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Supporting resource efficiency in chemical industries - IT-based integration of flow sheet simulation and material flow analysis

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Abstract

Substantial resource efficiency increase in material-intensive chemical industries requires an integrated analysis and optimization of complex production systems including raw material and energy use, resulting costs and environmental and climate impacts. This necessitates the integration of computer-aided process engineering methods including flowsheet simulation and heat integration with IT-based tools for industrial ecology, life cycle analysis in particular. The paper presents preliminary results of conceptual and case study-based research within the InReff project with particular emphasis on linking flow sheet simulation software used in process engineering and material flow network software applied in industrial ecology.

Keywords: process engineering; flow sheet simulation; material flow analysis; chemical process engineering; software development; Umberto; CHEMCAD

1. Introduction

The research project InReff (Integrated Resource Efficiency Analysis for Reducing Climate Impacts in the Chemical Industry) aims at providing a set of techniques and tools to support the analysis of resource efficiency in the chemical industry from ecological as well as economic perspectives. Focus is put on a reasonable integration of existing techniques and tools such that their practical benefit and applicability is improved especially for (but not limited to) small and medium sized enterprises (SMEs).

Continuous increase of resource efficiency, i.e. the minimization of natural resource input per unit of production output, will only be achieved if resource efficiency aspects are available on all levels of decision making with chemical industries. An initial analysis and first deduction of resource efficiency improvements for production and product systems can be based on average material and energy inputs and outputs of the respective system in a given time period. However, this black box approach is not sufficient anymore if resource efficiency measures require the adaptation of process parameters and programs, the inclusion of material loops and recycling, or the often non-linear interaction of various processes. In such cases, resource efficiency analyses need to dig down to the level of thermodynamic and physical causalities on the process design level.

For this purpose, a basic workflow for resource efficiency analysis in chemical engineering was proposed in an early project phase. As shown in Fig. 1, this workflow comprises at least four stages, where increasingly complex analysis techniques are applied to gain more insight into a process and possible means to improve its resource efficiency: (1) analysis of basic material and energy flows based on a coarse-grained material flow analysis (MFA) of the target system; (2) calculation of ecological impact and economic performance indicators based on results from step 1; (3) model refinement using methods from chemical engineering including flow sheet simulation and heat integration analysis; (4) application

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of algebraic or simulation-based optimization, e.g. to prioritize action alternatives. When conducting resource efficiency analysis in practice, these stages can be conducted subsequently, i.e. starting with simple models and proceeding to more complex stages only when the previous analysis could not provide sufficient information to identify appropriate action. .

Within this workflow, material flow networks (MFN) and flow sheet simulation (FSS) represent two important, complementary modeling techniques, each exhibiting characteristic strengths and weaknesses. MFA especially suits coarse-grained modeling of larger-scale processes and time periods with a focus on an economic and ecological analysis of the used materials and energy. FSS concentrates on detailed physical modeling of (typically smaller-scale) chemical processes in equilibrium state and takes into account thermo-dynamic models.

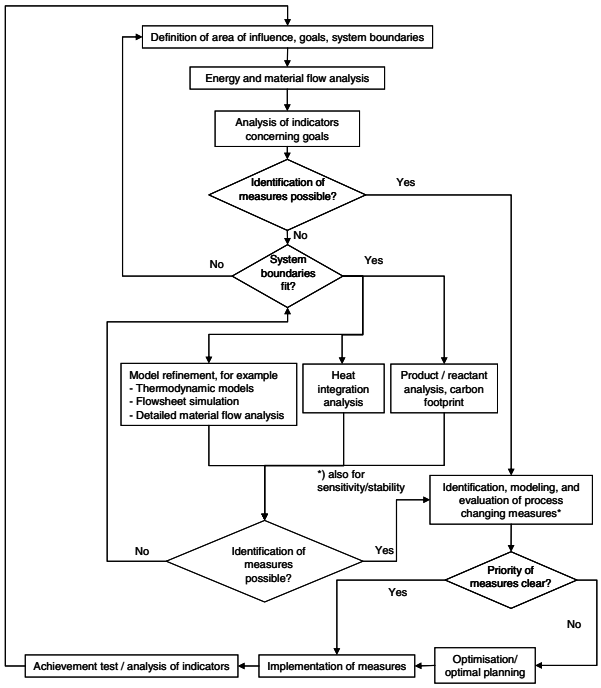

Fig. 1. Workflow for resource efficiency-directed analysis in chemical industries.

