

Practitioner's Section

Integrated Resource Efficiency Analysis for Reducing Climate Impacts in the Chemical Industry

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Reducing greenhouse gas emissions of the material-intensive chemical industry requires an integrated analysis and optimization of the complex production systems including raw material and energy use, resulting costs and environmental and climate impacts. To meet this challenge, the research project InReff (Integrated Resource Efficiency Analysis for Reducing Climate Impacts in the Chemical Industry) has been established. It aims at the development of an IT-supported modeling and evaluation framework which is able to comprehensively address issues of resource efficiency and climate change within the chemical industry, e.g. the minimization of material and energy intensity and consequently greenhouse gas emissions, without compromising on production performance. The paper presents background information on resource efficiency and the research project, an ideal-typical decision model for resource efficiency analysis, the conceptual approach for an IT-based integration platform as well as the case study design at the industrial project partners' sites. These first results are linked to future activities and further research questions are highlighted in the concluding section.

1 Introduction – Resource Efficiency in Chemical Industries

Mitigation of climate change is an inevitable challenge for manufacturing industries. Numerous efforts are made in reducing climate impacts caused by greenhouse gases. Isolated approaches to reduce greenhouse gases - for instance by increasing energy efficiency - are useful starting points but fail to explore the full potential of more holistic approaches. The latter require practice-oriented integrative methods which combine aspects

and concepts of process and chemical engineering, environmental life cycle assessment, managerial accounting and operations research. Such integrated approaches are still rare. One reason is a lack of adequate instruments for systematic consideration of the various environmental and climate impact categories in process engineering and design. Especially small and medium sized companies require support to keep track of possible climate protection and resource efficiency measures.

“Resource” is a rather broad term with a range of different meanings, including for instance man-

power (human resources), time, finance, raw materials or operating supplies. The term resource efficiency, though, is mostly used in the context of natural resources and sustainable development: "Resource efficiency means using the Earth's limited resources in a sustainable manner while minimizing impacts on the environment. It allows us to create more with less and to deliver greater value with less input" (European Commission, 2013). This particular understanding of resource efficiency has been appointed as one of the seven flagship initiatives under the European Commission's 2020 strategy (European Commission, 2011).

Looking at single topics within resource efficiency, like energy efficiency, there are already numerous guidelines or supporting programs available. In contrast, guidelines on integrated approaches for resource efficiency analysis are still rare or under development. The Association of German Engineers (VDI), for instance, currently develops standards and general guidelines on resource efficiency analysis to pursue the reduction of resource input and emissions and to increase resource productivity (VDI ZRE, 2013). A study mandated by the European Commission identified financial and information barriers, lack or insufficiency of knowledge on resource efficiency approaches in particular, as main obstacles for the application of resource efficiency analysis (Rademaekers *et al.*, 2011).

