Application of the Simultaneous Modular Approach in the Field of Material Flow Analysis (MFA)

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Abstract
Life cycle assessment (LCA) and material flow analysis (MFA) are two important modelling instruments in the field of industrial ecology. Different scientific communities develop and refine the underlying concepts and instruments. However, it has been already shown that it is possible to combine MFA and LCA. LCA as well as MFA-based cost accountings become evaluation methods of material flow models. On the input side of this models it is possible to enhance them so that a simulation-based modelling framework can be implemented for the analysis of material and energy flows and stocks of production sites, supply chains, eco-industrial parks, regions etc. A specific MFA instrument has to answer two different questions: (1) what kind of data or information should be provided? In this perspective, the MFA instrument is an accounting system. (2) The second question is how to establish the material flow models (modelling and calculation). In particular, the aspect of modelling is discussed in this contribution. The paper makes clear that core algorithms to material flow analysis can be adopted from process flowsheeting approach in chemical engineering, especially the sequential modular approach and the simultaneous modular approach.

1. Introduction
Life cycle assessment (LCA) has generated considerable interests as an approach that promises to cover several challenges in the field of sustainable development. By definition, life cycle assessment is an efficiency analysis (Guinée et al. 2002, Heijungs, Suh 2002, Möller 2000): LCA analyses the relationship between positive outcomes (functional units or reference flows respectively) and global environmental impacts. Users are understandably interested in instruments that perform these assessments, especially if they instruments provide single numbers – like product carbon footprinting does. Today, LCA is the most important instrument to analyse the industrial metabolism. However, LCA does not estimate all relevant attributes of those systems, for instance the role and time dependency of stocks. Several challenges of sustainable development stay in strong relationship with stocks: scarcity of raw materials, products in the use phase, and concentration of carbon dioxide in the atmosphere. In such a stock-centred perspective approaches of dynamic material flow analysis and continuous simulation come into consideration.

Somehow in between are modelling approaches, which do not explicitly include stocks as building blocks of models (like system dynamics does) but which can deal with nonlinear processes in connection with loops. The purpose of these instruments is to estimate steady states of material and energy flow systems. In sequential process chains without recycles this is no problem, but the approaches can deal with recycles in combination with nonlinear processes involved.

In this contribution, the basic ideas behind the loop-centred modelling approaches are discussed. The main purpose is to apply them in period-oriented material flow analysis. Such an instrument is not an alternative to life cycle assessment. It can be treated rather as a data provider for design- and future-oriented life cycle assessments, carbon footprinting and (life cycle) costing. This requires a systematic distinction between appropriate data structures and methods, which allow calculating the data sets. Appropriate data structures result in an accounting system, which not only serves as a data provider for evaluations steps like LCA but also close the gaps between LCA, steady-state MFA and dynamic MFA.

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So, MFA can be regarded in two different perspectives. The first is the accounting perspective, the second the modelling perspective. In the accounting perspective, we can treat material flow analysis as an accounting process. The result data sets, material flow analysis should provide, are categorized. We distinguish flows, transformations, and maybe stocks. The characterization of material flow networks as an accounting instrument in the field of period-oriented material flow analysis is already discussed (e.g. Moeller, Rolf 1995, Wohlgemuth et al. 1997, Moeller 2000, Moeller et al. 2001) so that the focus can be directed on the modelling perspective.

2. Material Flow Networks as a Modelling Framework

In the following, the question is discussed how we can fill the accounting system, mentioned above, with data. In this perspective, the accounting system becomes a modelling framework, which integrates several sub-models (modules, unit processes, unit operations...). Integration approaches are required, and in this regard, material flow analyses may apply approaches in chemical engineering: Process flowsheeting.

