Systems analysis of stock buffering: development of a dynamic substance flow-stock model for the identification and estimation of future resource, waste streams and emissions

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Chapter 2 Substance Flow Analysis – Background and Modelling Aspects

2.1 Introduction

Modelling is a powerful tool for describing, analysing, operating and evaluating complex systems. It provides an efficient means of communication within the scientific community and between it and policy makers. By definition, models are a simplification of reality and have been defined as ‘a description of the essential aspects of a system, which represent knowledge of that system in a usable form’ (Sinha and Kuszta, 1983). This reflects that models do not include everything, and that this simplification of reality makes models useful (Braat and Lierop, 1987 and Meadows, 2001).

This chapter provides information on modelling in general and substance flow analysis (SFA) models in particular. The following section provides general information on aspects of modelling, section 3 provides information on the SFA framework, section 4 provides a general background on modelling in SFA, which is at the core of this thesis, and section 5 provides general information on computer modelling and software tools used for physical models.

2.2 Model types and modelling aspects

2.2.1 Model types

Quantitative modelling techniques can be classified according to the purpose they are designed to fulfil. Braat and Lierop (1987) identify four different types:

- descriptive models that are used for to give a general overview of a given problem;
- explanatory models that are based on observation and used to clarify the system;
- predictive models that are used to forecast changes, which include prescriptive, control or management models, that are used for optimization, and;
- evaluative models that are used to assess alternatives.

Descriptive and explanatory models can be an end in themselves or a starting point for developing predictive models, which can either be simulation or prescriptive (optimization) models. Parameter estimates from descriptive models can be used for making predictions (Baron et al., 1990).

Predictive models can be further classified as (Meadows et al., 1974):

- absolute, precise prediction that give exact information about what will happen in the future such as those that predicting natural phenomena;
- conditional, precise prediction that give exact information about what will happen if something else has happened as those for example in process control;
- conditional, imprecise projections of dynamic behaviour that give information about changes in a system if something happens such as those of system dynamic models;
- summary and communication of current trends, relationships or constraints that may influence the future behaviour of a system, and;
- a purely philosophical exploration of the logical consequences of a set of assumptions.

The model developed in this thesis is a predictive model. In SFA, as in other economic and social systems, it is not possible to make precise predictions (in either the absolute or conditional sense) due to uncertainties in the system. In SFA these uncertainties are associated with the estimates of model variables and parameters, which are mainly related to the limited availability and reliability of data and problems of aggregation in the model. Therefore the dynamic SFA model developed in this thesis are time dependent models that can be classified as conditional and imprecise projections of a dynamic behaviour mode.

2.2.2 Temporal and spatial

Time and space are important aspects in modelling. In terms of time, models can be static or dynamic, continuous or discrete, deterministic or stochastic. Static systems have a direct and instantaneous link between their variables. Dynamic systems are those in which the variables change without outside influence and their value relies on earlier signals (Ljung and Glad, 1994). Continuous time models are mathematical models that describe the relation between time-continuous signals. They use differential equations to describe these relationships. Discrete time models describe the relation between sampled signals and use difference equations to describe thise relation. Deterministic models work with exact relations (i.e. without uncertainty). Stochastic models are those models that also work with concepts of uncertainty or probability (Ljung and Glad, 1994). In spatial terms models can be global, or cover a specific geographical region. The choice should be based on the nature of the problem at hand: as some problems are local or regional in nature and others are global.

2.2.3 Aggregation

The level of aggregation in model design is an important factor in determining the outcome. It may be important in several aspects of the model, such as scale (macro, meso, and micro levels) and time period (second, minute, hour, etc.). Aggregation can also be an issue in terms of the environmental issues at stake (Kandelaars, 1998).

2.3 Substance flow analysis

Substance flow analysis (SFA) has been described as a tool to investigate the metabolism of a single substance or group of substances (Udo de Haes, 2000). The current SFA framework was established by Udo de Haes et al. (1997) and contains three elements:

1- Goal and systems definition, in which the system's flows and stocks should be defined and system boundaries (in terms of space and time) established according to the aim of the study,
2- System flows and stocks quantification, in which the system should be quantified through either accounting or modelling,
3- Interpretation of the results, in which the overview of the system flows and stocks is transformed into policy relevant information.

SFA is based on the principle of materials balance, which enables different types of analysis. Substance flow accounts can be used to identify major flows and accumulations and to spot trends. Static models can be used to identify the causes of pollution problems and to assess the effectiveness of contra-measures (Baccini and Bader, 1996 and van der Voet, 1996a). Dynamic models allow the exploration of future flows and stocks (resources, emissions and wastes) (Bergback and Lohm, 1997) and provide a relevant input for strategic environmental policy planning.

