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 3 Dynamic Substance Flow-Stock Model

3.1 Introduction

Within the community of systems analysis, there are many interpretations of what a system is. In general, the term 'system' can be defined as a group of interacting, interrelated or interdependent elements forming a complex entity. Each element has specific properties that enable the system to function. A system can be a physical or social entity, or an abstract idea, and can be either open or closed.

In Substance Flow Analysis, the system is a physical entity, which is divided in two subsystems, the economic and the environmental. Sometimes, it is not clear where exactly to draw the border between the two. A landfill is situated in the environment but is still under human control. However, the choice of treating a landfill as part of the environment or of the economy will not make any difference in modelling terms or to the outcome of the SFA model. This is in contrast to, for example, LCA where the boundary between the technical subsystem and the environment has to be drawn as one of the system boundaries (Guinée et al., 1993), as it determines what to call "emissions". It is generally accepted that the emissions from landfill sites should be included in the inventory and therefore that the landfill sites should be included in the economic subsystem (Heijungs et al, 1992 & Finnveden et al, 1995). Likewise, agricultural soil may be treated as an environmental component or as part of the economic subsystem, due to the fact that it is also used as a mean of production.

The economic and the environmental subsystems are shown in figure 1. The economic subsystem includes several processes (extraction, production, consumption and waste management processes) and several flows and stocks. Economic stocks are contained in the production and consumption phases, landfill sites, and agricultural soil. The environmental subsystem includes several processes (leaching, evaporation and deposition), and also contains several flows and stocks. Environmental stocks are those in the non-agricultural soil and natural resource stock. The environmental components in the model are air, water and non-agricultural soil.

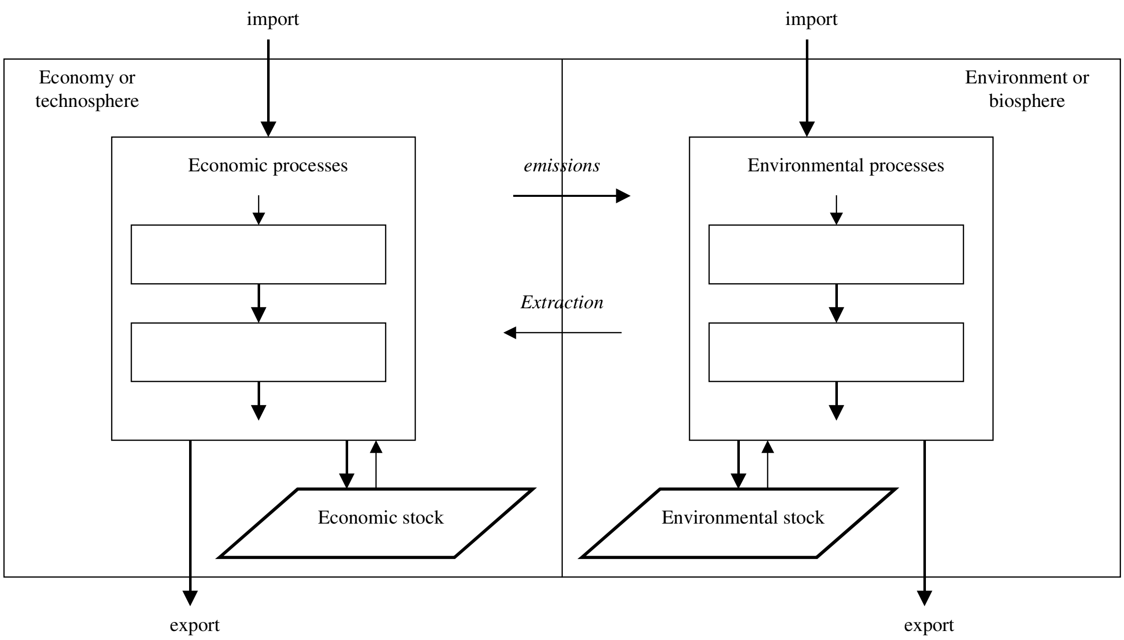

Fig. 1: The economic and the environmental subsystems and their components

SFA studies typically cover a period of one year. Flows of goods appear within this year and goods are transferred from one process to another. In the use phase, goods with a life span of longer than 1 year tend to accumulate: they do not flow out in the same year but remain for longer in the use-process. Such applications, with a life span of more than 1 year, are referred to as stocks. Although SFA typically covers a period of one year, a shorter time period can also be used (e.g., one month, one day, etc.). Goods with a life span longer than the time period taken in the model will be accumulating. This study uses a time period of one year.

SFA always focuses on investigating a specific substance. All flows and stocks therefore are regarded in terms of the substance as a chemical element and are specified in these terms. A substance may occur in a number of materials and in an even larger number of products. A substance stock therefore includes materials stocks, which in turn include product stocks. A careful distinction needs to be maintained between the stock of products, handled by producers and consumers, the stock of materials that those products are composed of, and the stock of a substance, contained within these products and materials and eventually resulting in emissions. The stock dynamics can be a result of developments at all three levels.

In the following sections, the economic and the environmental subsystems, their main components, their main variables and parameters and the most important aspects affecting their dynamic behaviour will be discussed.

3.2 Economic subsystem

3.2.1 General

The economic subsystem has three main component categories: processes, flows, and stocks. The flows and stocks represent certain economic goods. Flows refer to goods travelling from one process to another. Stocks are goods stored within the economic subsystem. Goods are transformed from one state to another through the processes. When this transformation takes place within the time period taken in the model (here one year), the goods will appear as flows in the SFA system. If this transformation takes a longer time, the goods will appear as stocks. Processes, flows and stocks in the economic subsystem are shown in figure 2.

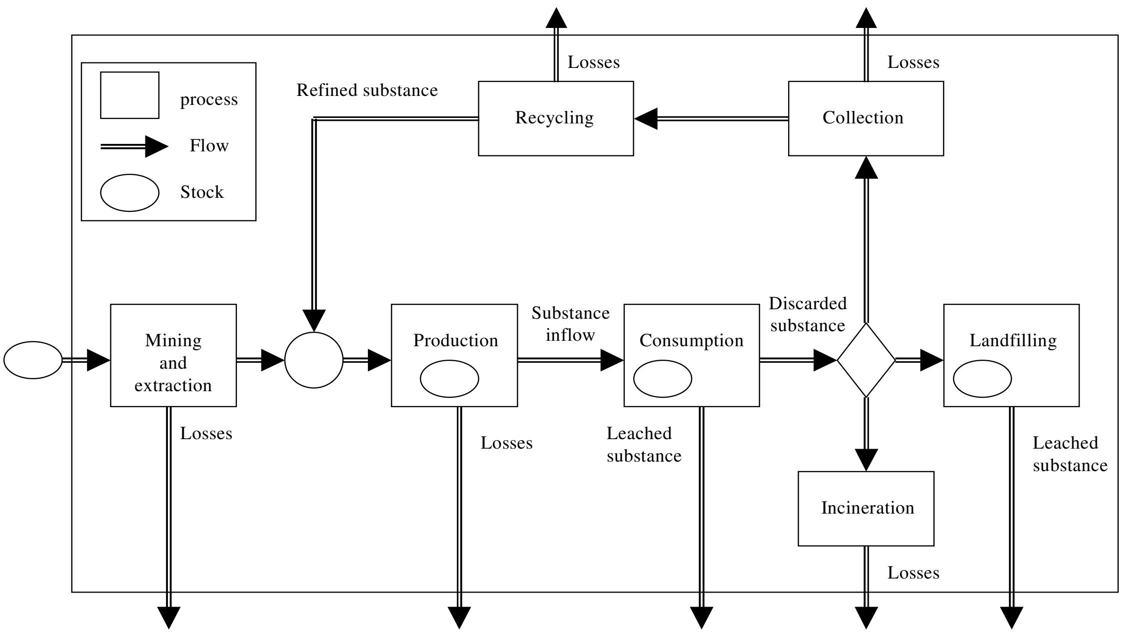

Fig. 2: The main processes, flows, and stocks in the economic subsystem.

Categories of processes

Mining and extraction, the processes through which raw materials are extracted from the biosphere or geosphere and transformed into materials that can be used in production and manufacturing. **Production and manufacturing**, the processes through which raw materials are transformed into finished goods. **Transportation**, the processes of transporting goods from one place to another, which does not involve any transformation. **Consumption and use**, the processes through which products are transformed into discarded products. These may involve a considerable time period. **Hibernation**, the processes involving storage of products no longer in use, but not yet discarded. **Waste treatment**, the processes involving the treatment of waste materials, thereby transforming discarded products into re-used products, recovered energy, recycled materials, landfilled waste, or emissions.

Categories of flows

Mined raw materials, the extraction or mining from the environment of a flow of raw materials containing the substance under study, which then enters into the economic subsystem. **Products**, the flow of different kinds of finished goods containing the substance into the consumption phase, either through production processes within the studied system or entering it through trade. **Discarded products**, the flow of discarded goods from the consumption and/or hibernating phases to the waste-processing phase. **Reused products/recycled materials**, the flow of goods recaptured from the waste stream and returned to the production or consumption phases. **Final waste**, the flow of materials with no economic value to be disposed of. At present disposal is either through landfill or incineration. Ashes and slag from the incineration process may be recycled or end up in landfill. Materials may also be emitted to the environment. **Emissions,** the flow of materials or substances from the economic subsystem to the environmental subsystem. Emissions represent losses from processes in the economic subsystem through corrosion, leakage or volatilization and can occur in all phases of the life cycle. The emissions themselves are not intended. By making changes to certain processes, they can be intentionally reduced or prevented. **Imported goods**, the flow of substances, materials, semi-manufactured and finished goods containing the substance entering the system under study from outside the system. These flows occur through trade with other countries or regions. **Exported goods**, the flow of substances, materials, semi-manufactured and finished goods containing the substance under study out of the system, again through trade.

Categories of stocks

Resource, the stock of the substance in the lithosphere or biosphere. **Product and material stock in industries**, the stock of goods and materials containing the substance under study kept in industries or in storage prior to use. **Product stock in use**, the stock of goods in use, containing the substance under study providing the service they were made for. **Hibernating products**, the stock of goods containing the substance under study that no longer provide the service they were made for but not yet discarded. **Substance stock in use,** the stock of the substance under study in the use phase. **Landfilled waste**, that is, the stock of final waste deposited at landfill sites.

The modelling of these processes flows and stocks in the economic subsystem will be described in the next sections. The starting point for the modelling is the consumption of applications containing the substance, mainly the demand for the substance being studied. Other aspects of the economic subsystem are mainly derived from this.

