A Toolbox for Building up Process-based, Macro-economic Material Flow Models

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Abstract

Using the example of CarboMoG, the Carbon Flow Model of Germany, structures and processes for process-based, macro-economic material flow models were analyzed. The aim is to create a toolbox, which can be used to assemble models of this kind from building blocks, to parameterize and calculate a model, and then to use the model for analysis tasks. It was investigated whether and how toolkits existing in the fields of material flow analysis and life cycle assessment could also be used for process-based, macro-economic material flow models. Unfortunately, it was found that no product could be used without massive adaptations. Thus, the development of an own toolbox was initialized.

1. Introduction

The development of strategies for dealing with climate change requires knowledge of the effects of anthropogenic impacts on natural, biogeochemical processes. The interdependencies among production processes imply that the cause-effect relationships are often not easy to grasp. Consequently, explicit and complete modeling of the processes and their interrelationships on an appropriate level of abstraction is helpful. Karlsruhe Institute of Technology (KIT) developed CarboMoG (Carbon Flow Model of Germany), a material flow model of the German carbon system (Uihlein/Poganietz/Schebek 2006, Poganietz/Feifel/Schebek 2008, Schebek/Poganietz 2011). Within the system frame of Germany, the model system underlying CarboMoG describes the material and energy flows of the whole economy, including flows across the system boundaries (import, export, withdrawals from and inflows into lithosphere, assimilation from and emissions into the atmosphere), and their links on the process level. By adding additional components (satellite systems), specific aspects, such as carbon flows, can be modeled. The latter was essential for CarboMoG.

CarboMoG currently describes German economy with about 300 processes and with flows of more than 300 different products (including services and waste) as a snapshot of a given year (2005). In the future, the model also is planned to be used to analyze developments over time and interrelationships of interdependent regions (regionalization). However, this is rather difficult due to the current implementation of the model in Microsoft Excel (with over 100 interlinked Excel data sheets). Therefore, we started to develop a flexible and extensible toolbox to set up CarboMoG in a new IT frame and extend it according to the previously mentioned tasks. With the help of this toolbox, it will be possible to implement not only CarboMoG, but also other models with an appropriate structure.

This paper describes the concept of this toolbox. Upon the completion of work, both the newly established CarboMoG and the toolbox itself shall be provided in a form suitable for general use.

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2. Components of the Toolbox

Certain tasks must be supported by the toolbox, such as describing and building up a model, filling the model with appropriate data, and supporting the modeler in the processing of interesting scenarios and application fields. The main components “data acquisition and processing”, “data generation” and “analysis model” are chained, i.e. the components are based on the results of the predecessor.

![Diagram of the toolbox components](image)

2.1 Data Acquisition and Processing

The component "data acquisition and processing" allows to define the data structures for raw data (sector^3 data, process data) and modeling data as well as appropriate mapping rules between them. Fig. 2 illustrates the data flow for sector data. This kind of data typically comes from statistics or studies and often does not correspond in granularity and physical units to the needs of the model. The toolbox therefore allows to configure a mapping of the sector data to the modeling data by several intermediate steps, consisting of aggregation, disaggregation, and some predefined but parameterizable conversion methods. Specific values are typically provided as time series.

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^3 Three Examples of sectors: Mining, industry, agriculture & forestry
For process data, which are process-specific input/output coefficients, rules can be defined to calculate values for a reference year based on sector data and fixed initial values. To obtain values for subsequent calendar years, learning curves can be applied.

The component will manage references to the sources of the raw data and will deliver the derived modeling data for the modeling period considered to the next component, i.e. data generation.

### 2.2 Data Generation

The “data generation” component provides functions to build up the model. The aim of data generation is to generate a consistent/coherent data set for the component “analysis model”, since the sources of the data used in “data acquisition and processing” are manifold and the raw data are collected in different factual connections. Inconsistencies cannot be compensated in this first component.

The basic building blocks in data generation are processes, which connect inputs with outputs, and products that can be used as inputs and outputs. Regarding the inputs, it is distinguished between energy inputs, needed to produce energy for running the process, and material inputs, which are used as primary products in this process. Each process can produce zero, which rather is the exception, or one main product, but several co-products.

The concept of a product is very broad and does not only include physical goods, but also services, such as transportation. Waste is not modeled as a physical good, but as a special kind of service, a service for waste disposal. The reason is an adaptation to the LCA methodology and a simplification of the calculation method (see below).

The following explanations describe the core of the modeling method and of the toolbox to be developed, but they are simplified to some extent, so that they are not more complicated than necessary.

