, this means not only recycling materials but also optimizing processes for efficiency and eco-friendliness. Accurate data on material and energy flows is essential for informed sustainability decisions (2). However, integrating CO<sub>2</sub> accounting with material and energy flow analysis is challenging due to data inconsistencies, making accurate modeling difficult. The complexity of steel production requires advanced tools to ensure data is useful for decision-making. Additionally, efficient CO<sub>2</sub> reporting is increasingly necessary, aligning with guidelines like the European Sustainability Reporting Standards (3). This paper introduces a novel methodology for physically consistent modeling of data driven material and energy flows, integrating CO<sub>2</sub> accounting and reporting. It uses a graphic interface to handle both known and uncertain data, serialized into a structured JSON format. This data is translated into a mathematical model for optimization-based reconciliation, ensuring physical consistency and robustness. The methodology, demonstrated through an Electric Arc Furnace (EAF) steelworks production case study, enables easy system modeling and analysis, offering insights for improved decision-making and environmental impact reduction.

## 1. VISION

The vision for a transforming, resource-efficient and sustainable steel-industry is based on an integrated materials energy process optimization system, that covers different levels within whole enterprises (Fig. 1).



**Fig. 1 – Concept for an infrastructure of an integrated materials energy process optimization for enterprises**

The image depicts a pyramid illustrating a vision for a five-stage integrated material, process, and energy optimization. The pyramid's apex, Level 1, focuses on material selection, offering advanced information for engineers through a Material Selection Application (MSA) that integrates with CAD software like NX or CATIA. This level underscores the importance of choosing suitable materials for sustainable and efficient manufacturing, helping engineers balance cost reduction, low carbon footprint, and lightweight design. Level 2 emphasizes accurate environmental data, including carbon footprint and energy consumption for semi-finished products, crucial for minimizing environmental impact. Level 3 highlights the need for physically consistent data as the foundation of the process chain, ensuring reliable information. Level 4 offers a detailed breakdown of process steps, focusing on ecological attributes like mass and energy flow, waste management, and GHG emissions, facilitating in-depth analysis and optimization to boost efficiency and reduce environmental impact. The pyramid's base, Level 5, represents system planning and optimization, adopting a holistic perspective. The guiding principles include physically consistent information, mathematical data reconciliation, process-to-engineering traceability, and a unified FOSS-based infrastructure, essential for sustainable and efficient material, process, and energy planning.

## 2. METHODOLOGY

### Graphic Notation for Substance and Energy Flow Modeling

To model complex interactions in steel production, a specialized graphic notation was developed. This notation visually represents flows like raw materials, energy, and emissions, as well as processes such as production and waste management. Further details of the processes can be added and customized if desired. Using distinct symbols for each flow and process, it provides a clear overview, facilitating analysis and understanding. It effectively handles both known and uncertain data, ensuring comprehensive system representation.

