

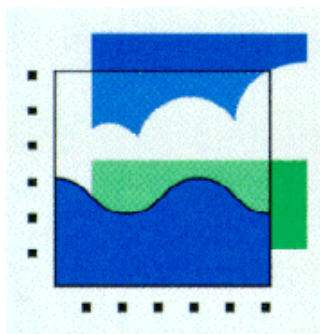
# **Dynabox: A dynamic multi-media fate model with applications to heavy metals**

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## II.5 Dynabox: A dynamic multi-media fate model with applications to heavy metals<sup>1</sup>

Reinout Heijungs

### II.5.1 Introduction

Many “integrated economic-environmental models” comprise a more or less sophisticated modelling of the economic subsystem, distinguishing various industries and households, describing import and export, and sometimes explicitly dealing with stock forming and time-lag in production and consumption (*e.g.*, Victor, 1972; Perrings, 1986). However, with respect to the environmental subsystem, these models almost always stop at the level of emissions, and do not explicitly address the subsequent pathways that pollutants traverse after they have left the economic subsystem. One reason is probably a misfit between the economy-wide character of most economic models, necessitating the lumping of pollutants with a subsequent loss of details, and the highly regionalised character of most environmental models, requiring very detailed information on nature and release pattern of pollutants. This chapter discusses the use of generic environmental models to make an assessment of potential hazards for men and the environment on the basis of moderately specific data, and can hence be seen as an attempt to bridge the gap.

A break-down of the mechanisms inside the environmental subsystem would require at least the following elements (*cf.* Van Leeuwen & Hermens, 1995):

- *exposure assessment*, *i.e.* the step from emission of pollutants to concentration in the environment or intake by or exposure of target organisms;
- *risk or damage assessment*, *i.e.* the step from concentration in the environment or intake by or exposure of target organisms to damage to the environment or target organisms;
- *value assessment*, *i.e.* the step from damage to the environment or target organisms to a judgement involving ethical considerations (like: birds are more important than worms).

This chapter is primarily devoted to the exposure assessment: it thus describes the *fate* of chemicals in the environment. Some aspects of the damage assessment are dealt with as well. The issue of value assessment is outside the scope of this chapter.

### II.5.2 Goal and scope of the model

This section starts with a concise overview of the risk assessment procedure and the idea behind the models that are used to support risk assessment of chemicals. The exposure assessment is the first topic of interest. The damage assessment is a second topic.

A chemical that enters the environment will in general not stay there. It will move to other compartments (*e.g.* from the atmosphere to the soil), it will disappear (*e.g.* by immobilisation in the sediment), and it will enter plants, animals and/or human beings (*e.g.* through drinking contaminated water). All these classes of transport phenomena may be described as environmental processes. A more systematic catalogue of environmental processes is the following:

- diffusive transport, through thermodynamic partitioning due to a chemical disequilibrium;
- advective transport, along with physical flows, such as river flows and rainfall;
- degradation, often by chemical reactions, but also by biological processes and photolysis;

<sup>1</sup> This paper is the concept version of a chapter of a book that is in the process of being published: E. van der Voet, J.B. Guinée and H.A. Udo de Haes (Eds.): *Heavy Metals: a Problem Solved? Methods and Models to Evaluate Policy Strategies for Heavy Metals*. 4th, Complete Draft 1-4-1999. Please contact the author for information on final publication details.