Flowsheeting is one of the most important modelling instruments in chemical engineering. The purpose of flowsheeting is “to perform steady-state heat and mass balancing, sizing and cost calculations for a chemical process” (Westerberg et al. 1979: 1). Even if steady state flowsheeting sounds like another accounting concept, main focus is on modelling and calculation. The calculation presupposes given unit models for each unit process and a flowsheet, which represents the flows between the unit processes. The unit models in chemical engineering are complex formal models. In general, the unit models exhibit a nonlinear behaviour and the evaluation requires a lot of computing time, for instance the determination of the chemical equilibrium of chemical reactors.

The calculation routines of computer-based flowsheeting tools use the unit models and given “feed streams” (input flows of the chemical process) to estimate the steady state of the chemical process, represented by the unit models and the flowsheet. Westerberg et al. (1979) mention three different approaches: the sequential modular approach, the simultaneous modular approach and equation-solving approaches.

The equation-solving approach assumes that the model is represented by a collection of nonlinear equations (Westerberg et al. 1979: 23, Westerberg, Piela 1994, Morton 2002). The unit models provide the model equations and the flowsheet the connecting equations. A solver is applied to calculate the results. The advantage of this approach is that the solution may include the estimation of parameters and design specifications: for given design specifications not only flows are calculated but as well the process parameters, under which the chemical process achieve the specifications. However, the equation-solving approach results in the challenge to solve a system of a huge number of nonlinear equations. Westerberg et al. estimate for chemical processes that “the number could become 50000 to 100000 or more” (1979: 161). Straightforward algorithms, which can deal with such systems of nonlinear equations, are not available. So, the solving routines include nested iterations and backtracking. This may result in a high time complexity and in particular a solution is not assured. Other authors argue that the equation-oriented approaches are not in line with images, modelling experts have in mind; they think the models step by step, so that a sequential modelling approach would ease model validation and the localisation of problems (Morton 2003: 321).

The modular approaches treat the unit models as black boxes or subroutines (Westerberg, Piela 1994: 3). Instead of providing the unit equations, the subroutines can be called to calculate unknown input and output flows for a set of given flows. The most important modular approach in practice is the sequential modular approach. Almost all flowsheeting tools implement the sequential modular approach as the basic calculation algorithm. Starting with given manual flows (feed streams), unit models of all processes are calculated step by step. In chemical engineering it is common that the feed stream are given on the input side of the process model. So, in the first step all unit models can be called, which require the feed streams as their input. The result of such a subroutine call is a set of new flows, in particular the output flows,
which can be used as the feed streams of other unit models. The method is successful, when all unit processes are calculated in a consistent manner.

Problems occur in case of recycle streams. Recycle streams play an important role in chemical engineering because the most important reference models in chemical engineering consist of the steps mixer, chemical reactor and separator (figure 1, Finlayson 2012: 120, Westerberg at al. 1979: 14). A separator is required in many chemical processes because in many chemical reactions the conversion from input to output is not 100 per cent. The mixture of inputs and outputs of a reactor is determined by the chemical reaction equilibrium (Finlayson 2012: 50). Recycling plays an important role in material flow analysis too, not because the output still contains raw materials, which we want to separate from the products and waste. Recycling is integral part of images and design patterns of material flow analysis (eco-industrial parks, “Verbund” production, Cradle-to-Cradle). It is necessary that modelling tools deal with recycling.

The problem is to determine steady states of the loops, which result in an overall consistency of the model. Therefore additional data is required to determine the process levels of the involved unit processes. In reference model mentioned above, the input of the mixer consists of the feed stream and the recycling stream. The output of the mixer can be calculated only, when both streams are known. In the sequential modular approach two techniques are combined to solve the problem: tearing of recycle streams and conversion methods. In a first step, we tear all loops so that loops do not longer occur in the system. Instead we can estimate the feed streams for the unit process, which use the tear streams as their data input. This estimation is called the first guess. Using this additional data input we can calculate the model. This results in new values for all tear stream (see figure 1). We are in steady state when there are no relevant differences between the guesses and the calculated values. We can stop the procedure.