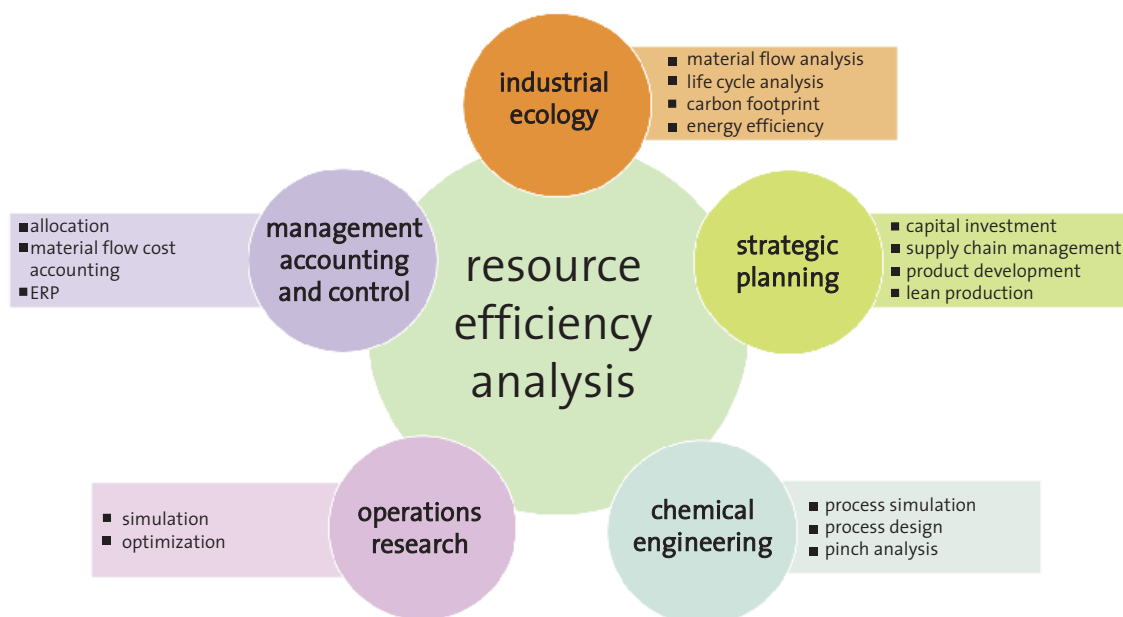
Achieving resource efficiency not only requires

integration of methods and tools from different disciplines, but also the inclusion of supply chain actors. Limiting resource efficiency analysis to single processes or production units is unlikely to fully explore reduction, recycling and symbiosis potentials within large industrial production networks. Within eco-industrial parks and highly integrated production networks, waste flows and heat losses from one company become valuable inputs for other businesses (Herczeg *et al.*, 2013). Hence, integrated resource efficiency analysis incorporates a holistic, system-wide perspective.

To meet these challenges, an interdisciplinary research project on *Integrated Resource Efficiency Analysis for Reducing Climate Impacts in the Chemical Industry* (InReff) has been designed and is partly funded by the German Federal Ministry of Education and Research (BMBF).

From an overall perspective this interdisciplinary research project aims at developing an IT-supported modeling and evaluation platform which is able to comprehensively address issues of resource efficiency and climate change within the chemical industry. Enhancement and integration of available concepts and methods, software prototyping, case study research, and knowledge transfer are essential parts of the project and conducted in close collaboration of one software solution provider, three industry partners, two universities and a wider range of associated organizations and experts. Well

Figure 1 Complexity range of integrated resource efficiency analysis.



established methods for process development and design, flow sheet simulation, heat integration, material flow analysis, material flow cost accounting and environmental assessments, including carbon footprinting and life cycle assessment, need to be combined in a coherent approach and supported by an IT-based environment for integrated resource efficiency analysis. The variety of potentially relevant methods and tools is presented in Figure 1.

This paper explores the project's conceptual approach on resource efficiency analysis (chapter 2), elaborates the concept for an IT-based framework for integrating relevant tools and methods (chapter 3), introduces the industrial case study design (chapter 4) and concludes by explaining the project's knowledge transfer conception and future research activities (chapter 5).

2 Conceptual Approach - Integrated Resource Efficiency Analysis

Based on a dialogue of chemical and process engineers, decision makers from industries and consultancy as well as academics in the field of chemical engineering and industrial ecology, an ideal-typical model for performing an integrated resource efficiency analysis has been developed. The dialogue took place on project workshops and included practitioners and academics from organizations outside the project. Figure 2 depicts the ideal-typical model including tools identified as highly relevant.

The model follows basic decision making model notations and thereby provides a sequence of steps that pursue continuous resource efficiency increase. Starting with basic considerations on the goals to be achieved and the relevant system boundaries (1), an energy and material flow analysis of the chosen system is performed (2). This analysis provides the basis for initial computation and assessment of key performance indicators and targets that quantify and benchmark the overall objectives (3). In some cases a basic energy and material flow analysis will reveal resource efficiency improvement potentials immediately (4a, 7, 8). Applying constant iteration to adapt target and system boundary (5, 4b), the model can be expanded and refined in order to find efficiency enhancing measures (6a-c). The refinement happens either within the energy and material flow model (6a) or integrates further tools like flow sheet simulation, heat integration analysis (6b) or carbon footprinting (6c). If multiple improvement potentials are identified, priorities need to be defined (8). Here, integrated optimization routines are beneficial to support the decision (9). The implementation of meas-

ures and control of its achievement (10, 11) either determines the analysis or initializes a new improvement circle (1).