3.2.2 Consumption of substance- containing applications

In general, the stock of a substance or material consists of all the products containing the substance or material that have a life span that exceeds the time period used in the model (1 year). This can involve a large number of products with widely differing characteristics. This implies that a substance stock model should contain two levels: the substance level and the product level, as shown in figure 3. Products have a given demand and life span, which may or may not be influenced by the substances it contains. A substance in a product may be substituted without changing the demand for the product. The substance in a waste product may be extracted and recycled, and subsequently used in different products. In this scenario the substance leaves the specific product stock but not society, and the life span of the substance may differ considerably from that of the applications in which it used.

3.2.2.1 Modelling the inflow of substances into the stock-in-use

The inflow of a substance into a stock-in-use is determined by the demand for products containing the substance and the substance content of products. The demand is influenced by socio-economic and economic factors such as Gross Domestic Product (GDP), per capita GDP, population size and growth, inter and intra-sectoral shares in GDP, price, consumer tastes and preferences, the possibilities of substitution and technical developments.

The model employs two approaches to model the inflow of a substance into the stock-in-use. In some cases the inflow of substances is modelled on the inflow of products multiplied by their substance content. In these cases the inflow of products and the inflow of the substance are modelled using two separate equations, determined by different factors as shown in figure 3.

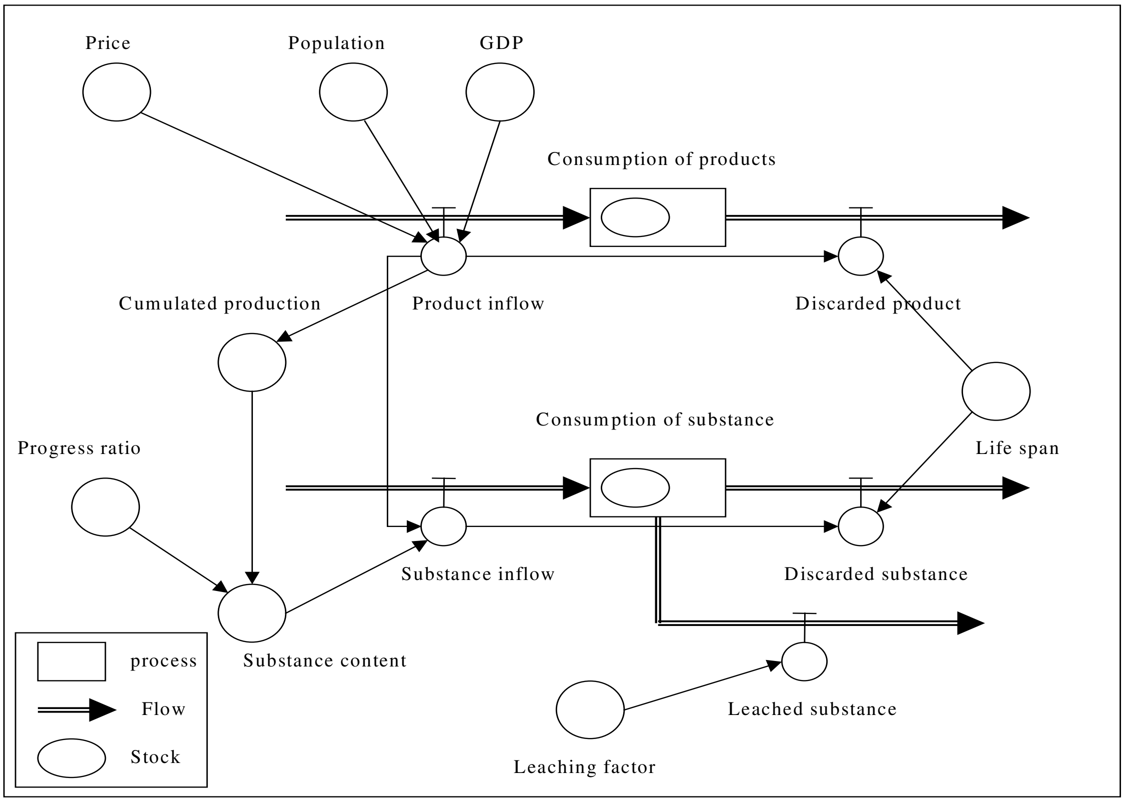

Fig. 3: The inflow of a substance into the substance stock-in-use, based on the product/substance approach

In the model, Eq. 1 is used to determine the inflow of products into the stock-in-use and is then multiplied by the substance content as given by Eq. 2. A regression model is used to establish the relative importance of the independent variables on the shape of the inflow curve over time. The substance content can be assumed to be either constant or to change over time. If the later is assumed, the substance content can then be modelled either as a function of the cumulated production (learning curve) or as a function of time. The model adopts the learning curve concept, as given by Eq. 3 and so models the substance content as a function of the cumulated production.

$$F_{PC,i}^{in}(t) = \beta_0 + \sum_{i=1}^{n} \beta_i X_i(t) + \varepsilon(t) \tag{1}$$

where $F^{in}_{PC,i}(t)$ is the inflow of product into the ith product stock at time t, n is the number of explanatory variables, $X_i(t)$ is the socio-economic variable at time t, β_i is the model parameter and $\varepsilon(t)$ is the model error at time t.

$$F_{C,i}^{in}(t) = SC(t) \cdot F_{PC,i}^{in}(t) \tag{2}$$

where $F^{in}_{C,i}(t)$ is the inflow of substance into the ith product stock at time t and $SC(t)$ is the substance content at time t.

$$SC(t) = SC_0 \cdot X(t)^{-r} \tag{3}$$

where SC0 is the initial content of the substance, X is the cumulated production and r is the experience index.

F, the progress ratio, can be defined as ($F=2^{-r}$)

The total inflow of a certain substance into a stock-in-use is the sum of all the inflows of the substance into products in which it is used.

$$F_{C}^{in}(t) = \sum_{i=1}^{n} F_{C,i}^{in}(t) \tag{4}$$

where $F^{in}_{C}(t)$ is the total inflow of the substance into the consumption phase at time t

In other cases, the inflow of the substance into the stock-in-use is modelled directly (as shown in figure 4) using different types of models (linear model, log-log model and the intensity of use technique). This approach is used when the data on the substance level directly available.

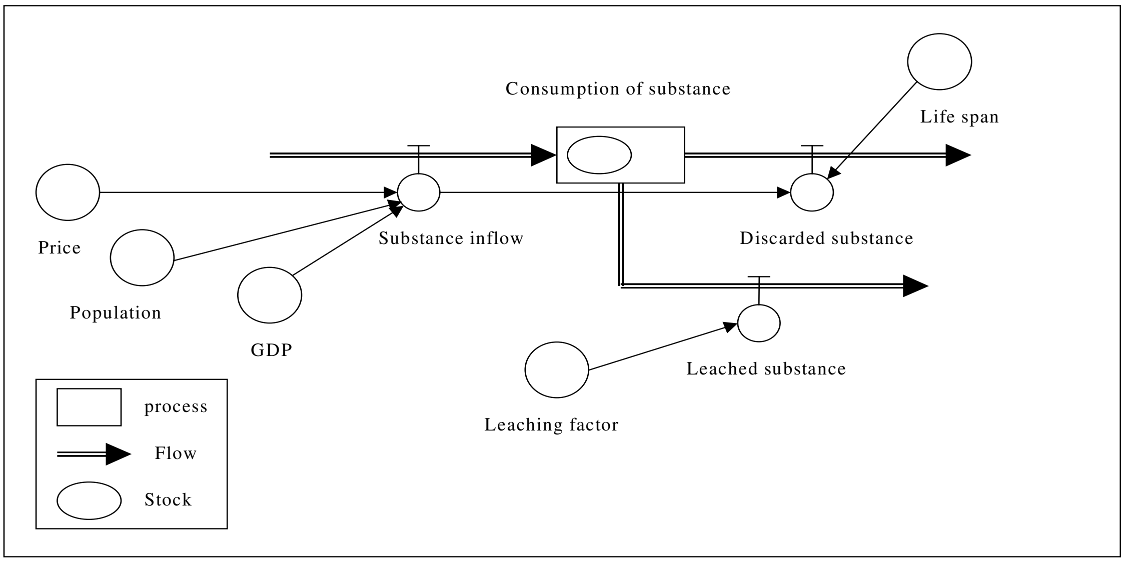

Fig. 4: The inflow of substances into the substance stock-in-use, based on the substance approach

3.2.2.2 Modelling the future inflow of substances into the stock-in-use

The derived inflow model can also be used to estimate the future inflow. This requires projected values of the influential variables. Some of the explanatory variables used in modelling the inflow, such as GDP, and population are exogenously determined. Others, such as the price, can be either exogenously or endogenously determined. Projections for GDP and population are available in different scenario studies (RIVM 2000, IPCC). The assumption then is that there will be no future discontinuity in the dependency of demand on the influential variables.

Approaches used to model the inflow of substances into the stock-in-use

- Linear model

The model uses a general linear function to describe the substance inflow (the product inflow multiplied by the substance content), which is separately fitted for each product based on past trend data:

$$F_{C,i}^{in}(t) = \beta_0 + \sum_{i=1}^{n} \beta_i X_i(t) + \varepsilon(t) \tag{5}$$

where $F^{in}_{C,i}(t)$ is the inflow into the *i*th product stock at time t, n is the number of explanatory variables, $X_i(t)$ is the socio-economic variable at time t, β_i is the model parameter and $\varepsilon(t)$ is the model error at time t.

The independent variables used in the model are Gross Domestic Product (GDP), Population (Pop), price (P) and a Time variable (T) that is used as a proxy for the combined influence of other variables on the inflow trend.

Sometimes the demand in a certain year does not correspond to the changes in the socio-economic variables in the same year, but to changes in these variables some years earlier. Apparently, there is sometimes a time lag between the driving forces and the response. Mathematically this time lag can be accounted for by Eq. 6:

$$F_{C,i}^{in}(t) = \beta_0 + \sum_{i=1}^{n} \beta_i X_i(t-j) + \varepsilon(t) \tag{6}$$

where $X_i(t\text{-}j)$ is the socio-economic variable at time (t-j), j is the time lag.

- Log-log model

Another possible model to determine the inflow of a certain substance into the use phase is the log-log model (Eq. 7). The estimated coefficients of this model can be interpreted directly as elasticities.

$$\ln\left[F_{C,i}^{in}(t)\right] = \beta_0 + \sum_{i=1}^{n} \ln\left[\beta_i X_i(t)\right] + \varepsilon(t) \tag{7}$$

- Intensity-of-use technique

Another possible approach for modelling the inflow in the use phase is to use the intensity-of-use technique. The approach separates the impacts of the intensity of use and GDP on consumption (demand) (Tiltone). Mathematically, the relation between consumption, the intensity of use and GDP can be expressed by Eq. 8.

$$D(t) = IU(t) \cdot GDP(t) \tag{8}$$

where *D(t)* is the consumption (demand) at time t, *IU (t)* is the intensity-of-use, and *GDP (t)* is the national income at time t.