Normally, that will be not the case. It is necessary to calculate the next “guess”. Here, the convergence methods come into play. The question is how to calculate the next estimation. The simplest method is direct substitution: we start the next iteration with directly with the calculated values. Another and very efficient method is the Wegstein method (Biegler 2000: 13). This method uses the results of the last two iterations. Wegstein’s method is the default algorithm in several flowsheeting tools. Other common procedures are Broydon’s method and Newton’s method (Barton 2000: 5, Broydon 1965, Finlayson 2012: 121). The difference between direct substitution and Wegstein on the one hand and Newton and Broydon on the other is that direct substitution and Wegstein do not recognize other loops (e.g. nested loops, inner and outer loops) to calculate the next estimation whereas Newton and Quasi-Newton convergence methods are based on the inverse of the Jacobian matrix.

Applying the sequential modular approach, we get a calculation procedure on two levels (2-tier Approach). The inner level addresses the calculation of input and output flows of unit processes. Because we can regard unit processes as black boxes in the modular approaches, it is possible to implement very different subroutines as unit process specifications: nonlinear equations between inputs and outputs, access to external data set like Excel, SAR ERP (common enterprise resource planning system in industry) or Aspen Plus, the utilization of scripting languages like Python etc.

The outer level of the calculation procedure tries to calculate step by step all unit processes, starting given manual flows or feed streams respectively. In case of loops tearing strategies and convergence methods are applied as outlined above.
Figure 1. Material flow network of a typical chemical process

Figure 1 shows an implementation of the sequential modular approach (using the prototype version of Umberto). To deal with the recycle streams one of the arrows is torn (between CP3 and the mixer). An initial guess (tear stream) must be specified, so that the mixer process can be calculated (step 1). As a result, the chemical reactor can be calculated (step 2). The last step (step 4) allows calculating the flow between the recycling process and the mixer. The system is in steady state, when this flow is the same as the initial guess. Otherwise, a next iteration is required with a new estimation. Convergence methods like Wegstein are applied to determine the new estimation. The stream table of the material flow between the recycling process and the mixer shows that in this example Wegstein’s method is applied and 4 iterations are required to determine the steady state of the chemical process.

Figure 2. Stream table for the material flow between the recycling process and the mixer

In the example manual tearing is applied. Several algorithms are developed to find out optimal tearing strategies for more complex flowsheets with several loops. In principle, these algorithms can be applied in the field of material flow analysis too. However, one important characteristic of (sequential) flowsheeting is “downstream thinking”. Calculations start with a given feed stream on the input side of the flowsheet. This is different to LCA. In LCA normally calculations start with products and services on the output side (“upstream thinking”). To allow both directions, material flow networks are not restricted to one calculation direction. It is possible that transitions can be evaluated if some output or input streams are given. Of-
ten, both directions are possible. The algorithms for automatic tearing (Gundersen, Hertzberg 1983) do not support this feature. They can be applied without enhancements only, if for a network a calculation direction is given.

3. Simultaneous Modular Approach as a Component in a Steady-State Material Flow Analysis Concept

The sequential modular approach with manual or automatic tearing is a straightforward enhancement of sequential approaches without tearing. They are easily to implement and they do not enforce the users to rethink their step-by-step modelling procedure. The equation-based approach as a simultaneous approach on the other hand requires for example an redesign for transition specifications in material flow networks because the specifications are not longer black-boxes: they have to provide nonlinear algebraic equations. Another problem of the sequential modular approach is the mix of upstream and downstream thinking in material flow networks. In combination with life cycle assessment and cost accounting calculations start with products and services (reference flows) and not with feed streams on the input side. This is a challenge for the sequential modular approach in combination with automatic tearing. Fortunately, an approach has been developed, which tries to combine the two different approaches: the simultaneous modular approach.