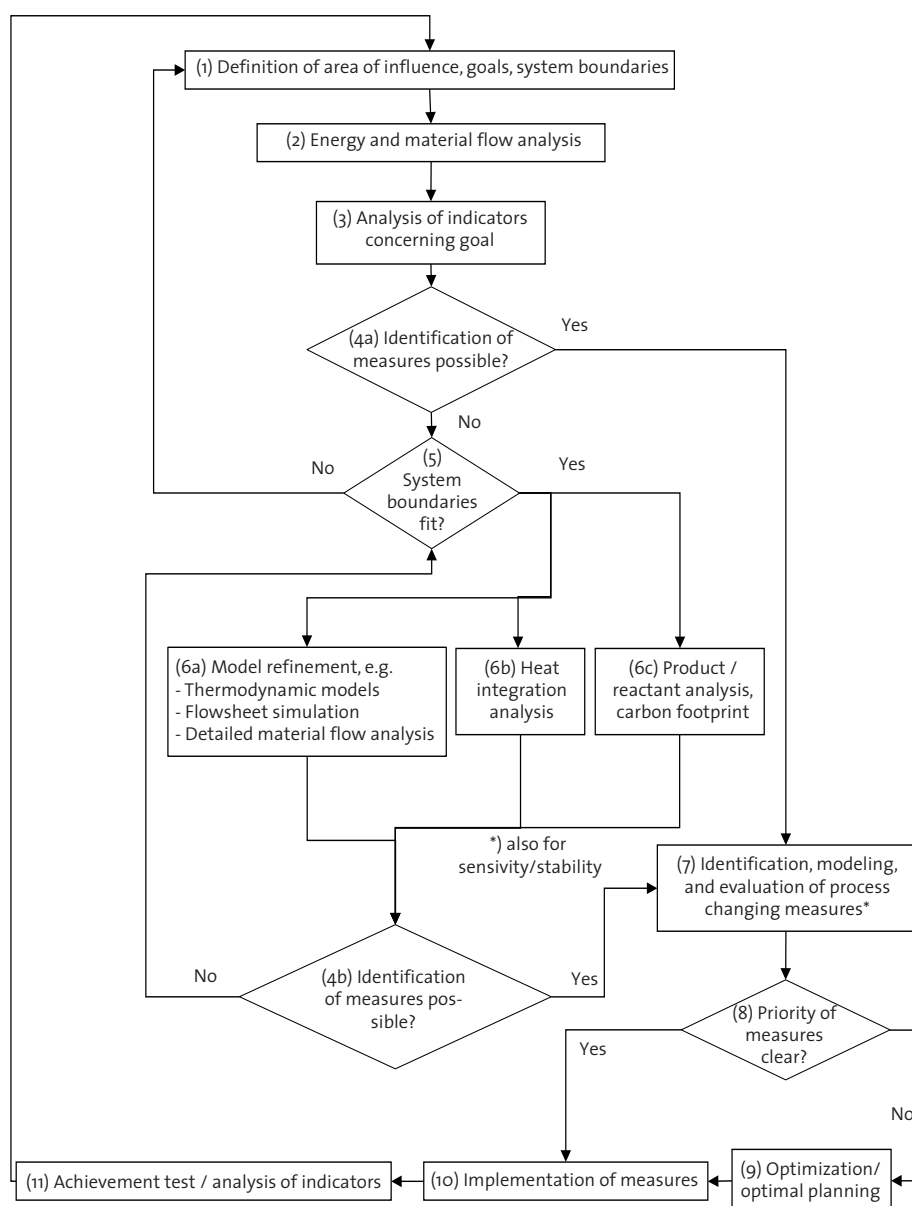
Material and energy flow analysis is a key component of the ideal-typical model and serves as the backbone for any process evaluation and optimization. Material and energy flow analysis accounts for material and energy inputs and outputs of processes, production units, chemical plants or even whole production networks and their interrelationships. This can be achieved by empirical input/output data (measurements and data records for batches or time periods) and provides a basis for several follow-up resource efficiency methods and their integration:

- *Environmental life cycle assessment methods*, in particular product and corporate carbon footprints (see ISO 14040, 2006; PAS 2050, 2011; GHG Protocol, 2011) to enable the inclusion of environmental impacts and objectives within and beyond company borders into resource efficiency decision making. For initial assessments, standardized life cycle inventory databases such asecoinvent (Ecoinvent, 2013) provide average datasets for purchased materials, auxiliaries and energy supply. Chemical engineers can use life cycle assessment methods to compute the whole life cycle impacts of product specification modifications or alternative process technologies. Thereby, environmental and resource efficiency aspects become part of product and process design decisions.
- *Computer Aided Process Engineering (CAPE)*, including flow sheet simulation, is a common working environment in process development and engineering (Beßling *et al.*, 1997; Braunschweig & Gani, 2002). Thermodynamic calculations result in consistent mass and energy balances which allow for proceeding steps like unit operation and equipment design, cost estimations or set-up of the process measuring and control strategy. One important point for the integration of CAPE tools is an easy to handle and generally accepted interface for data transfer to other resource efficiency applications. Furthermore, CAPE supports the integration of explanatory models into resource efficiency analysis, i.e. the definition of causalities and assessment of thermodynamic consequences of planned resource efficiency measures.
- Methods of *heat integration* for optimizing the interplay of heat sources and heat sinks in a production system. Data on warm and cold flows are collected and added to composite curves.

These curves can be analyzed regarding the potential of internal heat integration and the requirement for external heat supply. One well-known method for heat integration is the pinch point method (cp. e.g. Linnhoff & Hindmarch, 1983). Heat generation and cooling processes require large amounts of energy. Energy efficiency increases by means of heat integration reduce climate impacts and fossil fuel demands of chemical industries.

- Material flow cost accounting (MFCA) according to ISO 14051 (2011) makes use of material and energy flow analysis and aims at increasing resource efficiency by analyzing the particular cost of material loss and resource inefficiencies respectively. Chemical industry waste streams bear purchasing costs of lost material, processing and energy costs up to the point of loss and arguably even depreciation costs for used equipment and facilities. MFCA computes these lost values and hence provides figures on the potential gain that can be achieved by fur-

Figure 2 Ideal-typical model of integrated resource efficiency analysis (starting at top).



ther reducing waste streams and material losses.

- *Resource-efficiency oriented allocation methods* to treat multi-output processes adequately. By-products and multi-product processes are very common in chemical industries. Allocation methods have huge impacts on the results of ecological and economic product assessments and might lead to “subsidizations” of resource inefficient products and by-products if material and energy demands are not considered properly. Hence, resource efficiency analysis requires a thorough evaluation of existing allocation methods accompanied by new approaches such as game theory based allocation (Hougaard, 2009).
- The before mentioned methods are applied to derive ideas and measures for resource efficiency improvements. These options have to be evaluated within the given methods and against pre-defined indicators. Finally, *simulation-based optimization of material flow networks* can be applied to find optimal parameter settings for resource efficient production and products. Implementation and control of derived measures conclude the resource efficiency analysis and provide the starting point for continuous resource efficiency improvement at the same time.

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3 IT-based Framework

Software and IT support is an essential part of any type of analysis within this large array of relevant methods and tools related to resource efficiency, while its heterogeneity implies that an ‘one fits all’ software solution is neither feasible nor efficient. Hence, a clever combination and integration of formerly isolated software tools and methods is more promising. The overarching objective of the InReff project is the development of an IT-supported modeling and evaluation framework in order to receive decision-supporting information for increasing resource efficiency in a holistic but feasible manner.