The intensity of use follows a generally inverted U-shape trend (Tiltone, 1990). Although several functions can be used to capture this trend, the quadratic equation is the simplest (Roberts, 1996). The intensity of use is determined by the product composition of income, which depends on per capita income, and the material composition of products, which depends on technological change and long run price trends (Tiltone, 1990). It is possible to assume the IU as a function of per capita income (GDP/C) (Eq. 9) (Malenbaum) or as a function of time (t) (Eq. 10) (Roberts, 1996), which is used as a proxy of technological change and long run price trend. It can also be assumed as a function of both per capita income (GDP/C) and time (linear time (Eq. 11) or exponential (Eq. 12)) (Guzman, 2004).

$$IU(t) = a + b \cdot (GDP/C) + c \cdot (GDP/C)^2 \tag{9}$$

$$IU(t) = a + b \cdot t + c \cdot t^2 \tag{10}$$

$$IU(t) = a + b \cdot (GDP/C) + c \cdot (GDP/C)^2 + t \tag{11}$$

$$IU(t) = \left[a + b \cdot (GDP/C) + c \cdot (GDP/C)^2\right] \cdot e^{d \cdot t} \tag{12}$$

The parameters of these functions can be estimated by regression analysis

3.2.2.3 Modelling the leaching outflow of substances from the stock-in-use

The outflow of substances out of the stock takes place through two processes: leaching and delay (Van der Voet et al. 2002). Leaching occurs during use, due to corrosion or slow volatilization of substances from various stocks of applications. These emissions may end up in the soil, surface water, ground water or sewage system. The yearly emissions of a substance in a certain application can be modelled as a fraction of the total size of the stock by using linear or exponential emission coefficients. The model uses a linear emission coefficient, as given by Eq. 13.

$$F^{out}{}_{C,E,i}(t) = \alpha_i \cdot S_{C,i}(t) \tag{13}$$

where $F^{out}_{C,E,i}(t)$ is the outflow due to emissions at time t, α is the emission factor and $S_{C,i}(t)$ is the stock of the substance in product i at time t.

3.2.2.4 Modelling the delayed outflow of substances from stock-in-use

Delay is related to the discarding of products after use. The discarded outflow of a product depends mainly on the product inflow and its life span. Empirical data on the life span is often not available and as an alternative one can either assume an average life span or a certain life span distribution.

The discarded outflow can be modelled as a delayed inflow, corrected for emissions that occur during use, as given by Eq. 14:

$$F^{out}{}_{C,D,i}(t) = F^{in}_{C,i}(t - L_U) - \sum_{i=1}^{L_U} \alpha_i \cdot F^{in}_{C,i}(t - L_U) \cdot (1 - \alpha_i)^{i-1} \tag{14}$$

where $F^{out}_{C,D,,i}(t)$ is the outflow due to the delay mechanism at time t, α is the emission factor and L is the average life span of the product.

Or in the case of using a Weibull distribution, the discarded outflow at time t is a weighted sum of all past values of the inflow up to the present time, as given by Eq. 15.

$$F^{out}{}_{C,D,i}(t) = \sum_{j=0}^{\infty} W_j \cdot F^{in}{}_{C,i}(t-j) = \sum_{j=-\infty}^{t} W_{t-j} \cdot F^{in}{}_{C,i}(j) \qquad (15)$$

where the lag weights w are the probabilities of exiting the delay in any time period j and must sum to unity.

$$\sum_{j=0}^{\infty} W_j = 1$$

The total outflow at time t, F^{out} is given by Eq. 16.

$$F^{out}{}_{C,i}(t) = F^{out}{}_{C,D,i}(t) + F^{out}{}_{C,E,i}(t) \qquad (16)$$

The use of the delay model requires intensive historical information. In some cases it is possible to use the leaching model, which requires less information, as a proxy for the delay model (Van der Voet et al. 2002) using $\alpha_i=1/L_{ui}$. To use the leaching model as an approximation of the delay model, it must be possible to describe the inflow curve by an exponential function, the life span (L) is short and the parameter describing the direction and the steepness of the graph is small.

For some applications, use is sometimes equal to the emissions to the environment. This is the case with the lead applied in ammunition: once the bullets are used, lead is brought directly into the environment. In cases like this, an explicit borderline between the economy and the environment has to be made: Is the bullet, once shot, the emission, or is the emission only the corrosion once it is laying on the soil?

3.2.2.5 Modelling substances stock-in-use

The change of the magnitude of the stock over time is the difference between the inflow and the outflow, as given by the differential equation (Eq. 17).

$$\frac{dS_{C,i}}{dt} = F^{in}{}_{C,i}(t) - F^{out}{}_{C,i}(t) \qquad (17)$$

where $F^{in}{}_{C,i}(t)$ is the inflow into the *i*th product stock at time t, $F^{out}{}_{C,i}(t)$ is the outflow from the *i*th product stock at time t and $S_{C,i}$ is the *i*th product stock.

3.2.2.6 Modelling hibernating stock

The term "hibernating stock" refers to the stock of goods no longer providing the service they were made for, but not yet discarded. Some goods are stored for some time before being discarded. The main difference between the stock-in-use and the hibernating stock lies in the product life span. In the use phase, the life span is determined by the technical specification of the product. In the hibernating phase, however, the life span is determined by the consumer's decision. If a product is stored before being discarded, this hibernating time should be taken into account, either by adding the hibernating time (L_H) to the use time (L_U), if the entire discarded outflow enters the hibernating stock, or by modelling the hibernating phase separately. If the hibernating phase is to be modelled separately, the change of the magnitude of the hibernating stock is the difference between its inflow and outflow as given by Eq. 18.

$$\frac{dS_{H,i}}{dt} = F^{in}{}_{H,i}(t) - F^{out}{}_{H,i}(t) \qquad (18)$$

where $F^{in}{}_{H,i}(t)$ is the inflow into the hibernating stock at time t and $F^{out}{}_{H,i}(t)$ is the outflow from the hibernating stock at time t.

The inflow into the hibernating stock ($F^{in}_{H,i}$) is the discarded outflow of the stock-in-use ($F^{out}_{C,D,i}$), or part of it, as given by Eq. 19.

$$F^{in}_{H,i}(t) = \alpha_{H,i} \cdot F^{out}_{C,D,i}(t) \tag{19}$$

where $\alpha_{H,i}$ is the fraction of the discarded outflow of the stock-in-use which enters the hibernating stock.

The outflow from the hibernating stock is the outflow due to the emissions during hibernation ($F^{out}_{H,E}$) and the discarded outflow ($F^{out}_{H,D}$). The same mathematical equations used for modelling the outflow from the stock-in-use (Eqs. 13 and 14) can be used. L_U in Eq. 14 should be replaced by the hibernating time (L_H). Alternatively, Eq. 14 can be employed directly, with the life span being the use life span plus the hibernating life span.

3.2.3 Mining and co-production of substances

3.2.3.1 Mining and extraction of substances

The total amount of a substance taken from ore is determined by the amount required from primary production and emissions of the substance during the production processes.

$$F^{in}_{P}(t) = F^{out}_{P}(t) + \left[\alpha \cdot F^{out}_{P}(t)\right] = (1+\alpha) \cdot F^{out}_{P}(t) \tag{20}$$

The amount of a substance required from primary production is determined by the total demand for the substance (the flow of the substance into the production processes) and the available amount of secondary materials.

$$F^{out}_{P}(t) = F^{in}_{PP}(t) - \left[\alpha \cdot F^{out}_{R,R}(t)\right] \tag{21}$$

where F^{in}_{P} is the inflow of substances into primary production processes (the extracted flow) and F^{out}_{p} is the outflow from these processes (refined primary substances)

The outflow of secondary materials from recycling processes is either partly or completely used in producing new products. This is mainly determined by the price of secondary material compared to the price of primary material on the world market.

3.2.3.2 Co-production of substances

The amount of co-produced substances is estimated from the required primary production of the main substance and the co-produced material content of the ores.

$$F^{in}_{x}(t) = \alpha_{x} \cdot F^{in}_{P}(t) \tag{22}$$

where $F^{in}_{x(t)}$ is the inflow of the co-produced substance into the economy at time t, $F^{in}_{P(t)}$ is the inflow of the substance into primary production processes at time t, and α_x is the ratio between the substance and co-produced substance.

3.2.4 Production of substance-containing applications

3.2.4.1 Modelling the inflow of substances into the production processes

The total inflow of a substance into the production processes is the amount needed to produce the different required products, as given by Eq. 23.

$$F_{PP}^{in}(t) = \sum_{i=1}^{n} F_{PP,i}^{in}(t) \tag{23}$$

F^{in}_{PP} *(t)* is the total inflow of a substance into the production processes of all the applications at time t, $F^{in}_{PP,i}$ *(t)* is the inflow of the substance into the production process of product i at time t and n is the number of products .

For each application, the inflow of the substance into the production process is equal to the outflow of the substance in the produced product plus the other outflows from the production process (emissions to air and water, and waste flow), as given by equation 24.

$$F_{PP,i}^{in}(t) = F_{PP,i,P}^{out}(t) + F_{PP,i,A}^{out}(t) + F_{PP,i,W}^{out}(t) + F_{PP,i,L}^{out}(t) \tag{24}$$

$F^{in}_{PP,i}$ *(t)* is the inflow of the substance into the production process of product i at time t, $F^{out}_{PP,i,P}$ *(t)* is the outflow of the substance in the produced product i at time t, $F^{out}_{PP,i,A}$ *(t)* is the outflow of the substance to the air during the production process of product i at time t, $F^{out}_{PP,i,W}$ *(t)* is the outflow of the substance to the water during the production process of product i at time t, and $F^{out}_{PP,i,L}$ *(t)* is the outflow of the substance to the landfill sites from the production process of product i at time t.

The inflow of the substance into the production process of product i ($F^{in}_{PP,i}$) is estimated directly for each product as a balancing item of the production process as given by Eq. 29. The total inflow of the substance F^{in}_{PP} is estimated in Eq. 23. This implies that it is not supply, but demand (i.e. domestic and foreign demand for products containing the substance) that is the driving force.

3.2.4.2 Modelling the outflow of substances from production processes

The total outflow of the substance from the production processes is the combination of the substance in the produced products, the emissions from the production processes, and the waste flow to landfill. If the modelled system is large (global), imports and exports can be neglected. Consequently the outflow of the substance into the produced products is equal to the inflow of the substance into the stock-in-use (Eq. 25).

$$F_{PP,i,P}^{out}(t) = F_{C,i}^{in}(t) \tag{25}$$

The other outflows can be estimated as a fraction of the outflow of the substance in products as given by Eqs. 26, 27 and 28.

$$F_{PP,i,A}^{out}(t) = \alpha_{PA,i}(t) \cdot F_{PP,i,P}^{out}(t) \tag{26}$$

$$F_{PP,i,W}^{out}(t) = \alpha_{PW,i}(t) \cdot F_{PP,i,P}^{out}(t) \tag{27}$$

$$F_{PP,i,L}^{out}(t) = \alpha_{PL,i}(t) \cdot F_{PP,i,P}^{out}(t) \tag{28}$$

where $\alpha_{PA,i}$ *(t)* is the air emission factor at time t, $\alpha_{PW,i}$ *(t)* is the water emission factor at time t and $\alpha_{PL,i}$ (t) is the landfill factor at time t.