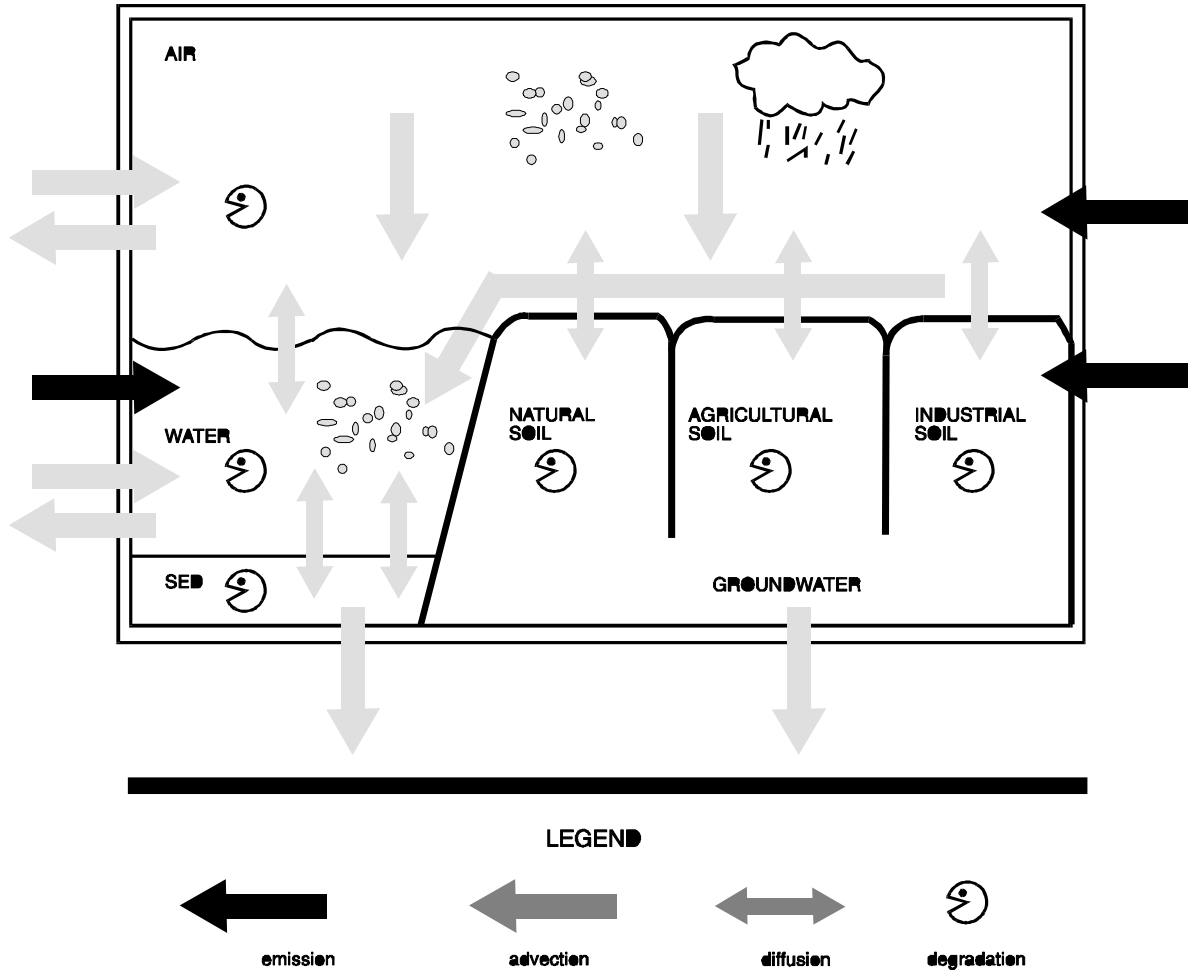
- immobilisation, for instance by burial in the deep sediment;
- intake, for instance through respiration, consumption of food and water, and through the skin.

The simultaneous taking-place of these environmental processes determines the fate of a chemical in the environment.

It will be clear that the fate of a chemical is extremely decisive in determining whether or not the chemical will exert a harmful influence on the environment, and, if so, on the magnitude of this influence. For instance, heavy metals have a much larger interaction with the lungs than with the digestive track. It is therefore of enormous interest to know to what extent a released heavy metal will reside in the air. Also, a substance like toluene is quite toxic but it has a short lifespan due to chemical instability on the other hand. There are many substances that are at least as toxic as heavy metals. One of the problems of heavy metals is that they share a relatively high toxic potential with an extremely long chemical stability. It is therefore essential to consider the fate of heavy metals in some detail.

The environmental processes that determine the fate of a chemical may of course be the subject of a modelling exercise. A widely recognised class of suchlike models is the multi-media fate model (see, *e.g.*, Cowan *et al.*, 1995). Multi-media fate models incorporate a number of environmental compartments (air, water, soil, groundwater, *etc.*) and describe the flows of a chemical between these compartments and the degradation within each compartment by means of mathematical equations for each environmental process. Figure II.5.1 illustrates what is involved in a multi-media model.