Due to this dichotomy, an application of both modeling techniques within the same study (or even model) might provide additional insight into the system under analysis. In doing so, a tight integration of both (sub-)models is desirable in order to avoid inconsistencies and redundancy of shared quantities and model elements.

This paper presents a concept and prototypical implementation for an interface between MFNs and FSS within the workflow depicted in Fig. 1. Following a brief review of both modeling techniques in the following section, requirements for an integration interface are discussed in Section 3. Section 4 explains the architecture of the prototype and substantiates the relevant architectural and technical design decisions. Section 5 exemplifies the outcome for a coupled material flow and flow sheet simulation model of a steam generator. Section 6 concludes the paper and provides an outlook on follow-up research activities.

2. Flow Sheet Simulators and Material Flow Networks

Material flow networks [1] and flow sheet simulation [2] are two techniques to model processes (not only) in chemical engineering that exhibit some commonalities but also several relevant differences. The main modeling concept underlying both techniques is a graph-based decomposition of the target system into connected model elements.

2.1. Flow Sheet Simulation

Flow sheet simulators like CHEMCAD [3], which was chosen for this study due to its widespread use in practice, provide a large number of predefined *unit operations* like pumps, flashes, or heat exchangers to model (parts of) a chemical facility. The unit processes are interlinked by connections and substances are fed into the network via feed streams.

FSSs typically include a large database of relevant substance properties and thermo-dynamic models to facilitate the calculation of further properties not explicitly specified in the model, such as pressure or enthalpy. Since numerous substance properties and thermo-dynamic relations must be considered, the calculation of complex FSSs does not necessarily converge, which makes the approach less suitable to model larger processes or whole facilities.

2.2. Material Flow Networks

Compared to flow sheet simulation, material flow networks, as described in [1], are a more abstract modeling technique based on the formalism of Petri nets (see e.g. [4]). Accordingly, a MFN is a bi-partite graph consisting of *transitions* as active nodes (e.g. unit operations), *places* as passive nodes (e.g. tanks), and *connections* to indicate paths of material and energy flow.

MFNs do not exhibit the event-based execution semantics of conventional Petri nets. Instead, the material and energy flow in the overall network is calculated from local *transition specifications* (i.e. which amounts of materials and energy are consumed and produced by a transition) in terms of linear coefficients, algebraic functions, or even program scripts. Material flow modeling with MFNs is supported by the software tool *Umberto* [4], which is also applied in this study.

Thus, the main differences between MFNs and FSS can be summarized as follows:

- The specification of processes in MFNs is often (though not necessarily) less detailed than in FSS; e.g. describing material flow in terms of linear coefficients.
- Due to this simplicity, convergence of calculations of large MFNs is not as much an issue as for FSS (though it is not guaranteed either).
- The focus of analysis in MFNs is not as much on technical properties of chemical processes as on ecological impact

assessment and cost accounting on the basis of calculated material and energy flows.
- The results of FSS are momentary *flow rates* calculated for the *optimal design state* of the modeled process. In contrast, MFA considers *material and energy balances* over longer periods of time (e.g. per month), possibly taking into account operational states like failures as well.

2.3. Benefits of Integrating MFNs and FSS

Integrated modeling with MFNs and FSS might provide several advantages for resource efficiency analysis in chemical engineering: Firstly, a coarse-grained model of a larger process (even a whole facility) can be set up as a MFN at the outset of a study. Sub-processes that require further investigation are then refined into detailed FSSs (see Fig. 1). Secondly, existing FSSs of different sub-processes can be coupled by representing the intermediate process stages in a simple linear MFN to improve the convergence of an overall calculation. The MFN calculation can also take into account non-productive operation states when transforming the flow rates from the FSS to the balanced period. Thirdly, material and energy flows calculated by the FSS can be further analyzed by means of cost accounting and impact assessment procedures stored in MFA tools like Umberto.

3. Integrated Platform Requirements

To integrate a MFN-based modelling tool like Umberto with a FSS like CHEMCAD, it is necessary to exchange flow data during the calculation of both models. This data exchange could, in principle, be performed manually by an experimenter. However, a higher degree of automation is inevitable in practice due to the large amounts of exchanged data and the possibly complex interaction of the overall model's calculation.