The simultaneous modular approach stands for a class of slightly different methods. One of these methods is the “All Stream Convergence” approach (Biegler 1983: 12, Chen, Stadtherr 1985: 1845). Here all data inputs of the unit models are torn streams and estimation about the flow levels. The unit models can be calculated (modular approach). These guesses allow calculating the unit models simultaneously. Moreover, we can vary the inputs to obtain derivatives (finite difference approximation). The approximation of the derivatives makes it possible to construct an approximation of the Jacobian matrix, which is necessary to apply Newton’s root finding algorithm (Newton or Broydon). In other words, we get again a 2-tier-approach with inner calculations (evaluation of transition specifications), but now with outer calculations based on Newton’s method (Biegler 1983: 13, Chen, Stadtherr 1985: 1847).

Two calculation steps of this approach are time-consuming: the approximation of the Jacobian matrix by calculating finite differences and the calculation of the inverse of the Jacobian matrix. Broydon’s method reduces this effort. In the field of material flow analysis, we are in a special situation because material flow analysis is linked to life cycle assessment. Several successful concepts in life cycle assessment can be applied in material flow analysis too, in particular the use of so-called databases. Databases like EcoInvent directly support life cycle assessment and therefor they have to provide linear specifications for all processes. This “linear thinking” has an important practical impact on the construction of material flow models: most of the process specifications are linear. Complex nonlinear process specifications, necessary e.g. to specify chemical reactors, are seldom. Often all processes are linear, e.g. if a pre-chain contains loops. In such a case, the approximation of the Jacobian matrix is very simple and requires no additional calculations. Another effect is that the resulting problem specification (see “formulation II” (Chen, Stadtherr 1985: 1848) and the “split-fraction concept” (Sinnott 2005: 172, Shacham et al. 1982: 82)) is very similar to the calculation of life cycle inventories (LCIs) based on material flow networks, so that we can enhance already exiting matrix methods (Heijungs, Suh 2002, Möller 2000) to implement the outer loop of the 2-tier-approach.

Figure 3 shows a simple example. Here, we start with the product output of transition “Delivery”. The sequential modular approach (without tearing) stops at connection place CP2, because the flows from the chemical reactor and to the recycling process are unknown.
The all stream convergence approach in connection with an assumption that all processes are linear allows using very simple first guesses. We calculate all processes simultaneously with non-zero guesses (e.g. between CP3 and the mixer 5000). In fact, in case of linear specifications a good initial guess is not required.

Figure 4 shows what can be expected: In case of linear specifications, the algorithm converges very well. This is a remarkable result, because the sequential modular approach (without tearing) cannot deal with this kind of loops. Software tools, which support life cycle assessment directly and apply matrix methods to calculate life cycle inventories (Heijungs, Suh 2002), seem to be more powerful because of the matrix method. This is not the case, as the example makes clear. In case of linear process specifications the calculation engines for material flow analysis are as powerful as the matrix methods in direct life cycle assessment. But they can deal with nonlinear specifications too.

The next example shows a small modification of linear specifications. This modification plays an important role in cost accounting and life cycle assessment. In particular, it is an approach to deal with attributional LCA and consequential LCA in a consistent manner. In the transition specifications, it is assumed that the flows consists of a fixed and a variable (linear) part. In cost accounting, we call these parts as fixed and variable costs. In other words, we use affine functions to specify the unit processes. The ma-
The stream table shows that several iterations are required to determine the steady state. This result is not surprising because the Jacobian matrix is still based on the assumption that the processes are linear. At least, very bad initial guesses result in stable behaviour. In the first step negative flows are calculated because the fixed part of the affine function is higher than the initial guess.

Already in case of affine function better approximations of the Jacobi matrix seem to be necessary. If we identify all specifications as linear or affine, we can simply use the variable parts of the affine functions as the derivatives, which constitute the Jacobian matrix. Again, the time consuming finite difference approximations, which require the calculation of all unit processes several times, can be avoided.