In SFA, the system is treated as a physical entity: a coherent set of elements that determine the flows of a certain substance or group of substances. Generally, the SFA system represents a geographically demarcated area: a country, region, group of countries, or even the whole world. In most cases, the SFA system is divided in two subsystems, the economic and the environmental. The economic subsystem is also called the 'societal subsystem', 'technosphere' or 'anthroposphere' – indicating that the system is not concerned with financial aspects. The environmental subsystem is also referred to as the biosphere.

The outcomes of SFA models can be transferred into policy relevant information. SFA is a useful tool for identifying potentially problematic substances at an early stage, for example in identifying the causes of pollution problems, assessing the necessity of action, the effectiveness of contra-measures and forecasting future developments. In this way it can provide an early warning of future problems.
SFA case studies have been carried out at a wide range of spatial levels: the international (Voet et al., 1994, Lanzano et al., 2006, Spatari, et al., 2003), national (Antikainen, et al., 2004, Tasaki, et al., 2004), and local and company levels (Burström, 1999, Lindqvist and Malmborg, 2004, Timmermans and Van Holderbeke, 2004, Van Holderbeke and Timmermans, 2002, Nilsson, 1995). SFA has proven to be particularly useful in spotting unintended flows: the occurrence of the substance as a trace contaminant in materials derived from fossil fuels, phosphate rock etc. (Guinée et al., 1999).

SFA can also be used as a basis for subsequent analysis. Environmental fate modelling is considered as a specific form of SFA. These models, which focus on environmental flows, are based on the physical and chemical properties of substances and environmental characteristics (Van der Voet et al., 2000). These models can be used as a starting point for risk analysis.

2.4 Modelling flows and stocks in SFA

The second element of the SFA framework, the one to which this thesis will mainly contribute, involves the description of the relations between flows and stocks in the economic subsystem. As discussed above, there are several aspects to such modelling. This section focuses on two main types: static and dynamic.

Static SFA models describe system flows and stocks, and present them as dependent on one another, through a set of linear equations that can be solved for a specific year by assuming a stationary state, i.e. one in which the flows do not change over time. The system is described in terms of nodes, sources and sinks. Flows can be fixed, determined by model relations, or provided by balancing equations. Static models, require a limited number of fixed flows and the outcome relies mainly on the distribution pattern implying that data are required on the production and environmental processes and the way substance flows are redirected by them (Van der Voet, 1996a). Although static models are more limited than dynamic models, they do have several advantages. They require far less data and the outcome is more robust, due to the exclusion of many uncertainties. Several static SFA models have been developed and applied to various substance groups, including heavy metals (Van der Voet, et al., 1994, Van der Voet, 2000), nutrients (nitrogen and phosphorous) (Schrøder, 1995, Van der Voet et al., 1996b, Van der Voet et al., 1996c, Nilsson, 1995, Antikainen, et al., 2004), and chlorine (Kleijn et al., 1993, Kleijn et al., 1997, Tukker et al., 1997).

Dynamic SFA models take into account changes in system flows and stocks over time. The dynamic models used in this thesis are time dependent models. It has recently been recognized that one of the main difference between static and dynamic SFA models is that the latter include stocks in society. By including the dynamic behaviour of the system, it is possible to explore future flows of emissions and wastes, based on past and future inflows and stock characteristics (Kleijn et al., 2000). Taking stocks into consideration is now recognized as important, and a number of specific substance stock databases or models have been developed (Baccini, et al., 1996, Boelens & Olsthoorn, 1998; Kleijn et al., 1998, Zeltner, et al., 1999, Kleijn, et al., 2000, Binder, 2001, Voet, et al., 2002, Ayres, et al., 2003, Elshkaki, et al., 2004, Müller, et al., 2004, Elshkaki et al., 2005, Spatari,et al., 2005, Elshkaki and Van der Voet, 2006, Binder et al., 2006).
The dynamics of stocks, which determine their change over time, and future flows of waste and emissions, depend on many variables. Among these are socio-economic aspects such as technological development and developments in population size, welfare, and markets. In addition to this the characteristics of substances and materials, such as degradability and volatility, also play a role: these determine emissions during use, corrosion, life span, recycling potential etc..

The future emission and waste flows from society to the environment can be described through two different forms:

1- The leaching model, in which the concentration of the substance is the driving force (e.g. the leaching of copper from water pipes through corrosion). In this case the outflow is described as a fraction of the stock.
2- The delay model, in which the age is the driving force (e.g. the generation of waste containing copper from discarded products). In this case the outflow is described as a delayed inflow.