In the context of the analysis workflow shown in Fig. 1, the following requirements for a platform to integrate MFA and FSS can be identified:
- The platform should provide an interface to exchange flow- and material property-related data between FSS and MFN.
- The platform should automatically synchronize the calculations of the flow sheet simulator and the MFA tool.
- The interface should perform conversions between flow rates calculated in the FSS and time periods calculated in the MFA; also taking into account non-optimal operation states.
- The interface should provide a re-usable structure to describe data typically exchanged between FSS and MFN.
- The exchanged quantities should be transparently documented to ensure traceability of the performed studies.
- Conceptually, the interface should not be limited to specific tools or models. Under practical considerations (i.e. existing software used by the participants of the *InReff* project) a solution based on Microsoft Windows is desirable. User-defined extensions, such as specific conversions between exchanged quantities, should be possible.
- The integration platform should enable (or at least not forbid) a combination with further analysis techniques like heat integration analysis or simulation-based optimization in the future.

4. Architecture and Implementation

To design and implement an integration platform, two important design decisions must be made. On one hand, an overall architecture has to be devised to meet the requirements stated above. On the other hand, a technical foundation for data exchange between the involved software tools must be identified. In the following, the available options for both tasks are presented and the resulting decisions are substantiated. On this basis, the principle design of the interface is presented without going into implementation details.

4.1. Architectural Options

One manifest option to couple different analysis tools within an engineering study is an *external integration platform* as described in the context of *scientific workflow* (SWF) management (see e.g. [6]). Different from business process modeling, scientific workflow modeling puts larger focus on the representation of data flow, integration of heterogeneous tools, and (often) distributed execution of complex calculations [7]. Though these focal points are in good accordance with the requirements of the *InReff* project, the effort of implementing such a general concept appears rather large: A SWF platform must be adopted or implemented, the involved software tools must be interfaced with this platform, and a choreography for an overall calculation must be set up.

The second option identified takes advantage of the specific structure that the coupled MFN and FSS models exhibit. As stated above, The MFN typically serves as the *main model* (e.g. representing a chemical facility) into which one or more FSSs are embedded as detailed sub-models. Therefore, the overall model can be calculated in a *master / slave* fashion where the MFN calculation requests data from the FSS when needed. The FSS models are thus represented by transitions in the MFN that, during their calculation, (1) pass input data to the FSS; (2) initiate the calculation of the flow sheet simulator while waiting for its termination synchronously; (3) read output data from the FSS back into the MFN.

Pondering these arguments, a coupling of MFNs and FSSs can, to the impression of the authors, be achieved with the *master / slave* approach more straightforwardly. Nevertheless, the integration of further analysis techniques like optimization and heat integration analysis might motivate the additional use of an external integration platform in the future.

4.2. Implementation of Data Exchange

Having chosen the *master / slave* approach as an architectural basis, the second design decision regards the technical implementation of data exchange between the material flow analysis software and the flow sheet simulator on the Microsoft Windows platform. For this purpose, three different

options were considered. These are displayed and rated with respect to four relevant requirements in Fig. 2.

Microsoft COM (Component Object Model, see e.g. [8]) is a general interface standard for the communication of heterogeneous software components and applications on the Microsoft Windows platform. Therefore, a domain-specific structure for process engineering would be implemented in a specialized interface layer. Ensuring traceability of the exchanged data requires custom implementations as well. COM is supported by many software applications (not only) in the engineering domain, including the tools applied in this study. Existing COM interfaces of software applications can be used straightforwardly via scripting languages like Visual Basic (see e.g. [9]) or Python (see e.g. [10]). However, extending a COM-based interface towards further, user-defined data exchange requires in-depth programming knowledge.

CAPE-OPEN [11], in contrast, is an interface standard specifically tailored towards the needs of computer aided process engineering (CAPE). Therefore, the domain-specific structure and understandability of the provided interfaces is higher compared to COM. However, the coverage of the CAPE-OPEN standard in existing software tools is still rather low which hinders its practical applicability.

The third (and finally chosen) option for data exchange between MFNs and FSSs is a rather pragmatic approach driven by the needs of the industrial partners in the *InReff* project. The good connectivity of software tools in the engineering domain to *spreadsheet* applications like Microsoft Excel [12] suggests to choose a spreadsheet-based approach for data exchange.

	Microsoft COM	CAPE-OPEN	Microsoft Excel
Domain-specific structure	low	high	low
Support by existing tools	high	low	high
Understandability of data exchange	low	medium	high
Extensibility	difficult for end users	difficult	simple for end users

Fig. 2. Ratings of three options to implement data exchange between MFNs and FSSs with respect to four relevant criteria.