Figure II.5.1. Overview of a multi-media fate model with the compartments air, water, sediment and three types of soil, with an indication of the different transport and degradation processes.



The structure of these model equations is in general a system of linear differential equations, based on mass-balance conditions and first-order kinetics. Multi-media fate models assume that there is a homogeneous mixing within every compartment, so that there are no local concentration gradients. This is a bold assumption, but it is certainly one that facilitates the modelling step.

As an example, consider a two-compartment model comprising air and water (taken from Heijungs, 1995). It is assumed that there is degradation of the chemical in air, and that it is proportional to the amount that is present in air, the coefficient of proportionality being  $kdeg_{air}$ . Further, it is assumed that there is a direct emission of the chemical to air of magnitude  $EMIS_{air}$ . And the exchange between air and water is assumed to be proportional with the difference in concentration between the two compartments, the coefficient of proportionality being  $\lambda$ . For the aquatic compartment, a similar reasoning can be held. The system of differential equations that govern the fate in this simple 2-media model is thence:

$$\begin{aligned} \frac{d\bar{m}_{air}(t)}{dt} &= -kdeg_{air}V_{air}C_{air}(t) + EMIS_{air} + I(C_{water}(t) - C_{air}(t)) \\ \frac{d\bar{m}_{water}(t)}{dt} &= -kdeg_{water}V_{water}C_{water}(t) + EMIS_{water} + I(C_{air}(t) - C_{water}(t)) \end{aligned} \quad (1)$$

For reasons that we will discuss later in this chapter, multi-media fate models are almost exclusively used to calculate steady-state concentrations. In that case, the lefthandsides of the differential equations are put to zero, and the system of equations is solved for  $C_{\text{air}}$  and  $C_{\text{water}}$ . This can easily be done by matrix inversion.

A more realistic multi-media model includes several compartments and many environmental processes. The structure, however, is similar to the one outlined in the example. The incorporation of exposure routes from the concentrations in air, water, *etc.* is straightforward when data on respiration, consumption of drinking water and food are known.

Concentrations in environmental compartments and intake by human beings are already much more meaningful than plain emission flows. But still, there is a large difference between 1 mg/m<sup>3</sup> mercury in the air and 1 mg/m<sup>3</sup> copper in the air. To account for these differences in intrinsic toxicity or hazard, risk assessment procedures extend a damage assessment to the exposure assessment.

A popular approach is the so-called PEC/PNEC approach. The predicted environmental concentration (PEC) is the concentration that is the output of the multi-media fate model, so  $C_{\text{air}}$ ,  $C_{\text{water}}$ , *etc.* The predicted no-effect concentration (PNEC) is the concentration at which it is believed that no more than 5% of the species of an ecosystem is affected to some extent. The PNEC is often for policy purposes, like prioritising toxic substances. The ratio between PEC and PNEC is sometimes called the hazard index. It is a critical ratio in the sense that it should not exceed 1 in a safe world. But is often used to indicate potential unsafe situations. For instance, a hazard index below 0.1 is regarded as under control, while a higher index should instigate more detailed research.

Within the Metals programme, a dynamic multi-media fate model *Dynabox* has been developed and implemented in software. *Dynabox* is largely based on existing steady-state multi-media models, that are moreover primarily intended for application to organic compounds. Most existing multi-media fate models do not address the issue of dynamics. Our motivation to introduce dynamics is as follows. For most organic chemicals, the degradation time is in the order of days or perhaps a few years, so that transient phenomena are not particularly relevant. For inorganic substances, the degradation times are often much longer, and for chemicals like heavy metals, degradation is absent or negligible on human time scales, and immobilisation in deep soil or sediment is the main mechanism of removal. What then is the policy meaning of a steady-state concentration if it is only reached after 100,000 years? It may for some purposes be much more interesting to know the dynamics of the concentrations or the resulting risks. With the dynamics, we mean questions like: What is the concentration/risk after 100 years? and: When is a critical concentration/risk level surpassed?

One sometimes reads or hears remarks that modelling of dynamics is extremely more difficult than modelling of the steady state. The next section will discuss to which extent this is true. It describes the development of a dynamic model from an existing steady-state model. And it will apply the newly developed model to a small number of metals.