3.2.4.3 Modelling the stock in production processes

In the production phase of the applications containing the substance in question, the change of the magnitude of the substance's stock over time is assumed to be 0, as given by Eq. 29. Therefore, the inflow of substances into the production of different applications is equal to the total outflow from the production processes (emissions and products).

$$\frac{dS_{PP,i}(t)}{dt} = 0 = F_{PP,i}^{in}(t) - F_{PP,i}^{out}(t) \quad (29)$$

where $F^{in}_{PP}(t)$ is the total inflow of a substance into the production processes of each application at time t, and $F^{out}_{PP}(t)$ is the total outflow of a substance from the production processes of all applications at time t.

3.2.5 Waste management of substance containing applications

Part of the discarded outflow (F^{out}_{D}) from the stock-in-use and/or the hibernating stock will be collected for recycling purposes and part will end up in final waste treatment, either on landfill sites or in incineration plants. Collected, incinerated and landfilled streams are modelled as fractions of the discarded outflow as given by Eqs. 30 and 31. Figure 5 shows the main factors determining the distribution of the substance in the waste management phase.

$$F_{SC,i}^{in}(t) = a_1(t) \cdot F_{C,D,i}^{out}(t) \quad (30)$$

$$F_{inc,land,i}^{in}(t) = F_{inc,DC,i}^{in}(t) + F_{land,DC,i}^{in}(t) = F_{C,D,i}^{out}(t) - F_{SC,i}^{in}(t) \quad (31)$$

Where $F^{in}_{SC,i}(t)$ is the amount of scrap waste material collected for recycling purposes, at time t and a_1(t) is the collection rate. $F^{in}_{inc,land,i}$ is the inflow of the substance into incineration plants and landfill sites from the discarded product i, $F^{in}_{inc,DC,i}$ is the inflow of the substance into incineration plants from the discarded product i, and $F^{in}_{land,DC,i}$ is the inflow of the substance into the landfill sites from the discarded product i.

3.2.5.1 Collection

In this phase the collected part(s) from obsolete products are gathered and stored for some time before entering the recycling processes.

The inflow of substances into the collection phase

The inflow of substances into the collection phase is a fraction of the discarded outflow from the stock-in-use and/or the hibernating stock. The stream of collected materials is mainly determined by policy, economic, technical and socio-economic aspects.

Economic factors, largely derived from the ratio of primary and secondary material prices, are the main determinants of the extent to which the recycling process is profitable. The price of secondary material can be used as a proxy for the cost involved at this phase (the cost of collection and transportation). The model can test and regulate the effects of policy through applying different policy measures, such as a landfill tax. The socio-economic and demographic factors are indicated by per capita GDP and population density.

Regression analysis is used to parameterise the relation between the collection rate (a_1 in Eq. 30) of each of the substance's applications and the different factors that influence this (the cost of collection and transport, population density, per capita GDP, Landfill tax, etc.). A general function similar to Eq. 1 is used to describe the collection rate. This can be fitted separately to each product according to the past collection rate trend data.

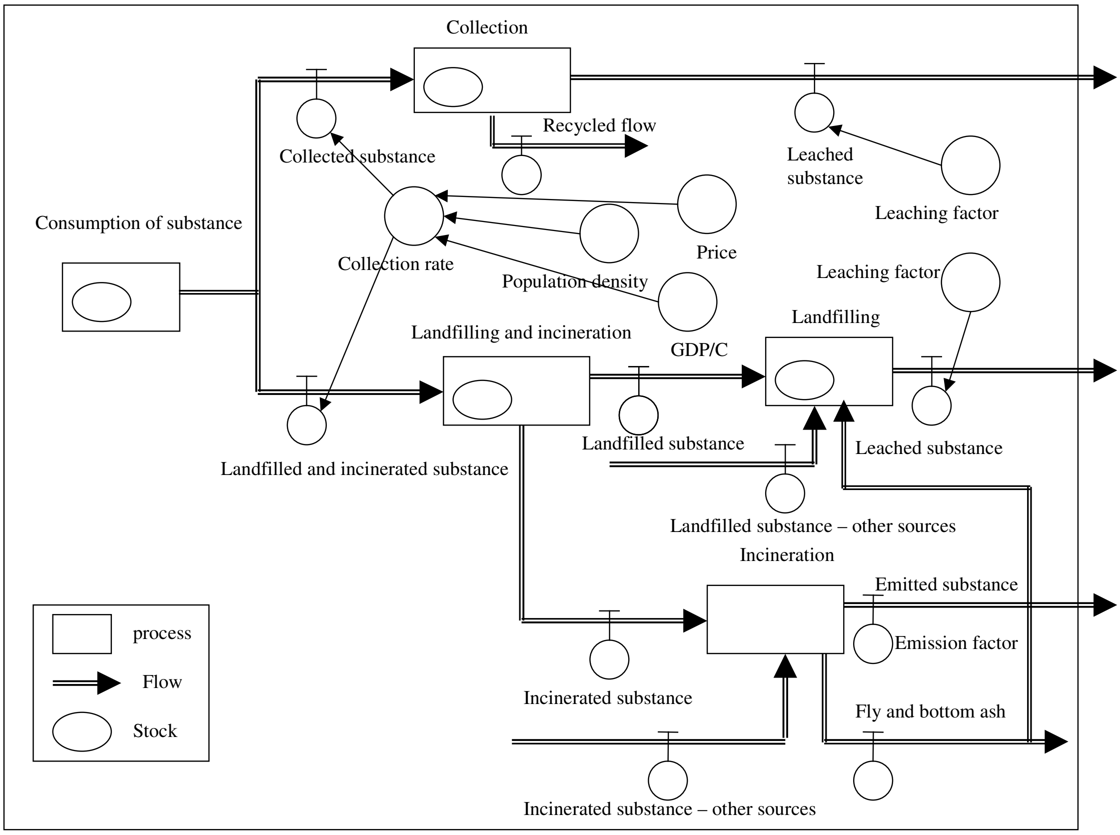

Fig. 5: The distribution of a substance between different waste management options

The outflow of substances from the collection phase

The outflow from the collection phase is due to emissions during storage time and the flow of substances entering recycling processes, as given by Eq. 32.

$$F_{SC,i}^{out}(t) = F_{SC,i,E}^{out}(t) + F_{SC,i,R}^{out}(t) \tag{32}$$

$F^{out}_{SC,i}(t)$ is the outflow from the collection phase at time t, $F^{out}_{Sc,i,E}(t)$ is the emitted outflow at time t and $F^{out}_{SC,i,R}(t)$ is the outflow going to recycling processes at time t.

The outflow to the recycling processes can be estimated as delayed inflow, by using an equation similar to Eq. 14. The storage time could range from 0 to a few years. The outflow due to the emissions during storage time can be estimated as a fraction of the stock using an equation similar to Eq. 13. α in Eq. 13 is the emission factor and L in Eq. 14 is the storage time of obsolete products in this phase.

Substance stock in the collection phase

The change in the magnitude of stock of the substance in the collection phase over time is the difference between the inflow (the part collected from obsolete products) and the outflow (the emitted outflow during storage time and the recycled flow) as given by Eq. 33.

$$\frac{dS_{SC}(t)}{dt} = F_{SC,C}^{in}(t) - F_{SC}^{out}(t) \tag{33}$$

S_{sc} is the stock of substance in the collection phase, F^{in}_{sc} is the inflow of the substance collected from obsolete products and F^{out}_{sc} is the outflow of the substance in obsolete products to recycling processes and emissions during storage.

3.2.5.2 Recycling

Recycling materials involves several interconnected processes. The recycling process begins with the collection of obsolete products, followed by sorting and separation activities and finishing (in the case of metals) with smelting and refining processes. Each process has its own requirements (material, energy), recoveries and losses (waste and emissions).

The recycling industry is driven by market-based factors, such as the cost of the different processes and the price of primary material compared to secondary material.

Inflow to the recycling processes

If the modelled system is large (global), the imports and exports can be disregarded. Consequently F^{in}_{R} can be estimated, as given by Eq. 34.

$$F_R^{in}(t) = F_{SC,R}^{out}(t) \tag{34}$$

Outflow from the recycling processes

The outflow from recycling processes is emissions during these recycling processes, the waste flow to landfill, the waste flow used for other applications (non-intentional flows of substance) and the useable secondary materials, as given by Eq. 35.

$$F_R^{out}(t) = F_{R,E}^{out}(t) + F_{R,W}^{out}(t) + F_{R,CNI}^{out}(t) + F_{R,R}^{out}(t) \tag{35}$$

$F^{out}_{R}(t)$ is the total outflow of the substance from recycling processes at time t, $F^{out}_{R,E}(t)$ is the emitted outflow at time t, $F^{out}_{R,W}(t)$ is the landfilled outflow at time t, $F^{out}_{R,CNI}(t)$ is the waste outflow used in other applications (non-intentional applications) at time t and $F^{out}_{R,R}(t)$ is the substance secondary outflow at time t.

Each of the outflows from recycling processes can be estimated as a fraction of the outflow of secondary materials as given by Eqs. 36, 37 and 38.

$$F_{R,A}^{out}(t) = \alpha_{RE}(t) \cdot F_{R,R}^{out}(t) \tag{36}$$

$$F_{R,L}^{out}(t) = \alpha_{RL}(t) \cdot F_{R,R}^{out}(t) \tag{37}$$

$$F_{R,CNI}^{out}(t) = \alpha_{CNI}(t) \cdot F_{R,R}^{out}(t) \tag{38}$$

$F^{out}_{R,R}(t)$ is the outflow of secondary materials from recycling processes within the country at time t and α*'s (t)* are the emission, landfilled waste and used waste factors at time t.

The stock of substances in recycling processes

The phase of recycling includes the sorting, smelting and refining of obsolete products. The change of the magnitude of the stock over time is assumed to be 0, as given by Eq. 39. Therefore, the inflow of obsolete products to recycling processes (the outflow from the collection phase) is equal to the outflow from the recycling processes (emissions, waste and useable secondary materials).

$$\frac{dS_R(t)}{dt} = 0 = F_R^{in}(t) - F_R^{out}(t) \tag{39}$$

3.2.5.3 Incineration

The inflow of substances into incineration plants

The inflow of substances into incineration plants mainly comes from the stock-in-use of different substance applications. For each application this flow is estimated in combination with the inflow of substances to be landfilled and is calculated as the difference between the total discarded waste stream from the stock-in-use of these applications and the flow collected for recycling, as given by Eq. 31.