While this technique appears simplistic at first sight, it offers several advantages in practice: (1) Both software tools used offer mature interfaces to write (read) calculation-related data to (from) cells in Excel, either via user-defined scripts in Umberto or so-called data maps in CHEMCAD. (2) Exchanged data is clearly and traceably represented in one or more spreadsheets; (3) To the experience of the authors, process engineers often possess deep knowledge of spreadsheet-based modeling. This enables them to customize the sheets used for data exchange. (4) In addition, predefined spreadsheets can serve as templates to conceptually structure the predefined data and perform common conversions. (5) Due to the scripting support provided by Excel itself, a synchronization of the MFN and FSS calculations can also be achieved via this channel.

4.3. Structure of the Prototype

Fig. 3 shows the structure of the prototype that integrates the software tools Umberto and CHEMCAD via Excel. Though the implementation is clearly tailored towards the specific toolset, the concept appears generic enough to work with other software as well, especially taking into account the good Excel connectivity of many tools in the engineering domain.

As described above, transitions in an Umberto model can be refined by a FSS modeled in CHEMCAD. During the calculation, these transitions write relevant data to specific spreadsheet cells using simple Python scripts and start the flow sheet simulation via a predefined Visual Basic script provided with CHEMCAD.

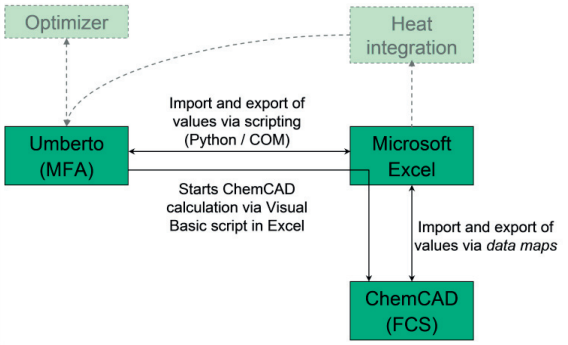

Fig. 3. Structure of the prototype to couple the MFA tool Umberto with the flow sheet simulator CHEMCAD via Microsoft Excel. Dashed elements indicate possible future extensions not implemented yet

The flow sheet simulator reads this data and returns selected results of the calculation to further spreadsheet cells. When control flow returns to Umberto, the respective transition reads the results and propagates them to the ongoing calculation in Umberto. The conversions between flow rates (calculated in CHEMCAD) and periods used in Umberto can on one hand be achieved with the aid of formulas implemented in Excel. On the other hand, a largely generic net template called time capsule has been implemented in Umberto in order to perform these conversions for the flows produced and consumed by an embedded subnet.

A technical challenge is posed by the need to synchronize the calculations in Umberto and CHEMCAD. In the first prototype used for the example described in Section 5, both calculations had to be initiated by the user in an appropriate order.

A further prototype, developed with the InReff-partner Sachtleben Chemie GmbH included an automated invocation of the COM-based API (Application Programming Interface) provided by CHEMCAD from a transition script in Umberto. For this prototype, new instances of MATLAB and Excel had

to be created in every simulation run. This proceeding largely increases computation times, especially in contexts like simulation-based optimization, where several simulations of the same model with different parameter settings are required. In consequence, the recent prototype starts a single instance of Excel and CHEMCAD beforehand, to which multiple simulation requests can be dispatched during calculation in the style of a service.

The dashed boxes and arrows in Fig. 3 indicate possible future extensions of the prototype towards an additional coupling with tools for optimization and heat integration analysis. A prototype for simulation-based optimization of Umberto models has been implemented as part of the research project KOMSA [13] and recently extended for use in the current project (see also [14]). This tool communicates with Umberto via COM directly. Therefore, parameters from the FSS, that should be subject to optimization, must be 'proxied' in Umberto and passed to the flow sheet simulator during calculation. This use of the MFN as a central place to manage parameters of the coupled model also seems plausible with respect to the process model shown in Fig. 1.