### Serialization in JSON

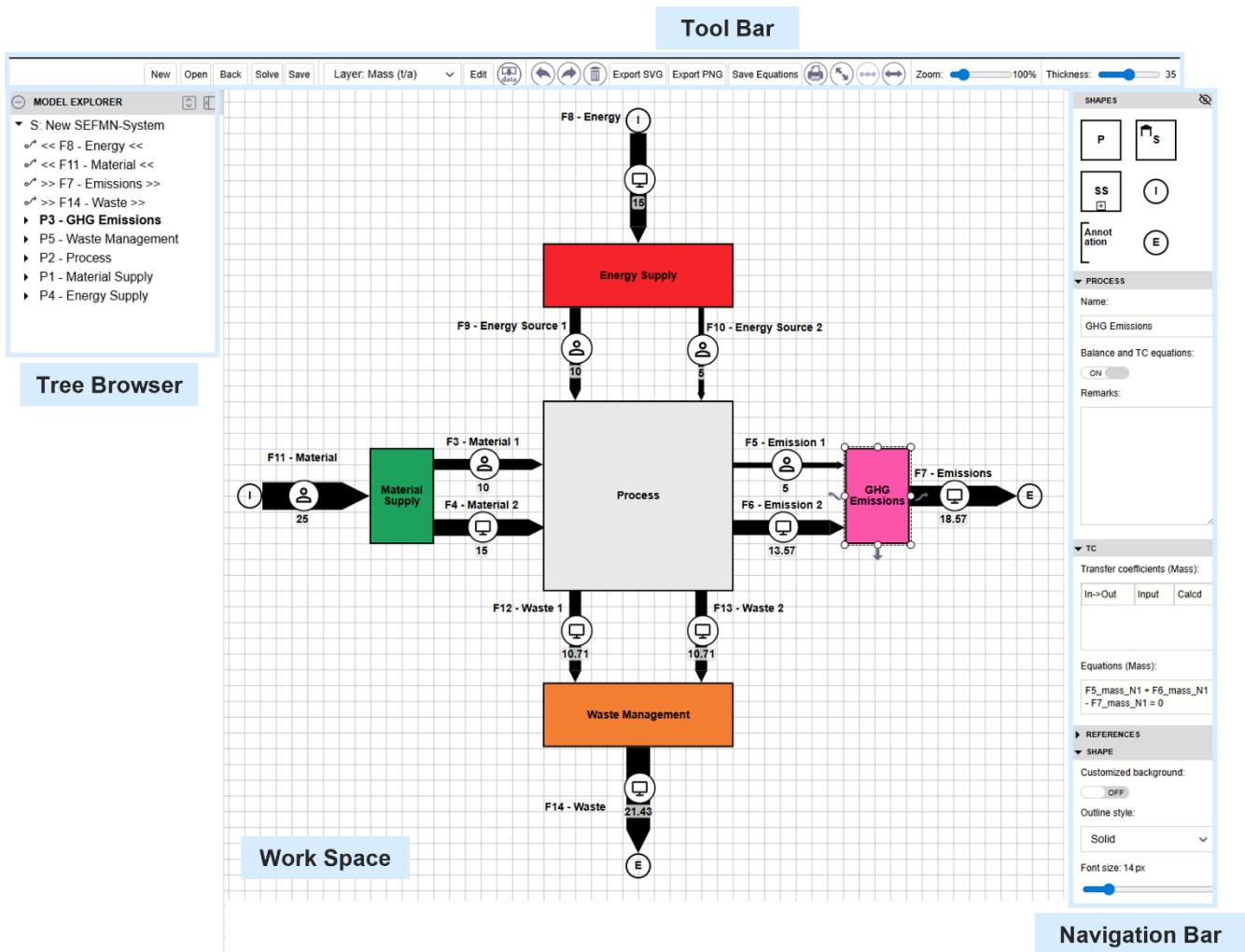
The graphic notation is serialized into a structured JSON format, ideal for capturing relationships and attributes within the system. This process translates visual elements into a JSON data model, detailing flow types, processes, and interactions. The resulting JSON format offers a standardized, flexible representation, easily integrated with various tools and platforms.

### **Mathematical Modeling and Optimization**

The JSON data model underpins a mathematical model incorporating mass and energy conservation principles, ensuring physical consistency. Optimization-based data reconciliation techniques address data discrepancies, minimizing differences between observed and predicted values under conservation constraints. This ensures the model is both physically consistent and mathematically robust. Advanced tools like the programming language Julia enable complex calculations, ensuring accurate physical behavior representation (4).

### **Software Application**

A user-friendly software application with a graphic user interface (GUI) and mathematical solver was developed for easy access. The GUI allows users to create and edit graphic representations of material and energy flow systems in a format with Sankey arrows, while the solver performs data reconciliation. Designed for intuitiveness, it enables efficient system modeling and provides tools for analysis. The solver handles complex calculations, ensuring model accuracy and reliability. Fig. 2 illustrates a generic ESRS-conform mass flow model example created with this application.