The inflow of substances into incineration plants from discarded products is estimated as a fraction of the total uncollected flow for each product, as given by Eq. 40. This fraction is determined by several factors, including policy and the characteristics of the waste stream. The model can employ different scenarios to estimate the inflow of substances into incineration plants.

$$F_{inc,DC,i}^{in}(t) = \alpha_{1,i}(t) \cdot F_{inc,land,i}^{in}(t) \tag{40}$$

$\alpha_{1,i}$ is the fraction of the total uncollected flow of product t that ends up in incineration plants

The total inflow of substances into incineration plants is the inflow of substances from discarded products and the inflow from other sources, as given by Eq. 41.

$$F_{inc,t}^{in}(t) = \sum_{i=1}^{n} F_{inc,DC,i}^{in}(t) + F_{inc,others}^{in}(t) \tag{41}$$

where $F^{in}_{inc,others}$ is the inflow of substances into incineration plants from sources other than discarded products.

Other inflows into incineration plants such as that of incinerated sewage sludge are estimated as model relations.

The outflow of substances from incineration plants

The total outflow of substances from incineration plants is equal to the inflow of these substances into incineration plants. The outflow of substances from incineration plants is contained in incineration residues (bottom and fly ash) and emissions from incineration (Eq. 42). Each of these outflows is estimated as a fraction of the total inflow of the substance into incineration plants, as given by Eqs. 43, 44, and 45. The distribution of substances between the different outflows is determined by the technical specifications of the incineration plants.

$$F_{inc,t}^{out}(t) = F_{inc,B}^{out}(t) + F_{inc,F}^{out}(t) + F_{inc,E}^{out}(t) \tag{42}$$

$$F_{inc,B}^{out}(t) = \beta_1(t) \cdot F_{inc,t}^{in}(t) \tag{43}$$

$$F_{inc,F}^{out}(t) = \beta_2(t) \cdot F_{inc,t}^{in}(t) \tag{44}$$

$$F_{inc,E}^{out}(t) = \beta_3(t) \cdot F_{inc,t}^{in}(t) \tag{45}$$

$F^{out}_{inc,,t}$ is the total outflow of substances from incineration plants, $F^{out}_{inc,,B}$ is the outflow of substances from incineration plants in bottom ash, $F^{out}_{inc,,F}$ is the outflow of substances from incineration plants in fly ash and $F^{out}_{inc,E}$ is the emissions of substances from incineration plants.

Stock of substances in incineration processes

The incineration of applications containing the substance in question is one option for the waste management of substances. The change of the magnitude of the stock over time is assumed to be zero as given by Eq. 46. Therefore, the inflow of substances into incineration plants is equal to the outflow of substances from these plants.

$$\frac{dS_{inc}(t)}{dt} = 0 = F^{in}_{inc,t}(t) - F^{out}_{inc,t}(t) \tag{46}$$

where $F^{in}_{inc,t}$ *(t)* is the total inflow of the substance into incineration plants from different sources at time t and $F^{out}_{inc,t}$ *(t)* is the total outflow from incineration plants at time t.

3.2.5.4 Landfilling

The inflow of substances into landfill sites

Substances flowing into landfill sites originate from different sources in the economic subsystem: the stock-in-use, recycling and production processes, and the consumption of non-intentional applications of substances.

The inflow of substances into landfill sites from the stock-in-use is estimated in combination with the flow of substances to be incinerated. They are jointly estimated as the difference between the total discarded waste stream from the stock-in-use and the flow collected for recycling, as given by Eq. 31. The inflow of substances into landfill sites from discarded products is estimated as a fraction of the total uncollected flow of each product, as given by Eq. 47.

$$F^{in}_{land,DC,i}(t) = (1 - \alpha_{1,i}(t)) \cdot F^{in}_{inc,land,i}(t) \tag{47}$$

where $F^{in}_{land,DC,i}$ is the inflow of the substance into landfill sites from the discarded product i and $F^{in}_{inc,land,i}$ is the combined inflow of the substance into incineration plants and landfill sites from the discarded product i.

The total inflow of substances into landfill sites is the inflow of substances from discarded products and from other sources, as given by Eq. 48.

$$F^{in}_{land,t}(t) = \sum\nolimits_{i=1}^{n} F^{in}_{land,DC,i}(t) + F^{in}_{land,others}(t) \tag{48}$$

where $F^{in}_{land,others}$ is the inflow of substances into landfill sites from sources other than discarded products.

Other inflows into landfill sites, including inflow from sewage sludge and from incineration residues can be estimated as model relations.

The outflow of substances from landfill sites

The outflow of substances from landfill sites is the amount of these substances that leach into the soil and ground water. The leaching outflow is estimated as a fraction of the stock of substances in landfill sites using a similar equation to Eq. 13.

The *stock of substances in landfill sites*

The landfilling of applications containing the substance in question is one option in substance waste management. In this phase, the change of the magnitude of the stock over time is calculated as the difference between the inflow of substances from different sources in the economic subsystem and the outflow of these substances to environmental media (soil and ground water), as given by Eq. 49.

$$\frac{dS_{land}(t)}{dt} = F^{in}_{land,t}(t) - F^{out}_{land,t}(t) \tag{49}$$

where $F^{in}_{land,t}\ (t)$ is the total inflow of the substance into landfill sites from different sources at time t and $F^{out}_{land,t}\ (t)$ is the total outflow from landfill sites at time t.

3.2.5.5 Sewage treatment

Sewage treatment is connected to several substance flows. Its inflows come from emissions during use, from the consumption of food and animal products and from industrial processes, notably the production of other heavy metals. Its outflows are effluent and sewage sludge. Part of the inflow of a substance will end up in sewage sludge and the remainder will end up in the effluent. The sludge can be distributed over soil (used as a fertilizer or soil improvement material), incinerated, sent to, landfill and other destinations.

Inflow of substances into sewage treatment

The input of the substance into sewage treatment plants originates from emissions of the substance during the use phase, production processes, the consumption of food and animal products and other sources, as given by Eq. 50.

$$F^{in}_{ST}(t) = F^{out}_{CE,ST}(t) + F^{out}_{PP,ST}(t) + F^{out}_{CFA,ST}(t) + F^{out}_{other,ST}(t) \tag{50}$$

Where $F^{in}_{ST}(t)$ is the inflow of the substance into sewage treatment plants at time t, $F^{out}_{C,E,ST}(t)$ is the flow of the substance originating from emissions during the use phase at time t, $F^{out}_{pp,E}(t)$ is the flow of the substance originating from production processes, and $F^{out}_{C,FA,ST}(t)$ is the flow of the substance originating from the consumption of food and animal products at time t.

The inputs of the substance to sewage treatment plants from different sources (consumption, production) are estimated as model relations in the substance use phase.

The input of the substance from the consumption of food and animal products is estimated from the amount of the substance taken by food and fodder from agricultural soil. The uptake of the substance by food and fodder is estimated as a fraction of the substance stock within agricultural soil.

Outflow of the substances from sewage treatment

The distribution of the substance between sewage sludge and effluent is mainly determined by the efficiency of the processes and the input volume of the substance.

$$F^{out}{}_{ST,SS}(t) = \alpha_1 \cdot F^{in}_{ST}(t) \tag{51}$$

$$F^{out}{}_{ST,W}(t) = F^{in}_{ST}(t) - F^{out}{}_{ST,SS}(t) \tag{52}$$

where $F^{out}_{ST,SS}(t)$ is the outflow of the substance from sewage treatment processes with sewage sludge at time t, $F^{out}_{ST,W}(t)$ is the outflow of the substance from sewage treatment processes with water at time t, and α_1 is the efficiency of the processes.

Sewage sludge

Sewage sludge is disposed of in different manners. Part is used as a soil improver, part is incinerated and the remainder is landfilled. The future development of disposal routes for sewage sludge can be estimated either by the general equation (Eq. 1) or by using different scenarios (assuming that the most recent values for different disposal routes will remain valid in the future).

$$F^{out}{}_{SS,S}(t) = \alpha_1 \cdot F^{out}_{ST,SS}(t) \tag{53}$$

$$F^{out}{}_{SS,INC}(t) = \alpha_2 \cdot F^{out}_{ST,SS}(t) \tag{54}$$

$$F^{out}{}_{SS,L}(t) = F^{out}_{ST,SS}(t) - F^{out}{}_{SS,S}(t) - F^{out}{}_{SS,INC}(t) \tag{55}$$

where $F^{out}_{SS,S}(t)$ is the flow of the substance in sewage sludge applied to soil, where $F^{out}_{SS,INC}(t)$ is the flow of the substance with incinerated sewage sludge, and $F^{out}_{SS,L}(t)$ is the flow of the substance with landfilled sewage sludge.

3.2.6 Additional issues related to non-intentional use

In addition to the intentional use of substances, they also exist as contaminants in applications. This presence is either due to the natural occurrence of substances in ores, such as the presence of lead in phosphate fertilizers, or in fossil fuels, or is due to anthropogenic sources, such as the presence of lead in sewage sludge, incineration and recycling residues.

For these non-intentional applications, the inflows into the economic subsystem are not related to the substance itself but rather to the application in which the substance occurs. In this case each application has to be modelled separately. For some applications there are well developed models and/or scenarios, which can be used directly. In other cases, however, a new model has to be made on the basis of related explanatory variables.

The non-intentional flows of a certain substance in the economic and environmental subsystems are partly related to the waste streams of intentional applications of the substance itself and partly to applications of mixed primary resources.

3.2.6.1 Mixed primary resources

The inflow of a certain substance through mixed primary resources (coal, oil, other metals ores, phosphate ores, etc.) is determined by the demand for these resources and the proportion of the substance that they contain. Demand for these resources is mainly determined by the demand for final output from the processes in which they are used (e.g. electricity, metals, fertilizer).

In the model a general function (Eq. 56) is used to describe past developments in the demand for the final output from the processes (electricity, oil, heavy metals, and phosphate fertilizers). The same function is used for the future with an assumption on the future development in the explanatory variables.

$$Y(t) = \beta_0 + \sum_{i=1}^{n} \beta_i X_i(t) + \varepsilon(t) \tag{56}$$

Y (t) is the demand for the final output from the processes at time t, *Xi's* are the socio-economic variables at time (t), *β's* are the model parameters and *ε(t)* is the model error.

An alternative approach, especially relevant when insufficient data are available or a discontinuity is expected, is the use of scenarios (Image team, 2001).

The input of the substance is modelled based upon the amount of the substance per unit of final output (e.g. per ton of produced metal, kwh electricity, or ton of phosphate fertilizers used) as given by Eq. 57.

$$F_{S,Y}^{in}(t) = Y(t) \cdot S_x \tag{57}$$

Where $F^{in}_{S,Y}(t)$ is the inflow of the substance at time t, and S is the amount of the substance

3.2.6.2 Reusing waste materials

The non-intentional inflows of a certain substance into the economy through intentional applications are due to emissions during the use phase, which partly end up in sewage sludge, and the processing of their waste streams. These flows are determined by the demand for the substance in intentional applications, their life span, the emission factors and the waste management of discarded products.