### II.5.3 Modelling principles and required data

A dynamic multi-media fate model has been developed on the basis of the steady-state model that is integrated in VROM (1994), which on its turn is based on Van de Meent (1991). This latter model, labelled *Simplebox*, also provided the inspiration for the name of the newly developed model:

*Dynabox*.<sup>1</sup> Below, the deviations from the original *Uses* model are described: the compartments, choice

<sup>1</sup> Meanwhile, a newer version of *Simplebox* has appeared (*Simplebox 2.0*: Brandes *et al.*, 1996), as has newer versions of *Uses* (*Uses 2.0*; Linders & Jager, 1997; *Euses 1.0*: EBC, 1997). These developments, however, came too late to be

of parameters for metals, the dynamics, the effect part, and some aspects of implementation. Readers interested in an overview of the basic principles of multi-media fate models are referred to Mackay (1991), Cowan et al. (1995) and to VROM (1994) for more information on *Uses*.

### *The compartments*

The *Uses* model comprises degradation in and transport between a number of compartments: air, surface water, soil, sediment, and so on. The newly developed model is extended to comprise the following compartments:

- the regional model: air, surface water, suspended matter, biota, sediment, natural soil, agricultural sand soil, agricultural peat soil, agricultural clay soil, pore water in sand soil, pore water in peat soil, pore water in clay soil, industrial soil, ground water;
- the continental model: air, surfacewater, suspended matter, biota, sediment, natural soil, agricultural soil, industrial soil, ground water;
- the sea model: air, seawater, suspended matter, biota, sediment;
- the outside world: deep soil, deep sediment.

The regional model is embedded in a larger system with which it may exchange substances through import and export. The concentrations at the continental and sea system are determined by the user. The outside compartments provide some ultimate sinks with which the regional system is not in steady state, but of which the concentrations are determined by equilibrium partitioning.

### *Adapting the model for metals*

Many parameters that find a place in the multi-media models are based on the intended use for organic degradable chemicals. This creates a barrier in the application of suchlike models for other substances, like metals. There are several reasons for this:

- Several models are able to estimate lacking parameters by means of other parameters or as a default, but only under certain restrictions which are often invalid for metals. In *Uses* 1.0, for instance, the default value for photodegradation in air is 160 days, and the estimation of bioconcentration factors provide values that are quite a bit off the empirical values.
- Certain models prevent the user for making certain mistakes by refusing to accept values that are improbable for organic substances. For instance, the degradation times should be at most 10,000 days (= 27 years) in *Uses* 1.0, which is quite unrealistic for metals.
- The calculation often involves parameters that are ill-defined for metals. For instance, the vapour pressure is essential in *Uses* 1.0, while it is undefined for metals.

The first point may be circumvented by putting more effort in data collection, so that estimation of missing parameters is not necessary. The second point could be solved by not implementing the restrictions on the domain of parameter values in *Dynabox*. The third point, however, is more difficult to avoid. One can try the effect of putting parameters to, say,  $10^{20}$  and checking if a value of  $10^{30}$  makes no significant difference. A useful reference in this context is Crommentuijn et al. (1997).

### *From steady-state model to dynamic model*

In general, multi-media-fate models calculate the steady-state concentrations of a pollutant in different compartments. As mentioned before, a policy-relevant application to metals requires a dynamic calculation. This subsection describes how such a dynamic model is obtained from a steady-state model.

#### a. The steady-state model

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incorporated into *Dynabox*. It is doubtful whether it would make much difference for the case of heavy metals, because *Euses* 1.0 is a refinement of *Uses* 1.0 that does not address the case of heavy metals and *Uses* 2.0 is mainly an improvement for pesticides.

We first describe the essentials of the steady-state model. This is done quite extensively, because the connection to a dynamic model would otherwise be unclear, and because most texts on multi-media models are less explicit in the mathematical structure of the general set-up.