**Fig. 2 – Generic example of a generally ESRS conform mass flow model**

The software application is implemented using modern software development practices and technologies, ensuring that it is robust, scalable, and maintainable. It is designed to be accessible to a wide range of users, from industry professionals to researchers, providing a powerful tool for improving the accuracy and reliability of environmental reporting in the steel industry.

### 3. RESULTS

#### Modeling of EAF Steelworks Production

To validate the effectiveness of the newly developed methodology, it was applied to a case study focusing on the Electric Arc Furnace (EAF) steelworks production process. The EAF process is a critical method for producing steel from scrap metal and involves a complex interplay of various material and energy flows (5). By modeling this process, it was aimed to demonstrate how the methodology can handle real-world industrial complexity and provide actionable insights. Using the graphic notation, a detailed representation of the EAF process, capturing the key flows and processes involved was created. This included raw material inputs, energy consumption,

emissions, and byproducts. The graphic notation provided a clear and comprehensive overview of the system, making it easier to understand and analyze the interactions between different components. The next step involved serializing this graphic representation into a structured JSON format. This serialization process captured the detailed relationships and attributes of the flows and processes, providing a standardized and flexible data representation. The JSON data model served as the foundation for creating a mathematical model of the EAF process, incorporating the principles of mass and energy conservation.