The input of the substance through sewage sludge originates from sewage treatment plants and the input of substances into sewage treatment plants is discussed in section 3.2.5.5.

The input of the substance into incineration plants originates from the waste stream of the products containing the substance which have been discarded from the stock-in-use, together with that part of the produced sewage sludge which is incinerated, as given by Eq. 58.

$$F_{inc}^{in}(t) = \sum_{i=1}^{n} F_{inc,DC,i}^{in}(t) + F_{inc,SS}^{in}(t) \tag{58}$$

The input from sewage sludge is estimated as a fraction of the substance in the sewage sludge. Other options for sewage sludge include disposal in landfill sites, application to the soil, and others as discussed in section 3.2.5.5.

The input from the discarded outflow from the stock-in-use is estimated from an assumption about the distribution between incineration, landfill and recycling as discussed in section 3.2.5.3.

3.2.6.3 Output of substances from different processes

Outflows of the substance from the production processes of final outputs (oil, electricity, other heavy metals) and the incineration processes are mainly determined by technical factors. These outflows are modelled as a fraction of the input, as given by Eq. 59. Mass balance is enforced by modelling one flow per process as a balancing item.

$$F_{S,x}^{out}(t) = \alpha_x(t) \cdot F_{S,Y}^{in}(t) \tag{59}$$

Where $F^{out}_{S,x}(t)$ is the outflow of the substance to a specific destination at time t, $\alpha_x(t)$ represents the emissions factor, the division of the substance between fly and bottom ashes, and the different disposal routes of sewage sludge at time t.

The emission factors are mainly determined by technological development. They are assumed either to be constant or to change over time. The emission data are fitted to a linear function similar to that given by Eq. 56, using time as proxy of technological development and other time-related variables, or they are fitted to an exponential function as given by Eq. 60.

$$\alpha_x(t) = \beta_0 \cdot e^{\beta_1 \cdot t} \tag{60}$$

The division of the substance to bottom ash and fly ash during incineration processes and electricity production is determined by technical factors and given in different sources (Hasselriis and Licata, 1996, Sandelin et al. 1999 & Sandelin et al. 2001).

The disposal routes of sewage sludge are mainly determined by policy aspects. These can be assumed to be constant and use the most recent values, or can be assumed to change over time, in which case they can be modelled based on Eq. 56. Time can be used as a proxy of the policy aspects and other time-related variables.

3.2.6.3 The agricultural cycle

Stock building of substances takes place in agricultural soil. Figure 6 shows the flows connected to the stock of substances in agricultural soil.

Inflow of substances into the agricultural soil stock

The inflow of a substance into agricultural soil originates from different sources, including the application of materials to agricultural soil (e.g. fertilizers, sewage sludge and manure) and deposition from the air.

$$F_S^{in}(t) = F_{AD,S}^{out}(t) + F_{F,S}^{in}(t) + F_{SS,S}^{out}(t) + F_{M,S}^{in}(t) \tag{61}$$

where $F^{out}_{AD,S}\,(t)$ is the deposited flow from the air $F^{in}_{F,S}\,(t)$ is the flow of fertilizers, $F^{out}_{SS,S}\,(t)$ is the flow from sewage sludge and $F^{in}_{M,S}\,(t)$ is flow of manure.

Outflow of substances from agricultural soil stock

The outflow of a substance from agricultural soil is the amount of the substance taken up by plants (food and fodder crops) plus the amount of leaching of the substance to the ground water. The flow of a substance taken up by plants further contributes to the substance stock in soil through loops within the subsystem, related particularly to animal production (manure) and food products (sewage sludge).

$$F^{out}{}_{S,FOOD}(t) = \alpha_1 \cdot S_S(t) \tag{62}$$

$$F^{out}{}_{S,FODDER}(t) = \alpha_2 \cdot S_S(t) \tag{63}$$

$$F^{out}{}_{S,L}(t) = \alpha_3 \cdot S_S(t) \tag{64}$$

where $F^{out}_{S,FOOD}\,(t)$ is the uptake outflow of the substance from agricultural soil to food, $F^{out}_{S,FODDER}\,(t)$ is the uptake outflow of the substance from agricultural soil to fodder, $F^{out}_{S,L}\,(t)$ is the leaching outflow of the substance from agricultural soil to water. α_1 is the uptake rate for food, α_2 is the uptake rate for fodder, and α_3 is the leaching rate.

Stock of substances in agricultural soil

The change of the magnitude of the substance stock in the soil over time is determined by the inflow of the substance into the soil through different sources and the outflow of the substance from the soil, given by Eq. 65.

$$\frac{dS_S}{dt} = F^{in}{}_S(t) - F^{out}{}_s(t) \tag{65}$$

where $F^{in}_S(t)$ is the inflow into the stock at time t, $F^{out}_S(t)$ is the outflow from the stock at time t

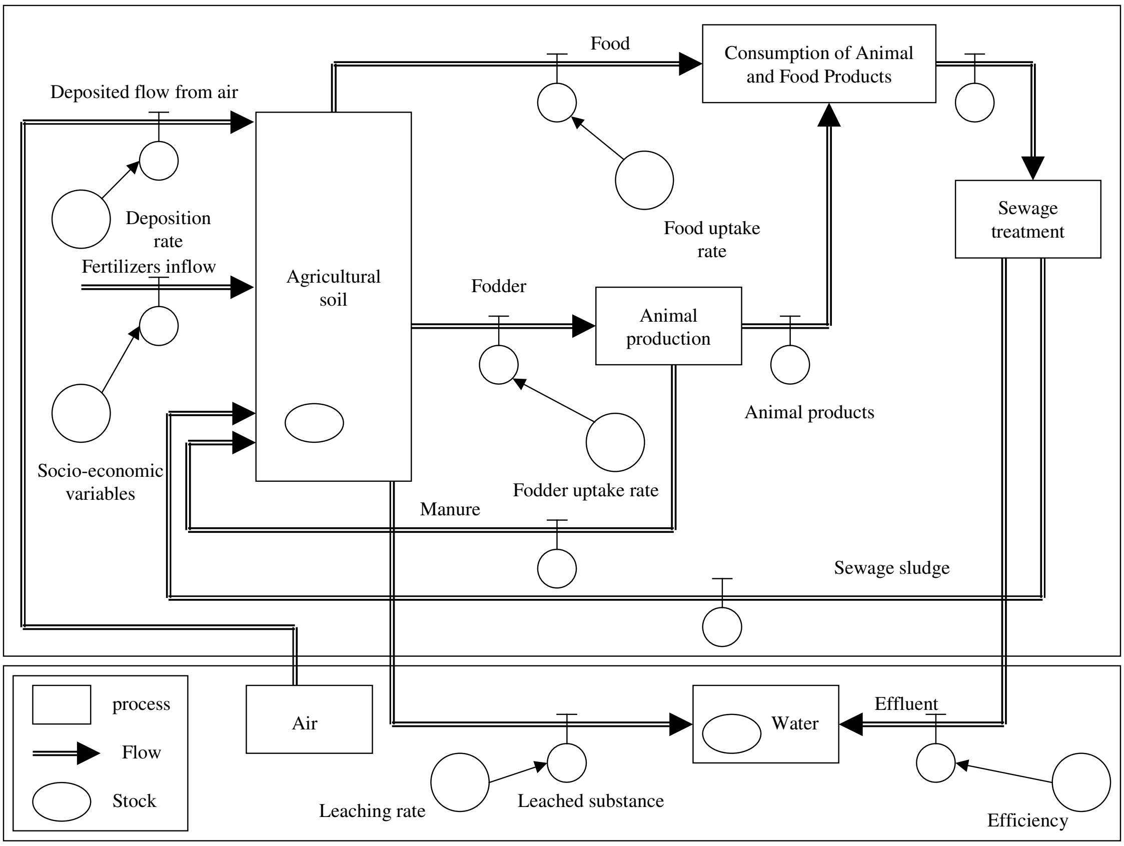

Fig. 6: The flows connected to the stock of substances in agricultural soil

Animal production

The inflow of a substance into animal production is the result of the output of the substance from the soil in the form of fodder. The outflow of a substance from animal production is the amount of the substance in manure plus the amount which goes to consumption of food and animal products (Eq. 66). The total outflow from animal production is equal to the total inflow into animal production.

$$F_{An}^{out}(t) = F^{in}{}_{CFA,An}(t) + F^{in}{}_{M,S}(t) \quad (66)$$

$$F^{in}{}_{CFA,An}(t) = \alpha \cdot F_{An}^{out}(t) = \alpha \cdot F_{An}^{in}(t) = \alpha \cdot F^{out}{}_{S,FODDER}(t) \quad (67)$$

$$F^{in}{}_{M,S}(t) = (1-\alpha) \cdot F_{An}^{out}(t) = (1-\alpha) \cdot F_{An}^{in}(t) = (1-\alpha) \cdot F^{out}{}_{S,FODDER}(t) \quad (68)$$

where $F^{out}{}_{An}(t)$ is the outflow of the substance from animal production, $F^{in}{}_{CFA,An}(t)$ is the inflow of the substance into the consumption of food and animal products from animal production, and $F^{in}{}_{M,S}(t)$ is the flow of manure from animal production.

Consumption of food and animal production

The inflows of a substance into the consumption of food and animal products, as given by Eq. 69, are the flows of the substance through food products, as given by Eq. 62 and the flows of the substance from animal production, as given by Eq. 66. The outflow from food and animal production enters sewage treatment, as given by Eq. 70, and is equal to the total inflow.

$$F_{CFA}^{in}(t) = F^{out}{}_{S,FOOD}(t) + F^{in}{}_{CFA,An}(t) \tag{69}$$

$$F_{CFA}^{out}(t) = F_{CFA,ST}^{out}(t) \tag{70}$$

where $F^{out}{}_{CFA,ST}(t)$ is the outflow of the substance from the consumption of food and animal products to sewage treatment .

3.2.7 Modelling imports and exports

Substance flow analysis can be carried out at different levels; international, national, and local. If the modelled system is small (national or local), the import and export of products, scrap and the refined substance should be taken into account. Figure 7 shows the processes, intentional flows and stocks in national or local economic subsystems.