#### 2.2.1 Processes

To build a model, different kinds of building blocks for processes can be used, i.e. there are different types of processes:

1. Production process (default): A normal production process has one or more inputs, exactly one main product (a physical good), and it may have one or more co-products. In principle, the modeler has to decide which of the products will be the main product. The volume of the main product determines the volumes of the inputs (demand-driven). The production volumes of co-products are driven by supply, i.e. the production volumes of co-products directly depend on the inputs. This basic logic can be flexibly parameterized and adapted by the modeler. The modeler will have to define formulas to connect the inputs with the outputs and eventually with stocks (e.g. acreage) and aggregated values.
2. Recycling process: In contrast to the production process, the amount of input determines the quantity of the main product (supply-driven).

3. Service or disposal process: Unlike the production process, the main products are no physical goods, but general services (e.g. transportation of persons) or specific services for waste disposal.

4. Consumption process: A consumption process determines the primary demand for certain products, e.g. for consumption goods like milk. These processes do not generate output, their inputs being the consumed product and normally waste disposal services.

5. Extraction process: This special case of a normal production process models the extraction of mineral, fossil, and metal resources.

6. Sector or difference process: If individual processes in certain sectors of the economy cannot or are not to be modeled completely or partly, the inputs can be described and put into the model in an aggregated form. Difference processes (subtype of sector process) are generated automatically as a difference between aggregated input values for a sector, given exogenously, and the input values of all modeled individual processes of this sector.

A concrete model is built up from a set of processes that are expressed as instances of different process types. One or more consumption processes are indispensable as a starting point for the calculations described below.

### 2.2.2 Linking of Processes

Macro-economic material flow models do not describe specific processes at site level. Instead, abstract average processes, i.e. the economy-wide produced, transported, and consumed volumes, are in the focus. Outputs and inputs of different processes are linked only indirectly on a higher balance layer. This layer ensures that the input of a certain product, summarized over all processes, is equal to the summarized output of the same product taking into account import, export, and recycling. In this way, material flows are modeled not as physical flows\(^4\), but as summarized, balanced flows. Fig. 4 shows the relationships in more detail.

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\(^4\) In the sense of paths of individual goods being tracked exactly.
Figure 4
Linking of processes using the example of a product $P_i$
(solid line: Demand for $P_i$; dashed line: Additional supply; dotted line: Demand-driven production)

In the sum over all processes, the inputs of product $P_i$ determine the total demand for $P_i$ within the system boundaries (in CarboMoG = Germany). The primary production that is directly required to meet the demand has to be calculated. The primary production equals the total demand, reduced by supply-driven produced quantities (main product in a recycling process or co-product). Export (additional demand) and import (additional supply) are other correction factors. The primary production of $P_i$ determines the production volume of the main product for the processes that produce the product $P_i$. If there is more than one such process, distribution coefficients have to be specified.

For waste, i.e. more accurately for waste disposal services, there is a similar procedure to describe and sum up the generation of waste and waste disposal across all processes.

2.2.3 Operating Procedures

The calculation process is based on the static model description of the processes, the product-related linking of processes, and the process-internal formulas connecting inputs with outputs. The time frame is a calendar year, i.e. total amounts for the reference year considered are required. Via a link to the component "data acquisition and processing", the model is supplied with initial values. In particular, these are the coefficients for process-internal linking of inputs and outputs, imports and exports for the reference year as well as the final demands for products (consumption) as total amounts. The filling of the model ("data generation") is an iterative process, as there may be loops in the model. The results of the calculation are consistent input and output quantities for all inter-related processes that are required to satisfy the final demands. In principle, the values are calculated in a demand-driven manner, as already described. Starting from the final demands, the inputs required for production will be calculated. They lead to intermediate demands and initiate a new cycle. Known production volumes for certain processes or aggregated structures, e.g. subsectors, can be used as fixed settings or for validation.
2.3 Analysis Model

As a result of the data generation, a consistent snapshot of the product-related production processes and material flows for a calendar year is obtained within the system frame under consideration. This already is a relevant result, but also the basis for the scientific analysis of the modeler. Questions of interest can be answered by modifications of the model and the observation of the resulting changes to the inputs and outputs of processes. The range of possible modifications reaches from simple parameter changes (such as changes of initial values, e.g. the primary demand) to more complex procedures, such as adding new, competing processes. Depending on the depth of modification by the modeler, two different approaches will be made available. Massive modifications of the model suggest to run the data generation again, a relatively time-consuming process. For simpler problems, the so-called "analysis model" is derived from the results of the data generation, a version of the model, where, in a first approximation, inputs are mapped directly to outputs. For this, certain properties of the model are fixed, e.g. the ratio of export / import and domestic production.