The heart of the multi-media fate model is a differential equation that expresses a mass balance

$$\begin{aligned} \frac{dm_i(t)}{dt} = & \left( \frac{dm_i(t)}{dt} \right)_{\text{from other media}} - \left( \frac{dm_i(t)}{dt} \right)_{\text{to other media}} + \\ & \left( \frac{dm_i(t)}{dt} \right)_{\text{through emission and import}} - \left( \frac{dm_i(t)}{dt} \right)_{\text{through degradation and export}} \end{aligned} \quad (2)$$

condition for each considered medium (compartment), i.e. air, water, soil, ground water, sea, etc.): where  $m_i(t)$  denotes the mass of a the substance under study in compartment  $i$  at time  $t$ . Three of the four terms on the righthand side of the equality-sign are constructed according to the principles of first-order kinetics:

$$\left( \frac{dm_i(t)}{dt} \right)_{\text{from other media}} = \sum_j (ADV_{ij} + DIFF_{ij}) \times C_j(t) \quad (3)$$

$$\left( \frac{dm_i(t)}{dt} \right)_{\text{to other media}} = \left( \sum_j (ADV_{ji} + DIFF_{ji}) \right) \times C_i(t) \quad (4)$$

$$\left( \frac{dm_i(t)}{dt} \right)_{\text{through degradation and export}} = (V_i \times kdeg_i + (ADV_{\text{outside},i} + DIFF_{\text{outside},i})) \times C_i(t) \quad (5)$$

while the fourth one contains two direct source terms:

$$\left( \frac{dm_i(t)}{dt} \right)_{\text{through emission and import}} = EMIS_i(t) + IMPORT_i(t) \quad (6)$$

In these equations,  $ADV_{ji}$  denotes a coefficient for advective transport from compartment  $j$  to compartment  $i$ ,  $DIFF_{ji}$  a similar one for diffusive transport,  $kdeg_i$  a degradation coefficient for compartment  $i$ ,  $V_i$  the volume of compartment  $i$ ,  $EMIS_i(t)$  the direct emission flow into compartment  $i$  at time  $t$ ,  $IMPORT_i(t)$  the transboundary flow into compartment  $i$  at time  $t$ , and  $C_i(t)$  the concentration in compartment  $i$  at time  $t$ . Furthermore, concentration and mass are related by the volume  $V_i$  of the

compartment by definition:  $C_i = \frac{m_i}{V_i}$ . Observe that the coefficients for advective and diffusive

transport and for degradation are time-independent (hence the qualification “quasi-dynamic” in Brandes et al., 1996), and that there are besides the masses (or equivalently: concentrations) other quantities that may be varying with time: the emission flow and the import flow due to concentrations in the outside world.

The general model structure is hence of the form



$$\frac{d\mathbf{m}(t)}{dt} = \mathbf{L} \bullet \mathbf{m}(t) + \mathbf{f}(t) \quad (7)$$

where  $\mathbf{m}(t)$  is a column-vector of all  $m_i(t)$  and  $\mathbf{f}(t)$  a column-vector of emissions and imports:

$$\mathbf{m}(t) = \begin{pmatrix} m_1(t) \\ \dots \\ m_i(t) \\ \dots \end{pmatrix}; \quad \mathbf{f}(t) = \begin{pmatrix} EMIS_1(t) + IMPORT_1(t) \\ \dots \\ EMIS_i(t) + IMPORT_i(t) \\ \dots \end{pmatrix} \quad (8)$$

Furthermore,  $\mathbf{L}$  is a vector of coefficients that determine the fate of the chemical (hence the term fate matrix in Heijungs (1997)):

$$\mathbf{L} = \begin{pmatrix} l_{11} & \dots & l_{1j} & \dots \\ \dots & \dots & \dots & \dots \\ l_{i1} & \dots & l_{ij} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \quad (9)$$

while for an arbitrary element of  $\mathbf{L}$  we have

$$l_{ij} = \begin{cases} \frac{ADV_{ij} + DIFF_{ij}}{V_i} & (i \neq j) \\ \frac{ADV_{ij} + DIFF_{ij}}{V_j} - \sum_j \frac{ADV_{ji} + DIFF_{ji}}{V_j} - kdeg_i + \frac{ADV_{outside, i} + DIFF_{outside, i}}{V_i} & (i = j) \end{cases} \quad (10)$$