The framework facilitates resource efficiency analysis as described in the previous chapter and provides the foundation for mapping the actual material, energy and cost flows, checking optimization potentials and giving a visual overview on the

effect of potential measures. The development of this framework includes selection of a suitable device, design of easy to handle interfaces for linking the relevant methods and tools, identification and integration of the required functionality for modeling, evaluation and optimization as well as specification of the navigation structure for user guidance.

At current stage, the framework interlinks software solutions for thermodynamic flow sheet simulation, software solutions for material and energy flow analysis including environmental and cost assessment, and algorithms for optimization.

3.1 Flow Sheet Simulation And Material Flow Network Interface

Material flow networks (MFN) and flow sheet simulation (FSS) are two complementary modeling techniques that serve different purposes in resource efficiency-directed analyses. As indicated in the workflow in Figure 2, MFN as the more abstract modeling technique is well-suited for the coarse-grained modeling of larger-scale processes up to the size of whole facilities. In contrast, FSS allow for physically valid modeling with regard to several substance properties and thermodynamic relations, typically stored in large accompanying substance databases.

An integration of MFN and FSS seems beneficial for several reasons: Firstly, an initial MFN can be set up with comparatively little effort in an early modeling phase; compensating missing data with broad estimations and simplistic (e.g. linear) relations to describe material and energy flow. This model can later be refined by replacing certain elements (i.e. transitions in the MFN) with data obtained from detailed FSS. Secondly, a MFN can serve as a link between different FSS sub-models. Due to the detailed modeling level, the simulation of large flow sheets is often computationally expensive and not guaranteed to converge. This situation might be improved by mapping only the most relevant processes to FSS and establishing linear input-/output-relations between these processes in an intermediary MFN. Thirdly, material flow analysis (MFA) tools like Umberto (cp. ifu Hamburg GmbH, 2014) allow to apply economic and ecological performance indicators to the calculated flows and to display the results using Sankey diagrams (Möller *et al.*, 2001; for Sankey diagrams cp. Schmidt, 2008; the relevance of MFN for efficiency increase in complex chemical production networks is discussed in Viere *et al.*, 2010). An integration of MFN and FSS enables the use of these analysis techniques on result data obtained from FSS as well.

As part of the IT-based framework, a prototyp-

ical interface between two exemplary tools for MFA (Umberto) and FSS (CHEMCAD, cp. Chemstations 2014) has been developed. The joint calculation is controlled by Umberto in a so-called master/slave fashion: A transition in the MFN can encapsulate a CHEMCAD model and initiate its simulation by calling CHEMCAD's COM (Component Object Mode, see e.g. Box, 1998) interface with the scripting language Python (cp. Python, 2014). Data between MFN and FSS is exchanged via a pragmatic spreadsheet-based interface, currently built upon Microsoft Excel. The use of spreadsheets enables a transparent and traceable data exchange between both process models. Furthermore, it allows for straightforward data conversion (e.g. from flow rates calculated by the FSS to larger time periods balanced in the MFN) and for predefined template spreadsheets that support users with the coupling of MFN and FSS models.