In the analysis model, the input volumes are calculated from the output volume for demand-driven outputs. For supply-driven outputs, the opposite is true. The direct input-output relationships are coupled by demand (product-specific sum of primary and intermediate demand caused by inputs) and supply (demand minus supply-driven outputs). Due to the coupling of the input-output relations, an iterative calculation method is also necessary to solve analytical problems. Decoupling of the input-output relations, i.e. including the upstream processes in the equations, by mathematical methods (matrix inversion) seems to be impossible from the current point of view because of special characteristics of the model type considered, e.g. the coefficient matrix is not quadratic.

3. Investigation of Implementation Alternatives

The model type used in process-based, macro-economic material flow analysis (pmMFA for short) is a special case of models in material flow analysis (MFA) (Brunner / Rechberger, 2004) and resembles models used in life cycle assessment (LCA) (Klöpffer / Krahl, 2009) in many aspects. Therefore, it is reasonable to investigate whether existing LCA or MFA tools can be used directly or with certain extensions for pmMFA, and especially for rebuilding CarboMoG. Three tools were put on the shortlist, namely, STAN (IWA 2012), a software for material flow analysis, Umberto (IFU Hamburg 2012), a commercial product for LCA, and OpenLCA (GreenDeltaTC 2012), an open source LCA software. For all three tools, not only the system properties and modeling capabilities were analyzed, but we also tried to implement parts of the CarboMoG model as a test. For openLCA, which proved to be the most promising candidate, a study was carried out together with the developing company GreenDeltaTC GmbH, to explore the potentials of the tool in greater detail.

The analysis of the MFA and LCA methodologies in general and the existing tools in particular revealed the following equalities and similarities to process-based, macro-economic material flow models:

- “Process” is a central concept of a model.
- Different processes are linked by their inputs and outputs (external interlinking) to process chains.
- The internal process logic, i.e. the process-internal linking of inputs and outputs, describes the manufacturing process. A crucial point is the functionality and flexibility of the linking options. The available tools are relatively limited in this respect.
- Quantitative data can be given in various physical quantities and units. Conversions are possible.
- The calculation method should be based on the primary demand (demand-driven) in principle. Only OpenLCA meets this restriction completely.
- One of the outputs can be distinguished as the main product. Only OpenLCA meets this restriction (quantitative reference).
- It can be distinguished between goods and waste.
- Imports and exports can be integrated into the model (for the tools considered, this is only partly possible).
- Models may include loops.

However, there are also major differences, such as:
- In pmMFA the product is in the foreground, as it will be balanced product-specifically within the system boundaries. Products as independent entities are difficult to model or cannot be modeled at all with the examined tools. Instead, the flows, i.e. the direct connections between the processes via inputs and outputs, are central elements of the models. These flows do not exist in pmMFA.
- Linking processes via a separate balance layer cannot be modeled with these tools.
- Stocks as a parameter for process-internal logic are not provided.
- No distinction can be made between different types of processes. In particular, no process without a main product (e.g. consumption) can be defined.
- No distinction can be made between material and energy inputs.
- No distinction can be defined between physical products and services.
- Aggregated processes (difference processes) are not provided.
- A sector-oriented hierarchization is missing (sector, sub-sector).

Unfortunately, it was found that for different reasons all tools were inapplicable or applicable with an unreasonably high expenditure only. For OpenLCA, as an open system, chances had been best. However, major modifications of the core functionality are necessary. They would not be compatible with the main line of development of the product. Taking into account the effort required, it was decided to implement the toolbox for process-based, macro-economic material flow models directly with a Java framework.

The toolbox will be based on the Eclipse's RCP (Rich Client Platform)\(^5\) which allows the development of any application using the dynamic plug-in model of Eclipse. For each component of the toolbox (see section 2), a separate plug-in will be available with common access to a relational database system (e.g. MySQL from Oracle Inc.) via the JPA (Java Persistence API) implementation Hibernate. The plug-ins will provide a comfortable user interface to manage the product and process data using Eclipse’s Standard Widget Toolkit (SWT) and JFace libraries.

4. Status and Outlook

The analysis of the model structures and the design of an IT-model are completed, with the exception of certain aspects of analysis models. Currently, the implementation of the component "data acquisition and processing" is in progress. As a next step, practical testing of the data acquisition and processing component and further implementation of the other components are planned. They are aimed at replacing the current CarboMoG implementation in Excel.

In the longer term, methodological extensions of the toolbox in different directions will follow, such as a balance level for carbon flows, a supplementary component for emissions, dynamic aspects (time series, trends over several calendar years), coupling of models (e.g. flows between regional models), and coupling with geographic information systems.

Bibliography