5. Case Example: Steam Generator

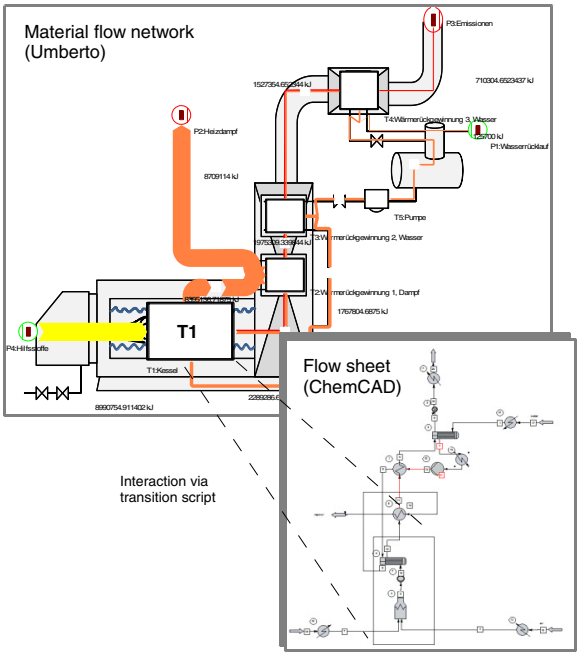

Fig. 4. Coupled model of a steam generator: The overall model is represented as a material flow network in Umberto. Enthalpy flows are shown in the Sankey diagram. Only the transition representing the boiler (T1) is refined by a flow sheet simulation in CHEMCAD.

For exemplification purposes, the first application of the integration platform has been the model of a steam generator inspired by actual processes running at a facility of one project partner (H.C. Starck GmbH). Three variants of this example were implemented to show the different coupling possibilities:

(a) overall steam generator modelled as MFN employing user defined functions to represent thermo-dynamic relations;

(b) overall steam generator modelled as flow sheet in CHEMCAD using Umberto only to display results in a Sankey diagram ;

(c) central process (boiler) modelled in CHEMCAD and overall network including peripheral processes (heat exchangers) represented in Umberto.

Variant (c), which seems to outline the most common application scenario for the integration platform, is depicted in Fig. 4 and briefly explained in the following.

In the example, the required amount of generated steam is predefined as a manual flow in the MFN, i.e. the overall calculation proceeds in backward direction (see Section 2.2). When the MFN calculation gets to transition T1, a user defined transition script is run that performs the following steps to exchange data with the embedded FSS of the boiler:

1. The predefined mass of steam is written to a cell in the Excel sheet that serves for communication and monitoring.
2. Based on previous FSS data Excel calculates upper and lower iteration bounds for the amount of natural gas expected to generate the required steam. These bounds are necessary to control the input-streams in CHEMCAD according to the amount of required steam as output steam.
3. To generate adjusted data the flow sheet simulation has to be executed manually in this prototype. As mentioned above, more recent prototypes allow starting CHEMCAD by calling its COM API via predefined Excel routines. The MFN calculation then synchronously waits while control flow is passed to CHEMCAD.
4. CHEMCAD reads the input amount and the iteration bounds into the simulation using a custom Excel data map.
5. The CHEMCAD simulation is iterated over the given bounds until a stable state is reached and the results meet the measured boundary conditions like temperature of exhaust gas.
6. CHEMCAD writes the resulting mass and enthalpy streams including temperatures and specific heat capacities for further calculations in the MFA to cells in the Excel sheet. The required conversions (see Section 3) between FSS and MFA are performed by Excel.
7. To load the appropriate/recalculated data into the MFA the calculation of the network has to be executed again including data import and export. In our recent prototype, the CHEMCAD simulation would simply terminate and pass control flow back to Umberto.

Further developments of the data exchange interface have enhanced its usability regarding automation of the execution of CHEMCAD during calculation and reducing the time required for multiple calculations within the same network (see Section 4.3).

6. Conclusion and Outlook

This paper proposes a concept and a prototypical implementation of a platform to integrate MFN and FSS for improved resource efficiency analysis in chemical process

engineering. The modeling techniques of MFN and FSS complement each other well: MFN enable coarse-grained modeling with a focus on economic and ecological analysis. FSS supports the detailed, thermo-dynamically valid representation of the most relevant sub-processes in the system.

To efficiently apply this integrated approach in practice, a tight coupling of MFN and FSS is required. A pragmatic master/slave architecture has been applied based on transition refinement and data exchange via spreadsheets. The approach was prototypically implemented using the software tools Umberto, CHEMCAD, and Microsoft Excel and successfully applied to the example of a simple steam generator.

To improve the practical utility of the presented prototype, several extensions will be required in the future, including the design of re-usable template spreadsheets to pre-structure data exchanged between FSS and MFA for typical model classes, and improved error-handling in MFN calculation to better cope with convergence failures and other issues in sub-ordinate FSS.

Applying integrated MFN and FSS modeling to larger industrial case studies is an important direction for future work that has already been taken by the project's industrial partners at Sachtleben Chemie GmbH. In this context, the project partners will also investigate methodological differences between MFA and FSS (such as flow rate- vs. period-based analysis) in larger detail.

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