Prototypes with different degrees of automa-

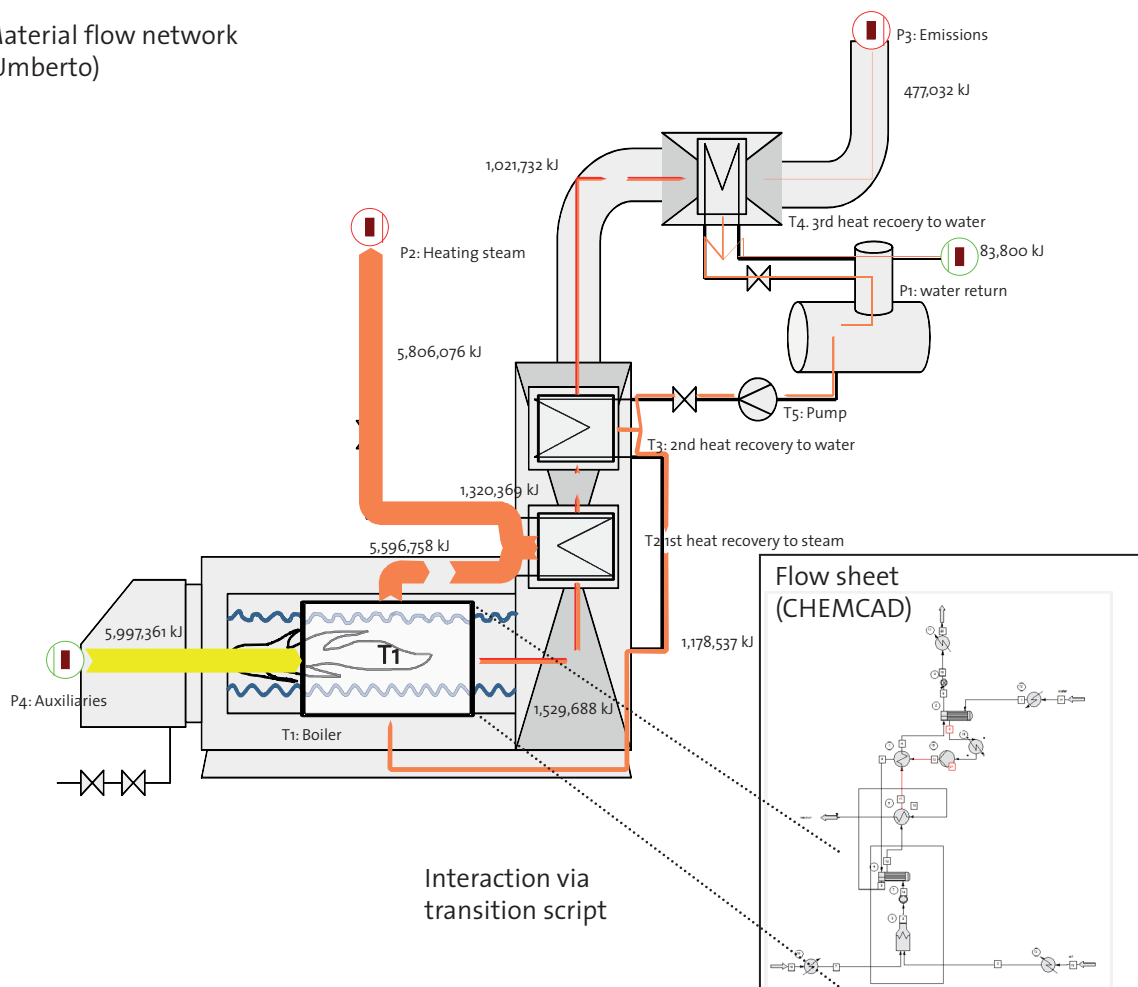
tion concerning data exchange and simulation control have been implemented at example models based on real processes from the InReff partners Sachtleben Chemie GmbH and H.C. Starck GmbH. Figure 3 depicts a first model of a steam generator where the transition T1 in the MFN is refined by a flow sheet in CHEMCAD (for a detailed elaboration of the prototypical interfaces cp. Denz *et al.*, 2014).

3.2 Simulation-Based Material Flow Network Optimization

Simulation-based optimization is an optimization approach for simulation models (Fu *et al.*, 2005). A simulation model is a model of a real system in which model variables are varied to analyze the system (Shannon, 1975). Model variables utilized for optimization are called decision variables. Simulation-based material flow network optimization aims at finding values of the decision variables

Figure 3 Integrated modeling with MFN and FSS at the example of steam generation (adopted from Denz *et al.*, 2014, Fig 4).