The differential equation (7) is in most multi-media fate models taken as a starting point, but with the addition that a steady-state situation is assumed:

$$\frac{d\mathbf{m}(t)}{dt} = \mathbf{0} \quad (11)$$

so that the time index  $t$  then refers to the situation after an infinitely long transition time, while the emission flow is taken to be time-independent:

$$\mathbf{f}(t) = \mathbf{f} \quad (12)$$

The result is a simple matrix equation:

$$\mathbf{0} = \mathbf{L} \bullet \mathbf{m}(\infty) + \mathbf{f} \quad (13)$$

which is easily solved by matrix inversion:

$$\mathbf{m}(\infty) = -\mathbf{L}^{-1} \bullet \mathbf{f} \quad (14)$$

This procedure corresponds to those of *Simplebox* 1.0 (van de Meent, 1991 (p.50-51)), *Simplebox* 2.0 (Brandes et al., 1996 (p.118-119), and, more implicitly, of Mackay (1991, p.177) and *Uses* 1.0 (VROM, 1994 (p.160)). It should be stressed that (14) only makes sense when  $\mathbf{L}$  is invertible. Although this condition is not discussed in the above references, it is not a trivial one; see the appendix of Heijungs (1995).

#### b. The dynamic model

If we wish to deviate from this normal practice of describing a steady state and seek to describe a dynamic concentration pattern, we need to solve the differential equation (7), either numerically or

analytically (cf. Mackay, 1991 (p.183-184), Van de Meent, 1991 (p.57-58) and Brandes et al., 1996 (p.123-125)).

Let us first consider the numerical approach. Simple stepwise integration (Euler's method<sup>1</sup>) yields

$$\mathbf{m}(t + \Delta t) \approx \mathbf{m}(t) + \frac{d\mathbf{m}(t)}{dt} \times \Delta t \quad (15)$$

By taking  $\Delta t$  sufficiently small, we will be able to approximate the time series  $m(t)$ ,  $m(t+\Delta t)$ ,  $m(t+2\Delta t)$ ,  $m(t+3\Delta t)$ , ... with a reasonable accuracy. The operational formula is then simply

$$\mathbf{m}(t + \Delta t) \approx \mathbf{m}(t) + (\mathbf{L} \bullet \mathbf{m}(t) + \mathbf{f}(t)) \times \Delta t \quad (16)$$

By comparison with the steady-state calculation (equation (14)), we see that there is, besides the more or less arbitrary integration stepsize  $\Delta t$ , one additional data requirement:  $m(t)$ , i.e. the amounts (or concentrations) of pollutant in the starting year. Environmental agencies or statistical bureaus often possess these background data for some initial year, usually a few years earlier, like 1990 or 1995.

Another important direction is that of leaving the field of numerical approximation, and trying to find analytical solutions of the differential equation (7). It is not difficult to derive a general solution in which  $\Delta t$  may assume any value, so also non-infinitesimal small values:

$$\mathbf{m}(t + \Delta t) = e^{(t+\Delta t)\mathbf{L}} \bullet \left( \mathbf{m}(t) + \int_t^{t+\Delta t} e^{-s\mathbf{L}} \bullet \mathbf{f}(s) ds \right) \quad (17)$$

This expression, however, is difficult to work with in practice for two reasons: it contains an integral that needs to be computed for the specific emission pattern  $\mathbf{f}(t)$ , and it contains an exponent with a matrix. If we simplify the problem to the extent that a constant emission flow is assumed, we are able to solve the integral and obtain

$$\mathbf{m}(t + \Delta t) = e^{(t+\Delta t)\mathbf{L}} \bullet (\mathbf{m}(t) + \mathbf{L}^{-1} \bullet \mathbf{f}) - \mathbf{L}^{-1} \bullet \mathbf{f} \quad (18)$$

but are still left with a matrix in the exponent. Although possibilities exist to deal with this (see, e.g., Apostol, 1969 (p.201 ff.) and Brandes et al., 1996 (p.124-125)), the mathematics indeed gets rather involved (cf. Mackay, 1991 (p.184)), and it will do so even more when the assumption of constant emission flows is dropped. The current version of *Dynabox* is based on Equation (13).