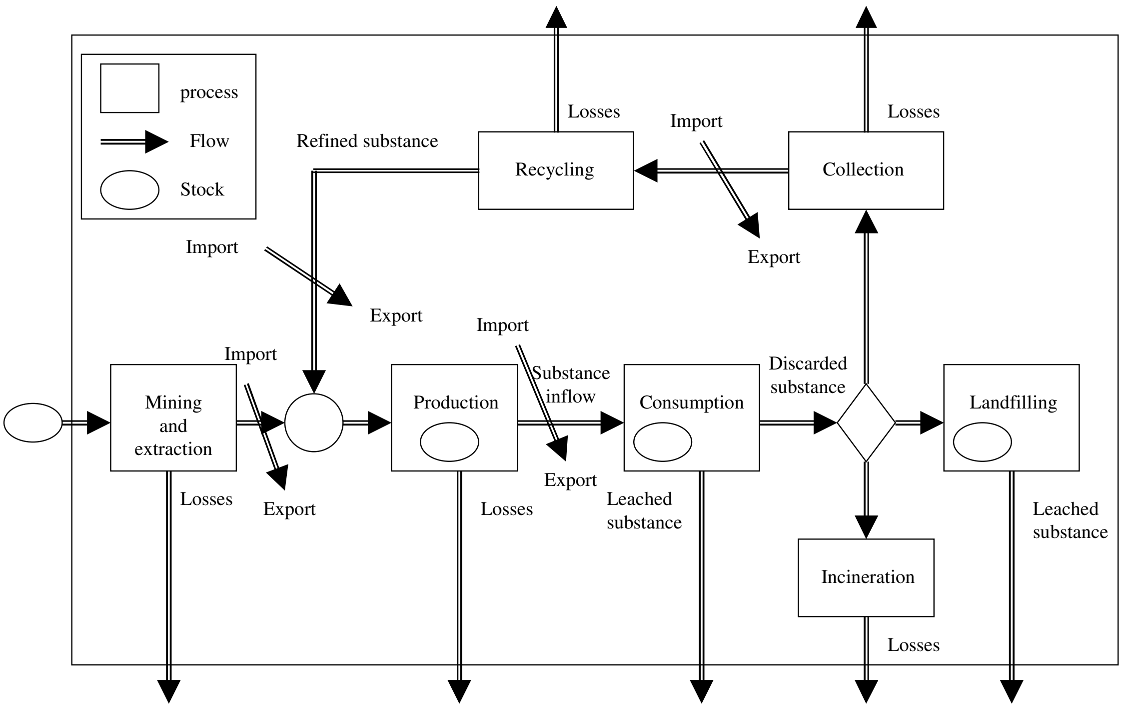

Fig. 7: The main flows, stocks and processes in a national or local economic subsystem.

3.2.7.1 Imports and exports of products

The inflow of a substance $F^{in}{}_{C,i}$ into the stock-in-use in a country is equal to the amount of the substance in the products produced in the country $F^{out}{}_{PP,i,P}$ plus imported products minus exported products, as given by Eq. 71.

$$F_{C,i}^{in}(t) = F_{PP,i,P}^{out}(t) + import(t) - \exp ort(t) \tag{71}$$

The import and export of products is estimated as the difference between the products produced in a country and the inflow of products into the consumption phase from Eq. 71 (i.e. as a balancing item between the production and consumption phases). It is difficult to separate the estimated value for imports and exports, and therefore the estimated value is kept as one variable, net imports. Eq. 2 gives the inflow of the substance into the use phase. In the model, a general function similar to Eq. 1 is used to describe the outflow of the substance within products $F^{out}_{PP,i,P}(t)$ based on the past trend data.

The production of a certain product in a specific country is determined by the global demand for products and the competition in the world market, which are affected by energy and labour costs, indicated by GDP/C, and the cost of disposing of any residual materials. The substance content of a product is determined by substitution and technical developments.

3.2.7.2 Imports and exports of obsolete products

The import and export of obsolete products are estimated as the difference between the products collected in a country and the inflow of obsolete products into recycling processes from Eq. 72 (i.e. as a balancing item between the collection and recycling phases). It is difficult to estimate the value of imports and exports separately, and therefore the estimated value is kept as one variable, net imports.

$$F_R^{in}(t) = F_{SC,R}^{out}(t) + import(t) - \exp ort(t) \tag{72}$$

The outflow of obsolete products to recycling processes is estimated in Eq. 32. The inflow of obsolete products into recycling processes is estimated as a balancing item for recycling processes. In this case, it is not possible to estimate the outflow from recycling processes (as given by Eqs. 34 and 35). Instead, the usable secondary material (one of the outflows of recycling) can be estimated on the basis of explanatory variables. A general function similar to Eq. 1 is used to describe the outflow $F^{out}_{R,R,}$ which is based on past trend data.

The most influential factors in this respect are: the costs of sorting and transformation, of disposing of any residual material, of energy and labour indicated by GDP/C, together with global demand for the material, and the price of secondary material compared to that of primary material.

3.2.7.3 Import and export of primary and secondary refined substances

The inflow of a substance F^{in}_{PP} into the production processes within a country is the amount of the substance (primary and secondary) produced in the country plus the imported amount of the substance minus the exported amount as given by Eq. 73.

$$F_{PP}^{in}(t) = F_{R,R}^{out}(t) + F_{R,P}^{out}(t) + import(t) - \exp ort(t) \tag{73}$$

where $F^{out}_{R,R}(t)$ is secondary refined substance in the country at time t, which is known from recycling processes, $F^{out}_{R,P}(t)$ is the primary refined substance in the country at time t.

The import and export of primary and secondary substances can be estimated as the difference between the primary and secondary refined substance produced in a country and the inflow of substances (primary and secondary) into the production processes of the substance-containing applications (i.e. as a balancing item between the recycling and production phases). In most cases, it is possible the estimate the production of refined substances (primary and secondary) in the future. Data about the inflow of these substances into the production processes of their applications is generally not directly available, but it is possible to estimate the inflows as described in section 3.2.4. By estimating the inflow directly from Eq. 24, the value of imports minus exports can be estimated from Eq. 73. As it is difficult to estimate the values of the imports and exports separately, the estimated value is presented as one variable, net imports.

3.3 Environmental subsystem

Substance flows and stocks in different environmental compartments originate from the substances used in economic activities (production, consumption, and waste management), whether these activities are related to the intentional use or non-intentional use of a substance. Figure 8 shows the environmental stocks and flows. The environmental subsystem includes several components; air, water, non-agricultural soil, sediment, ground water and sea water. In this study air, fresh water and soil are distinguished as separate components in the model. The environmental subsystem includes two stocks; stocks in non-agricultural soil and resource stocks. The substance flows and stocks in the different environmental components are inter-connected, with flows from one to another. These flows and stocks are only partially included in the model – more detailed modelling of these flows and stocks can be done through multi-media fate modelling (Heijungs, 2000).

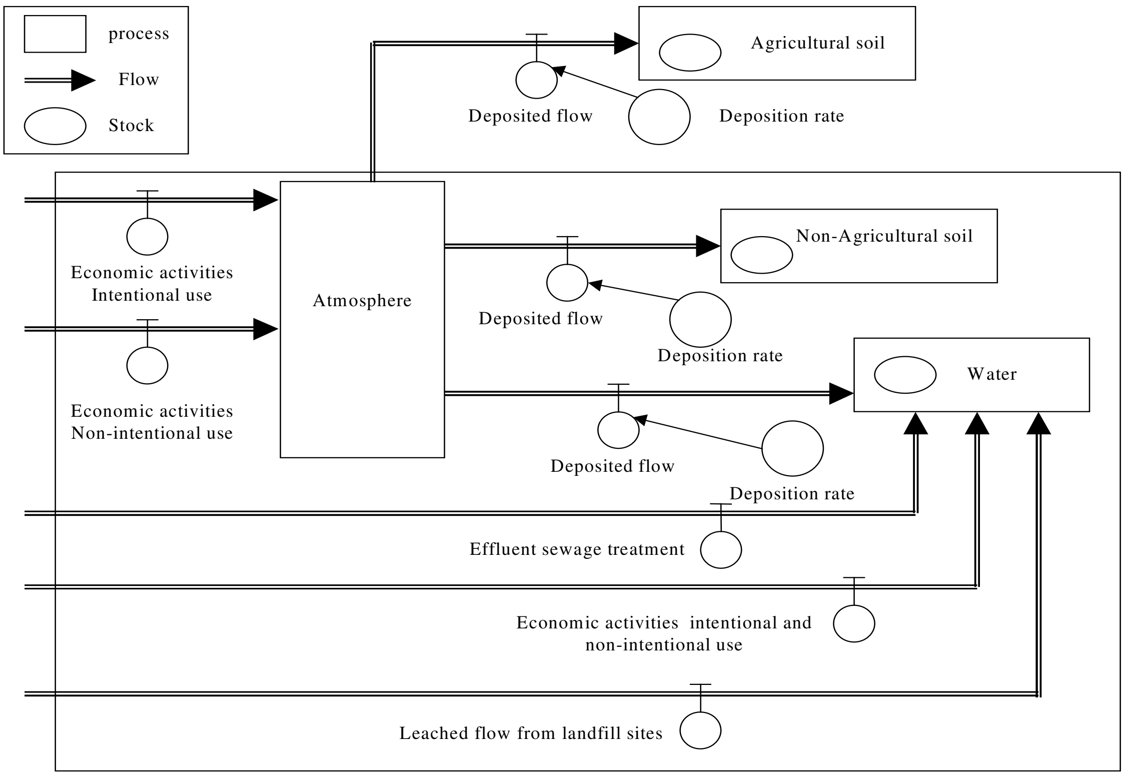

Fig. 8: Stocks and flows in the environmental subsystem.

3.3.1 Air

Inflow of substances into air

The inflow of a substance into the air originates from different sources, some of which are related to the intentional use of the substance and others to non-intentional use.

$$F_{A}^{in}(t) = \sum F_{PP,i,A}^{out}(t) + F_{inc,A}^{out}(t) + F_{R,A}^{out}(t) + F_{C,E}^{out}(t) + F_{NIU,A}^{out}(t) \quad (74)$$

where $F^{out}_{PP,I,A}$ is emissions from the production of different applications, $F^{out}_{inc,A}$ is emissions from the incineration process, $F^{out}_{R,A}$ is emissions from recycling processes, $F^{out}_{C,E}$ is emissions from use of different applications, $F^{out}_{NIU,A}$ is emissions from non-intentional use.