Material flow network
(Umberto)



that minimize or maximize the objective of the objective function of the optimization problem. The objective might be the minimization of the production costs or CO₂ emissions per product unit or the maximization of the benefit per product unit. Decision variables are defined within the material flow network and they have a strong impact on the objective of the optimization. Decision variables can be either technical or chemical parameters such as yield, temperature, and pipe diameter or material and energy flows.

To support simulation-based optimization within MFN and in combination with FSS, an interface prototype has been developed that steers the optimization process. The prototype applies optimization algorithms to MFN and the underlying FSS (for a detailed description cp. Zschieschang *et al.* 2014). At current stage it uses a commercial solver (OptQuest, see Laguna, 2011), that provides multiple search algorithms suitable for simulation-based optimization. Search algorithms explore the solution space for the optimal set of decision variables. The prototype will be enhanced to include further search algorithms and to identify best possible algorithms in terms of accuracy and computational effort depending on specific optimization problems.

4 Industrial Case Studies

To constantly evaluate the practical relevance of conceptual developments and prototypes, case studies are being conducted throughout the project. These case studies comprise the analysis of barium sulfate production at Sachtleben Chemie GmbH (Duisburg, Germany), tungsten manufacturing from scraps at H.C. Starck GmbH (Goslar, Germany), and aqueous alkyd resin production at Worlée-Chemie GmbH (Lauenburg, Germany). In the following, the case study design and first case study results are presented.

4.1 Barium Sulfate Production

Sachtleben Chemie with its production sites in Germany and Finland develops and produces white pigments and functional additives for customers in a wide range of sectors all over the world. For more than 130 years, Sachtleben has been one of the leading manufacturers of high-quality white pigments and excels with its expertise and quality.

One of these functional additives is barium sulfate whose production line in Duisburg (Germany) is to be analyzed in terms of resource efficiency. During the production, caulk stone is deoxidized in rotary kilns to barium sulfide and afterwards

precipitated with sodium sulfate to high-purity barium sulfate. This barium sulfate is dried, milled and packed in the post-treatment.

Initial analysis has identified several resource efficiency potentials that are currently under detailed investigation. These include energy saving potentials, e.g. by exhaust gas recirculation, substitution and variation of raw materials (petrol coke vs. natural gas), e.g. by process optimization, and an optimized and material flow based cost allocation rule for the production network using simulation-based optimization and the FSS-MFN interface (see 3.1 and 3.2).

The InReff case study at Sachtleben Chemie GmbH in Duisburg has so far revealed several improvement potentials at various points within barium sulfate production. These include for instance process engineering measures like optimizing fuel usage by heat integration at the day ring dryer. It also comprises business measures, such as an optimized cost allocation for multiple incurred in a process step and end-products. This improved cost allocation builds on the material flow models developed within the InReff project.

4.2 Tungsten Manufacturing

H.C. Starck GmbH is a world-wide operating company with over 2800 employees. At its major production site in Goslar (Germany), the company is established as an operator for production processes of hard-metal powder.

A batch production line is considered as the benchmark process. It includes the smelting of feed materials (ores, power or length metal scraps), followed by roasting and dissolving as well as purification process steps. Additionally, extraction and crystallization steps are necessary to separate the value components. Different products can be generated subsequently by operating beneficiation processes like calcinations, reduction and carburizing.

Characteristics of the production line are deviating feed material qualities combined with resource scarcity, high process temperatures and spatial separation of the different process stages at production site. Therefore, large potentials for improvement, especially in regard to resource and energy consumption, are expected. For this reason a systematic identification and quantification of potentials combined with climate protection measures is needed. Expected results of this resource efficiency measure are decreasing carbon dioxide emissions and energy consumptions per unit of intermediate products.

For the InReff project, a top-down approach has been used to gather all available material and ener-

gy flows of the process. Initially, no consistent mass and energy balances for the different process stages were available. In a first step, data gaps had to be filled by using databases, measurement data, and assumptions. Based on the derived consistent material flow model of the tungsten line (including energy demand and material losses) first saving potentials have been identified. For the most relevant process stages detailed models have been generated with tools like ChemCAD and Excel.