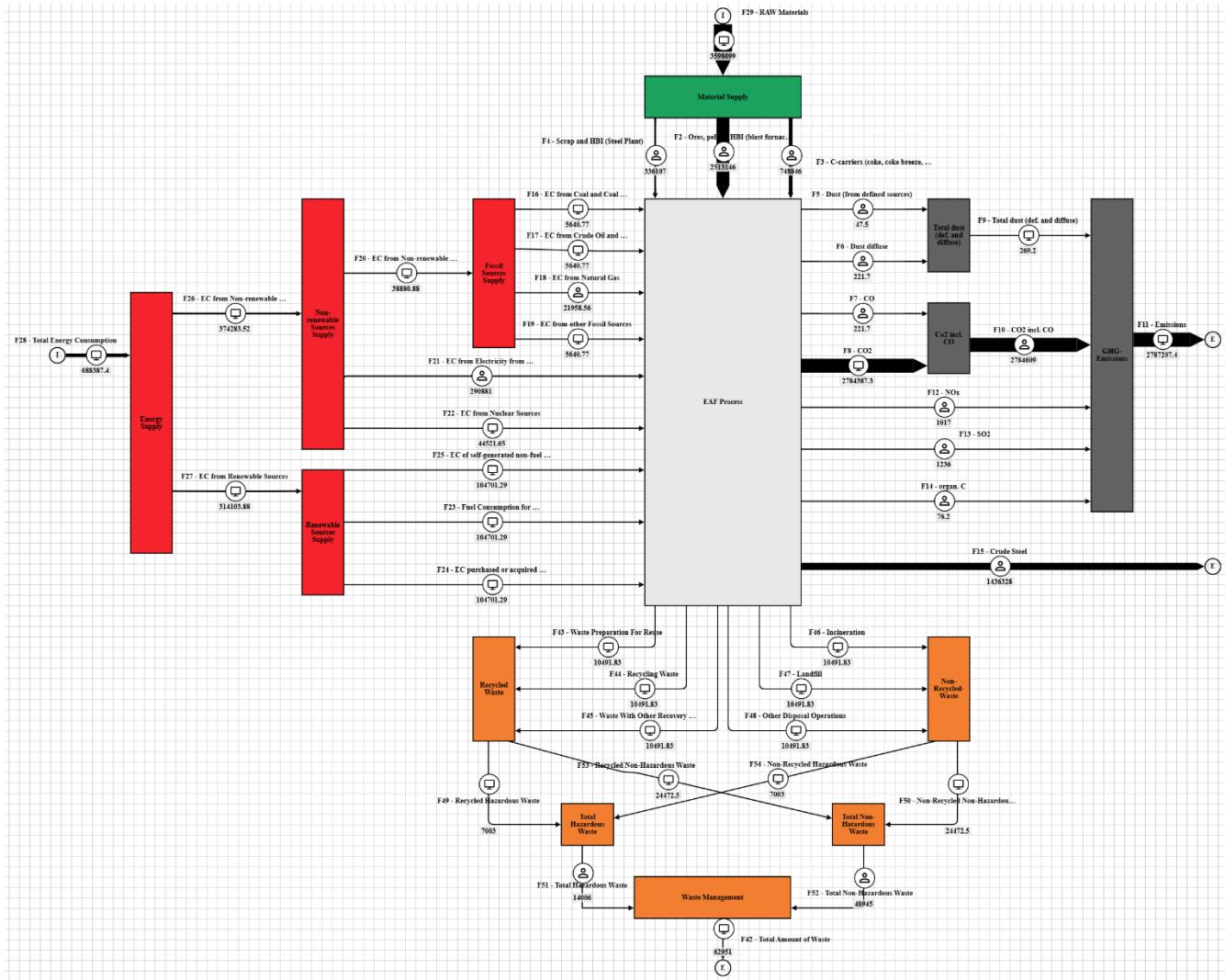
### **Physical Consistency**

Ensuring physical consistency in modeling complex industrial processes like EAF is challenging. The principles of mass and energy conservation must be strictly adhered to, and any data discrepancies must be reconciled. The optimization-based approach successfully addressed this, providing a physically consistent and mathematically robust model. The optimization process minimized differences between observed and predicted values, ensuring the model accurately represented the system's physical behavior and offered reliable insights into the EAF process. The model's robustness was demonstrated using a Julia-based solver, handling incomplete or contradictory data and uncertainties through data reconciliation.

### **ESRS Compliance**

The methodology aligns with the European Sustainability Reporting Standards (ESRS), emphasizing physically consistent and traceable information. Compliance with ESRS enhances the accuracy and reliability of environmental reporting in the steel industry. The EAF process case study demonstrated the methodology's application to real-world industrial processes, meeting ESRS requirements and providing valuable insights for better decision-making to enhance sustainability. The clear overview of material and energy flows, combined with the physically consistent model, offers insights into the system's behavior, enabling industry professionals to identify improvement and innovation opportunities.

Fig. 3 illustrates the ESRS-compliant EAF Steel Works Production Master Model. According to ESRS guidelines, mass and energy flows are divided into material supply, energy supply, GHG emissions, and waste management, each subdivided into detailed reporting areas. This complexity is integrated into the model, enabling automatic generation of ESRS-compliant reports. The model's visualization supports understanding through Sankey arrows representing flow values and indicating calculated or manually entered flows.



**Fig. 3 – ESRS conform EAF Steel Works Production Master Model**

## 4. DISCUSSION

### Benefits of Physically Consistent Modeling

The methodology presented offers significant benefits, particularly for environmental reporting and sustainability in the steel industry. By adhering to mass and energy conservation principles, it ensures accurate and reliable data for decision-making, crucial for environmental reporting like ESRS. Physically consistent modeling enhances data traceability, providing a clear overview of material and energy flows within a system. This traceability is essential for identifying improvement areas and optimizing resource efficiency and environmental performance, which is especially important in the complex steel industry.