Two approaches can be used to model the stock that is in use, the inflow of substances into the stock and the outflow of substances from the stock.
The first approach starts from historical data on the inflow into the stock and the product lifetime to estimate the past and future outflow from the stock and the stock-in-use (Baccini, et al., 1996, Zeltner, et al., 1999, Kleijn, et al., 2000, Van der Voet, et al., 2002, Ayres, et al., 2003, Elshkaki, et al., 2004, Elshkaki et al., 2005, Spatari, et al., 2005, Elshkaki and Van der Voet, 2006, Binder et al., 2006). For the future, the inflow into the stock-in-use is either assumed (Kleijn, et al., 2000) or estimated based on socio-economic variables using different techniques, such as intensity of use and regression analysis (Elshkaki et al., 2004).
The second approach starts from historical data on the stock-in-use and the product lifetime to estimate the past and future outflow and the future inflow (Binder, 2001, Elshkaki, et al., 2004, Müller, et al., 2004). The future stock is related to the service provided by the product and estimated based on socio-economic variables (Elshkaki et al., 2004, Müller, et al., 2004).

2.5 Software tools

A crucial aim of modelling the dynamic behaviour of systems is to improve understanding of the system elements and actors and how these affect the system's behaviour, thus enabling better forecasts.

In the mathematical and statistical world, several techniques are available for analysing dynamic systems. A few of these have been used in the field of Substance Flow Analysis (Kleijn et al. 2000). Software tools are an important aid in the successful implementation of such mathematical and statistical modelling techniques. These software tools can play an important role in SFA models. They facilitate the organising and analysing of data, deal with uncertainty, and are useful in modelling, and calculating (standardised) performance indicators. Moreover, they provide the possibility for scenario analysis, graphical presentation of the systems and the possibility of linking to other types of models.

A number of models have been developed and dedicated to substances and products analysis tools - SFA, MFA and LCA (Boelens & Olsthoorn, 1998). These software models can run on a PC under the ms-dos or Microsoft Windows platforms. These vary in their purposes and structures and include (to mention just a few): SFINX (Van der Voet, 1996a), SIMBOX (Baccini and Bader, 1996), ORWARE (Dalemo et al., 1997), FLUX (Olsthoorn and Boelens, 1998 and Boelens and Olsthoorn, 1998), DYNFLOW (Elshkaki, 2000), GaBi (IKP and PE Europe GMBH, 2006) and UMBERTO (IFU, 2006).

To date the existing SFA software tools have focused on the static, linear or non-linear, types of modelling. Dynamic modelling has mostly been neglected or inadequately included. Yet there are many well-known systems dynamic modelling software packages, including SIMULINK, STELLA, POWERSIM, and VENSIM. These can enhance the modelling and the simulation of complex dynamic systems.

Some of these software packages have been used to model ecological and economic systems such as STELLA, and VENSIM (Costanza and Gottlieb, 1998 and Ford, 1999) and others such as MATLAB and its extension SIMULINK, have been used to model environmental and technical systems (Eriksson et al., 2002 and Kumblad et al., 2003).

The software model used in this thesis uses MATLAB and SIMULINK as a starting point. They were chosen for several reasons. SIMULINK is an advanced extension of MATLAB software that assists in modelling, simulating, and analysing complex dynamic systems. It supports linear and non-linear systems, modelled in continuous time, sampled time or a hybrid of the two. SIMULINK provides features such as block libraries, hierarchical modelling, signal labelling, and subsystem masking, which makes it a powerful dynamic systems simulation tool. Its block library consists of over one hundred blocks. These are grouped into libraries according to how they function in the system. These blocks are the basic elements from which SIMULINK models are built. The user can model virtually any dynamic system by creating and interconnecting blocks in appropriate ways. SIMULINK provides a graphical user interface for building models as block diagrams, using click and drag mouse operations. With this interface, users can draw the model as they would with pencil and paper. The visual block diagram interface offers a simple method for constructing, modifying and maintaining complex system models. The user can also create custom blocks in two programming languages, C^{++} and FORTRAN, and add them to the SIMULINK block library. SIMULINK provides a convenient feature for customizing subsystem blocks, called masking. It gives a high degree of flexibility for customizing the SIMULINK modelling environment, as well as the behaviour and user interface of any block.
Although SIMULINK requires programmers to provide additional model structures that can be automatically created in other software, this gives them more control over specific aspects in the modelling process. For example, if a parameter needs to be estimated by using a value that should be lagged in time, circular dependencies appears in other dynamic software packages (Rizzo et al., in press).

A new software tool, called DYNFLOW, which is based on MATLAB and its extension SIMULINK has recently been developed by Elshkaki (2000). DYNFLOW is dynamic system software for substance flow analysis. It combines a dynamic modelling core with a user friendly interface and possibilities for graphical presentation. DYNFLOW uses the features of SIMULINK to not only model dynamic SFA models but also to structure and model static SFA cases (Elshkaki, 2000).

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