It is helpful to distinguish different transition specifications. This is already the case in Umberto. Umberto provides linear process specifications as well as so-called user-defined specifications. The user-defined specifications allow specifying nonlinear processes. It could be useful to introduce at least a new specification type to deal with affine functions. As mentioned above, affine functions play an important role to deal with fixed and variable parts of material flows and costs. In the following a list of useful specification types are presented:

1. Linear specifications as already implemented, maybe parameterized (the parameters allow adjusting the linear processes, they do not result in a nonlinear specification, so that parameters of nonlinear specifications are more powerful),
2. Affine specifications, which support fixed and variable parts. The user interface should look very similar to user interfaces and forms in the field of future-oriented cost accounting,
3. User-defined specifications as the most flexible specification type. This type requires the finite difference approximations.
4. Processes as “black-boxes”, which provide an interface to modelling tools like Microsoft Excel (Excel provides the calculation engine for the inner calculations but not equations and their derivatives) or an interface to external calculation engines (e.g. web services and mapping components of ERP systems). Note that only in case of 3 and 4 the time consuming finite difference approximation is required. The entries of the Jacobian matrix, which results from linear and affine specifications, can still be determined very easily.

From a calculation perspective, another specification type between 2 and 3 could reduce the calculation effort: a specification type, which uses are restricted set of functions to specify the nonlinear equations. Useful functions like an if-function or a pick-function are not allowed. The reason is that a restricted set of functions like sin, cos, sqr, sqrt etc. allows symbolic differentiation. We do not use the equations themselves as an input string of a expression interpreter to approximate the Jacobian matrix. Instead, we determine first the derivative functions (as strings) and use them. The jacobian matrix becomes a hybrid matrix.

4. Conclusions

The approaches to steady-state material flow analysis, discussed here, are already in use in chemical engineering. Process flowsheeting tools help to design complex chemical processes with several unit processes like mixer, chemical reactors and flash units. It is very common that recycle streams have be modelled, for instance between flash units and mixers. Tearing strategies and convergence methods together allow estimating the levels of processes and the resulting streams. The torn loops make it possible to apply sequential modular approaches. But it is necessary to converge the ends of the torn loops with aid of fixed-point iterations or root finding algorithms respectively.

The approaches can be applied as core algorithms of a calculation engine of steady-state material flow analysis too. This makes it possible to apply all scientific research in the field of chemical engineering in material flow analysis, for instance the different approaches, the sequential modular approach, the equation-based approach and the simultaneous modular approach. However, the purposes of the models are quite different, so that a direct application is not useful. In some cases, this is a challenge (automatic tearing) but often the situation is not as complex as in chemical engineering. Material flow analysis is normally applied on a higher level than approaches in the field of chemical engineering, for instance on the level of supply chains or eco-industrial parks. On this level, process optimization (based on process flowsheeting) is not in the focus, rather the effectiveness of the resulting material and energy flow network (the effective exchange of by-products, energy etc.). As a consequence, often linear or affine functions are used to specify the unit processes. This again has an influence on the selection of appropriate approaches. In particular, the simultaneous modular approach comes into play. In case of linear and affine functions, it is easy to determine the entries of the Jacobian matrix, which is required to apply Newton’s root finding algorithm.

However, all this is true only, if an overall steady state can be determined. On the level of chemical reactions and single chemical processes this can be assumed, on the level of eco-industrial parks not. But a combination with material flow networks as the underlying accounting system, it is possible to combine steady state material flow analysis with dynamic material flow analysis. Here, a place type comes into consideration: the storage place. This place type divides a material flow network into different parts. Such a partition of a material flow network allow identifying subnets, in which steady state flowsheeting can be applied, and the links between them. In dynamic material flow analysis these partitions can be treated as single processes. This reduces the complexity (it is a challenge in practice to deal with more then two or three stocks in dynamic material flow analysis, as practical experiences with system dynamics demonstrate). However, this requires further research: to combine steady state material flow analysis with dynamic material flow analysis in an efficient and effective way.
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