### Role in circular economy

The tool offers also valuable insight into the recycling processes for the circular economy. This can already be implemented with the product design process and used to analyze the different compositions of components in a product. While the steel production process in an EAF is already presented, the upstream processes of the process are also applicable. The energy consumption of a shredder process can be measured and used as a baseline for the energy and CO<sub>2</sub> already invested into the scrap waste stream. Followed by sieving and magnetic sorting processes this represents additional resource investment into the treatment of steel scrap. Depending on the definition and view of a company, this can be Scope 1 / 2 emissions for the recycling company or Scope 3 emissions from the initial manufacturer of the product (6). When other materials, residues or waste are present in the material the processing costs will increase along with the energy consumption and CO<sub>2</sub> emissions. Therefore, if designed right, the product shall be dismantlable in a way that there is minimal harmful or inert material in the process. Therefore, the process is more efficient, which has a positive impact for the CO<sub>2</sub> footprint of the recycled steel. That said, it is also possible to determine the main CO<sub>2</sub> and cost drivers in the production process of materials.

For a product with different assemblies and parts in those assemblies, an automated influence analyses, with standardized recycling process templates, can be utilized via the JSON structure. Changes in the material amount and composition of the assembly can be determined by the system. When more detail is needed, analysis of different parts and their influence on the process can be simulated. For a holistic analysis it is possible to estimate the influence of a new module towards the product level. In case there is information about the exact recycling process of the material the product can even match to that exact process. This gains efficiency and liberties in the design process, if the composition is not harmful for that process.

This allows developers to design the product along specific processes and determine the emissions within the life cycling for each step to a certain degree. Within a circular economy, knowledge about the emissions is crucial, lest one critical processes with high CO<sub>2</sub> does impact to much of the CO<sub>2</sub> budget.

### **Practical Applications**

The methodology has numerous applications in the steel industry, particularly in environmental reporting, where it improves report accuracy and reliability. Furthermore, the approach helps to transform a reporting obligation into a benefit in terms of deeper process knowledge. It can be applied to process optimization and resource management, providing insights into system behavior and identifying improvement and innovation opportunities. For example, it can optimize raw material use, reduce energy consumption, and minimize emissions and costs. Additionally, it supports the development of new technologies and processes, enabling researchers and industry professionals to explore new ideas confidently. This will lead to more efficient and sustainable steel production processes, enhancing the industry's environmental performance.

### **Challenges and Limitations**

Despite its benefits, the methodology faces challenges, particularly the complexity of modeling steel industry systems with vast material and energy flows. Accurate and comprehensive data capture is daunting, requiring sophisticated tools and a deep understanding of processes. Data quality and availability also pose challenges, as data can be incomplete or inconsistent. While the optimization-based approach addresses these issues to some extent, high-quality data is still needed for model accuracy and reliability. This necessitates robust data collection and management practices, along with ongoing efforts to improve data quality and availability.

## **5. CONCLUSION**

In this paper, we presented a novel methodology for integrating CO<sub>2</sub> reporting with physically consistent material and energy flow analysis in the steel industry. Our approach leverages a new graphic notation designed to handle both known and uncertain data, which is serialized into a structured JSON format. This JSON data model is translated into a mathematical model that forms the basis for optimization-based data reconciliation by the programming language of Julia, ensuring that the data is physically consistent and mathematically robust. The methodology is implemented through a user-friendly software application that includes a graphic user interface (GUI) and a mathematical solver. This application allows industry professionals to easily model and analyze their systems, providing valuable insights into the material and energy flows and supporting better decision-making to improve resource efficiency and reduce environmental impact. To demonstrate the effectiveness of our methodology, we applied it to a case study of Electric Arc Furnace (EAF) steelworks production. The results of the case study highlight the practical applications of our methodology in the steel industry, showing how physically consistent modeling can enhance the accuracy and reliability of environmental reporting. This approach showed numerous and varied benefits whereas some challenges and limitations remain. Future research directions could include extending the methodology to other industries and applications, as well as further refining the optimization techniques and data reconciliation processes.

## **ACKNOWLEDGEMENTS**

Selected activities of this work regarding the modelling part were supported through funding from the “Federal Ministry for Economic Affairs and Energy” within the project “Green-AI-Light”. We also want to thank Mr. Oliver Cencic from the Vienna University for his contribution to this topic.

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