Summarising the differences between steady-state and dynamic models for different classes of people:

- the *user* needs to specify one additional data item: the amounts or concentrations of pollutant in the different environmental compartments (air, water, etc.);
- the *user* will be confronted with a problem of interpretation: instead of one result, a whole time series of results will be obtained;
- the *modeller* that constructs the multi-media fate model sees no difference: it is his or her task to specify the matrix  $\mathbf{L}$ , and that matrix is the same for both types of model;
- the *software engineer* needs to design appropriate routines for numerically integrating systems of differential equation, or to go into the theory of exponents with matrices.

### *The effect part*

<sup>1</sup> Of course, we may also deal with the topic in a more sophisticated way. Euler's method of integration may be replaced by more accurate methods, like those of Runge-Kutta, and with a possible adaptive stepsize  $\Delta t$  (see, e.g., Press et al., 1982). This is, however, beyond the scope of the present chapter.

As stated in the Introduction, this chapter and *Dynabox* primarily describe the exposure assessment. However, in order to give an indication of damage, an effect module (cf. Jager & Visser, 1994) has been added. It is based on the “PEC/PNEC” approach, where “PEC” stands for the predicted environmental concentration, and “PNEC” denotes the predicted no-effect concentration. For humans, the ratio of the predicted daily intake and the acceptable daily intake (PDI/ADI) is used. These ratios are also referred to as the hazard quotient (and their reciprocal value as the margin of safety). In theory, a hazard quotient below 1 is an indicator for a safe situation, while a value larger than 1 indicates a hazardous situation. The real interpretation is obviously different, for instance, since a value below 1 does not necessarily indicate a safe situation due to uncertainties in substance parameters, environmental parameters, model assumption, and so on. The hazard quotient must therefore be regarded as an indicator that is the outcome of a screening tool.

Despite these words of caution, the results in Parts III and IV are simply based on the PEC/PNEC, without sensitivity analysis, and without further study in a more detailed risk analysis. As a justification for this we might say that the entire programme was of an explorative nature, and that all results provide mere indicative trends and no hard facts. The model calculates PEC/PNEC values for aquatic and terrestrial ecosystems, as well as PDI/ADI values for human beings. Different types of PNEC for ecosystems can be introduced, such as the reference value, the limit value and the maximum permissible concentration.

#### *Implementation in software*

The model has been implemented in a software code. The source code was written in Turbo Pascal. An executable code runs on MS-DOS, and is freely available.<sup>1</sup> For reasons of comparison with the original *Uses* 1.0, an option has been incorporated, which allows the user to investigate the differences in modelling results between the original and modified multimedia fate model. A further feature that deserves to be mentioned is an option that enables the user to choose between steady-state computation (Mackay’s level III) and a dynamic computation (level IV).

### **II.5.4 Results and interpretation**

Results of the model for real-world situations on cadmium, copper, lead and zinc can be found in Parts III and IV and in Guinée et al. (**in press; of wellicht al verschenen?**). Comparison with the *Uses* model yields a large difference for the steady-state values, mainly due to *Uses*’ limitation of the degradation time to 27 years. With this value, *Dynabox* computes results that are quite similar to that of *Uses*. The differentiation of agricultural soil into sand, peat and clay does not affect the overall picture. However, it introduces differences in soil concentrations of a factor up to 10. The results for soil are in reasonable agreement with those of Moolenaar (1998). A more complete discussion of the results of *Dynabox* is in preparation (Heijungs et al., in prep.).

### **II.5.5 Links to other models**

*Dynabox* needs emission flows as an input. The emission data are entered through a menu. Emission data may, however, also be read from an external file, for instance, produced by a model of the economic subsystem. A link with Flux **refrefref** is thus easy to realise. But also connections with the national statistics (input-output tables, emission inventories, etc.) are in principle possible.

The model gives concentrations in environmental media (air, surface water, etc.) and intake of humans as an output, or PEC/PNEC-like hazard quotients. Concentrations/intakes may be calculated as a

<sup>1</sup> Contact the web-site <http://www.leidenuniv.nl/etcetcetc>.

steady-state value, at any moment in time, or the whole time series may be exported. Any of these forms of output may become the input of valuation models. This aspect has, however, not been studied.

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