For the smelting step, mass and energy balances of the ovens have been compiled in Excel. Based on the results high energy demands and losses were identified. Operation at the particular site requires recycling streams that are mechanically processed and then retreated in the furnace process. Through better process control and adjustment of process parameters, a complete avoidance of such inefficient recycling streams appears to be feasible. At present, various thermochemical modeling studies are carried out to improve process control. Furthermore, so-called empty trips are analyzed in detail. During such empty trips, caking and unreacted material need to be treated without any production of valuable intermediates. H.C. Starck is currently optimizing its oven to further reduce or even fully avoid empty trips. Expected benefits are energy savings, simplified process design and possibly even capacity increase.

4.3 Aqueous Alkyd Resin

Worlée-Chemie GmbH is a medium-sized manufacturer of high-value additives, binders, and resins for the production of colors and varnishes (Worlée, 2013). The major production site of the long-established company is located at Lauenburg, close to Hamburg. During the last decade, Worlée has been engaged in several environmental protection activities including a commitment to and several awards achieved in the *Responsible Care* initiative of the German Federation of the Chemical Industry (VCI, 2014). Furthermore, Worlée is member of 'Climate Protection Enterprises' (Klimaschutz-Unternehmen e.V.), an association of German companies committed to voluntarily achieve measurable and ambitious targets in respect to climate-protection and energy efficiency.

Several measures have already been taken to improve the company's production line in the past; including heat insulation and recovery, use of renewable energies and primary products, coupling of thermal oil supplies, and flue gas cleaning by means of thermal post-incineration. For process analysis, pinch methods as well as material and energy flow analysis and visualization have already been applied using a proprietary software tool.

Thus, the main research question pursued in the case study is: If and how the workflow and tools of integrated resource efficiency analysis enable further improvements in a setting where several measures have already been implemented and relevant methods are already known. The modeling focuses on a production line for Aqueous Alkyd Resin in the first place. A material flow model of the main process and auxiliary processes like the thermal post-incineration has been set up and is currently refined with respect to process specification and data collection. This model will be the basis for further analysis steps that will include the application of LCA methods, material flow cost accounting (MFCA), alternative allocation methods, and optimization with the aid of algebraic reformulation of the MFN. Due to the early modeling stage, results for this study are not available yet.

5 Conclusion and Outlook

This paper has presented the conceptual approach as well as first results of research on Integrated Resource Efficiency Analysis for Reducing Climate Impacts in the Chemical Industry (InReff). Within the project, an ideal-typical model for resource efficiency analysis as well as prototype features for an IT-based modeling and evaluation framework have been developed, including the integration of material flow networks and flow sheet simulation as well as simulation-based optimization of both, ecological and economic performance targets. Next necessary steps comprise the feasibility and practicability enhancements of these prototypes and integration of further requirements, heat integration in particular. Industrial case studies at three different companies have been introduced and are used for evaluation and enhancement of the IT-based framework and prototypes.

Furthermore, the case studies as well as several workshops within the project including non-project participants from chemical industries and academia, foster knowledge transfer. In near future, project results and developments will be discussed with and disseminated to various actors in chemical industries including small and medium-sized enterprises (SME). As part of such knowledge transfer, a training concept on integrated resource efficiency thinking is to be developed and expected to meet requirements of multinational chemical companies and SME alike. This requires a flexible approach to software application allowing large enterprises to integrate their in-house solutions while enabling small companies to execute a resource efficiency analysis within reasonable time and effort by using less sophisticated software solutions.

Current results and conceptual developments support the authors' expectations that an integrated resource efficiency analysis is feasible and beneficial for chemical industries. Further work is required to substantiate this impression, to provide further case study evidence and practical guidance to chemical industries, and to initialize continuous resource efficiency analysis in chemical companies of all sizes.

6 Acknowledgements

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