Outflow of substances from the air

The outflow of a certain substance from the air, which is equal to the total inflow, is the amount of the substance deposited in water, soil (agricultural and non-agricultural) and outside the region (trans-boundary flow).

$$F_A^{out}(t) = \sum_{i=1}^{n} F_{A,i}^{out}(t) \tag{75}$$

$$F^{out}{}_{A,DS}(t) = \alpha_1 \cdot F_A^{in}(t) \tag{76}$$

$$F^{out}{}_{A,DW}(t) = \alpha_2 \cdot F_A^{in}(t) \tag{77}$$

$$F^{out}{}_{A,TF}(t) = F_A^{in}(t) - F^{out}{}_{A,DS}(t) - F^{out}{}_{A,DW}(t) \tag{78}$$

where $F^{out}{}_{A}$ is the total outflow from of the substance from the air, $F^{out}{}_{A,DS}$ is the deposited flow of the substance in the soil, $F^{out}{}_{A,DW}$ is the deposited flow of the substance in water, and $F^{out}{}_{A,TF}$ is the deposited flow of the substance outside the modelled system

3.3.2 Water

Inflow of substances into water

The inflow of a certain substance into water originates from different sources, some related to the intentional use of the substance and others to its non-intentional use.

$$F_W^{in}(t) = \sum F_{PP,i,W}^{out}(t) + F_{R,W}^{out}(t) + F_{NIU,W}^{out}(t) + F^{out}{}_{A,DW}(t) + F_{land,W}^{out}(t), F_{ST,W}^{out}(t) \tag{79}$$

$F^{out}{}_{PP,i,W}$ is emissions from the production of different applications, $F^{out}{}_{R,W}$ is emissions from recycling processes, $F^{out}{}_{NIU,W}$ is emissions from non-intentional use, $F^{out}{}_{A,DW}$ is deposition from the air, $F^{out}{}_{land,W}$ is leaching from landfill sites, $F^{out}{}_{ST,W}$ is effluent from sewage.

3.3.3 Non-agricultural soil

Soil is divided into two component parts, agricultural soil, which is treated in the economic subsystem and non-agricultural soil. The change of the magnitude of the substance stock in non-agricultural soil over time is determined by the inflow of the substance into the soil from different sources and the outflow of the substance from it as given by Eq. 80. The model treats non-agricultural soil as a sink, from which there is no outflow from stock.

$$\frac{dS_S}{dt} = F^{in}{}_S(t) - F^{out}{}_s(t) \tag{80}$$

where $F^{in}{}_S(t)$ is the inflow into the stock at time t, $F^{out}{}_S(t)$ is the outflow from the stock at time t and equal to zero in the model.

Inflow of substances into non-agricultural soil

The inflow of a substance to non-agricultural soil originates from different sources, some related to the intentional use of the substance and others to its non-intentional use.

$$F_S^{in}(t) = \sum F_{C,E}^{out}(t) + F_{NIU,S}^{out}(t) + F^{out}{}_{A,DS}(t) + F_{land,S}^{out}(t) \tag{81}$$

where $F^{out}_{C,E}$ is emissions from the use of different applications, $F^{out}_{NIU,A}$ is emissions from non-intentional use, $F^{out}_{A,DS}$ is deposition from the air, $F^{out}_{land,S}$ is leaching from landfill sites.

3.3.4 Resource stock

The change in the stock of a substance resource in ores is determined by demand for the substance from primary resources and consequently the amount being extracted from the ores and the addition to the stock, which is determined by the initial resource stock taken in the model. Two types of resources can be classified; identified resources and current reserves (USGS and USBM, 1980). Current reserves include all substance resources that are economic to extract at the current market price using existing technology. Identified resources include economic, marginally economic and sub-economic resources.
If the identified resources are used as the measure of the resource, this in principle gives a fixed amount and additions to the stock are assumed to be zero. If, however, the economic current reserve is taken as the measure, the resource stock can change with changes in techniques or prices. In this case, the addition to the stock will be the part of the identified resources, which is currently not economic or technically feasible to extract.

$$\frac{dS_{\mathrm{Re}\,s}(t)}{dt} = F^{in}_{\mathrm{Re}\,s}(t) - F^{out}_{\mathrm{Re}\,s}(t) = F^{in}_{\mathrm{Re}\,s}(t) - F^{in}_{P}(t) \tag{82}$$

where $F^{in}_{Res(t)}$ is the addition to the stock of resources at time t, $F^{out}_{Res(t)}$ is the outflow of the substance from the stock of resources at time t, and $F^{in}_{P(t)}$ is the inflow of the substance into primary production processes at time t.

3.4 Methods used in the evaluation of model variables and parameters

Several mathematical and statistical methods are used in the evaluation of some of the model's variables and parameters, such as the inflow of substances into the stock-in-use, the substance content in products, emission factors, and product life spans. These methods are briefly described below.

3.4.1 Evaluating the equation used in the inflow of substances into the stock-in-use

Regression analysis

Regression analysis is used in several scientific fields as a statistical tool to analyze the relation between variables. For example, it has been used to describe the demand for electricity, metals and other commodities as a function of socio-economic variables such as GDP, population, price and other specific variables for each commodity (Burney, 1995; Ranjan and Jain, 1999; Mohamed and Bodger, 2005; Roberts, 1996; Moore et al. 1996).

Regression analysis is used in the analysis to establish the relative importance of the independent variables on the shape of the inflow curve over time. It identifies the most significant variables, which contribute most to the shape of the inflow curve. It also examines the combined effect of significant variables. The fitting algorithm that determines the regression parameters ($\beta^{'s}$) uses the ordinary least square (OLS) criterion (Gijbels and Rousson, 2001).

The adequacy of the regression model and the significance of the variables can be described in statistical terms. The adjusted coefficient of determination (R^2adj) and F-statistics can be used to determine the overall goodness of the regression model. T-statistics can be used to evaluate the significance of the individual variables in the model.

R^2 is a measure of how much of the variance in the dependent variables is explained by the independent variables in the regression model. Large values of R^2 indicate better agreement between the model and the data. However, R^2 will always increase as more variables are added to the model. As an alternative, R^2adj can be used when more than one variable is combined in the model and this takes into account the number of independent variables. F-statistics indicate whether adding another variable to the regression model significantly improves the quality of the fit. T-statistics indicate whether or not each regression coefficient is significantly different from zero. For F-statistics and T-statistics, the critical value indicating the significance of the model, or its individual variables, at different probability levels can be found in statistical books.

Learning curve concept

The learning or experience curve concept is an analytical tool that can be used to provide a quantitative, mostly exponential, relation between a certain input to a process (Y) and a cumulative output (X) (Eq. 83). The parameter (-r) is referred to as the experience index and is defined by the progress ratio (F) and the learning rate (L). Eq. 84 and Eq. 85 give the progress ratio and the learning rate.

$$Y = a \cdot X^{-r} \tag{83}$$

$$F = 2^{-r} \tag{84}$$

$$L = 1 - 2^{-r} \tag{85}$$

where a in Eq. 83 is the value of Y for the first unit produced

The progress ratio (F) shows how an input Y will be reduced when the cumulative output is doubled. For instance, when F= 90% and L=10%, the input Y will be reduced to 90% of its previous level each time the cumulative output is doubled. In general, the progress ratio may increase over time for some technologies (Junginger et al., 2003, and Karaoz and Albeni, 2005).

The learning curve concept is used to model the relation between cost and cumulative production (Junginger et al 2005, Tsuchia and Kobayashi, 2004) and the relation between the energy consumption and cumulative production (Ruth, 1998, Ayres et al., 2003, and Ramirez and Worrell, 2006).

In the present model, the learning curve concept is used to model the possible reduction in the substance content of a product or material over time, the possible reduction in energy use in mining, smelting and refining processes, and possible reductions in ore grade over time.

3.4.2 Evaluating the distributions of the discarded outflow from the stock-in-use

In most studies, the life span of products is assumed to be a fixed number, an average value of several randomly occurring life spans. In reality however, products may have different life spans, depending on their technical specifications and the way they are used by consumers. To overcome the uncertainty associated with the assumed average life span, statistical distributions are performed to mathematically describe or model a certain life span behaviour. The probability density function (p.d.f.) is a mathematical function that describes this distribution. Common types of distribution are normal, lognormal and Weibull distributions. The Weibull distribution, which is also called lifetime distribution, was formulated by Professor Wallodi Weibull and is commonly used for analyzing life span data. This model uses the Weibull distribution, as it has been shown experimentally that it provides a good fit to the life span of many types of products (Melo,1999). The Weibull distribution is characterized by three parameters, the shape parameter β, which defines the shape of the curve, the scale parameter α, which defines where the bulk of the distribution lies and the location parameter a, which defines the location of the distribution in time. The mathematical formulas for the Weibull distribution are given below.

Probability density function (p.d.f.) of the Weibull distribution is given by

$$p.d.f = \alpha\beta^{-\alpha}(t-a)^{\alpha-1}\exp\left[-\left((t-a)/\beta\right)^{\alpha}\right] \tag{86}$$

$$P_t = \int_t^{t+1} f(x)dx \tag{87}$$

$$f(x) \Rightarrow p.d.f \tag{88}$$

The probability that a product has a life span of t years is given by

$$P_t = \exp\left[-\left((t-a)/\beta\right)^{\alpha}\right] - \exp\left[-\left((t+1-a)/\beta\right)^{\alpha}\right] \qquad a \le t < b \tag{89}$$

To determine the value of the parameters α and β the following equations can be used (Melo, 1999)

$$\gamma = 1 - \exp\left[-\left((b-a)/\beta\right)^{\alpha}\right] = 0.997 \tag{90}$$

$$\alpha \ln\left(\frac{b-a}{m-a}\right) + \ln\left(\frac{\alpha-1}{\alpha}\right) - \theta = 0 \tag{91}$$

where a is the minimum life span, b is the maximum life span and m is the most likely life span.

$$a + \beta\left(\frac{\alpha-1}{\alpha}\right)^{1/\alpha} = m \qquad \alpha \ge 1 \tag{92}$$

With the knowledge of parameters α and β, the mean and the variance of the distribution can be determined.

$$\mu = a + \frac{\beta}{\alpha}\Gamma\left(\frac{1}{\alpha}\right) \tag{93}$$

$$\sigma^2 = \frac{\beta^2}{\alpha}\left\{2\Gamma\left(\frac{2}{\alpha}\right) - \frac{1}{\alpha}\left[\Gamma\left(\frac{1}{\alpha}\right)\right]^2\right\} \tag{94}$$

with Γ(x) as the Gamma function

$$\Gamma = \int_0^{\infty} t^{x-1} e^{-t} dt \tag{95}$$

3.4.3 Evaluating the emission factors of processes

The emission factors for some processes are taken directly from the literature. For others, however, the emission factors have been evaluated in different manners. For example, the emission factor for producing catalytic converters (CC) is estimated using several parameters: the number of vehicles with CC, the average driving distance per vehicle, the emissions per km, and the platinum loading per CC. The platinum emission factor was estimated for three countries, and the average was used in the model.

3.4.4 Solving the differential equations

The differential equation given by Eq. 17 can be solved numerically by stepwise integration (Euler's method)

$$S(t+\Delta t) \approx S(t) + \frac{dS}{dt}\Delta t \tag{96}$$

$$S(t+\Delta t) \approx S(t) + [F^{in}(t) - F^{out}(t)] * \Delta t \tag{97}$$

By knowing the initial value of the stock at time t and the inflow, it is possible to calculate the stock as given by Eq. 98.

$$S_c(t+1) = S_C(t) + F_C^{in}(t) - F_C^{out}(t) \tag{98}$$

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