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Original Research

Modeling of Behavior of Organic Pollutants in Aquatic and Related Ecosystems

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Abstract

Approaches related to modeling chemical compound migrations in the environment are discussed. Models related to both closed and open systems in steady-state or non steady-state conditions are characterized. Methods of building the models and the review of the most important types of models with adequate examples, as well as the results possible to achieve using these groups of models are presented. The review also contains the division of models with respect to the way of presenting chemical transport, the complication level and the range of modeled area. Risk evaluation, abiotic and biotic approaches are discussed as well. Special attention was put on the complexity of abiotic models based on the fugacity concept.

Keywords: environmental fate modeling, environmental pollutants, transport, types of models, xenobiotics migration

Introduction

Mathematical models are widely used in many aspects of life. The careful monitoring and modeling of natural systems has turned out to be one of the most useful tools not only for assessment of the real state of the human environment but also for taking political decisions, often with global impact. However, environmental data include high variability due to various influences like geographical location of the monitoring sites, dynamic conditions in the atmosphere and hydrosphere, geological limitations, and many anthropogenic pollution sources. Usually, the output of the monitoring process is a large table with numbers indicating concentration levels at the sampling sites involved. Very often it is still generally accepted that satisfactory information could be extracted if the monitoring results are simply compared to allowable threshold values officially introduced by decision-making institutions. No need to say that this is an outdated approach. The monitoring data obtained should be considered in their entirety. Since manual consideration of a large data set is practically impossible, the only reasonable method of data mining is modeling and/or application of environmetric techniques. Simplification and approximation desirable by modeling are based on the following principle: a model has to imitate the real world, but it should focus on the specific aspects that are considered significant, and reject those that are not significant [1]. A mathematical model can adequately describe the environment and the processes undergoing in it. Models are created because of a number of reasons, i.e. in order to understand the environmental processes, or to determine qualitative and quantitative migration (in more than one medium or phase) and behavior of chemical compounds in the environment [2]. Models are also formulated to make pre-

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dictions in time about the compartment-specific concentration of a selected chemical compound whose given amount (i.e. known or assumed, and equivalent to pollutant load) is being released into the environment [3, 4]. The main purpose of migration models is to establish where (i.e. in the air, seawater, sediment, fish, etc.) and in what proportions the chemical compounds will end up in the environment [5]. Because of potentially serious hazards related to the presence of many chemical compounds in the environment, especially persistent organic pollutants (POPs), migration models are still a subject of active research [6-10]. By using a proper model one can predict, for example, lindane concentration in fatty tissue of the human living in a given coastal area and consuming a specified number of fish. These fish are caught at sea into which a known amount of lindane has been discharged via dry and wet deposition, direct spill, river runoff and leaching from the fields. By using the model, it can be calculated to what level the lindane load discharged into the environment should be reduced in order to decrease the chemical's concentration to a specified level in the waters of a given sea, or even in a human body.

Modeling of Environmental Processes to which Pollutants are Subjected

Environmental migration models for chemical compounds are constructed in order to obtain qualitative and quantitative determination of dispersion or spreading (in more than one medium or phase) and behavior of chemicals in the environment. By means of proper modeling, the environmental migration and behavior of specific chemical compounds can be studied which, in turn, allows us to address the question about the fate of pollutants in the environment. The behavior and spread of a chemical compound depends on the compound's molecular structure, the method of introducting it to the environment, and also on the characteristics of the environment into which it is being released [11]. Models serve as a tool for integrating information about multifaceted processes of transport and chemical transformations, and allow presenting the behavior and migration of a chemical compound in the environment in an understandable and clear way [12].

In this part general notions related to modeling chemical compound migration in the environment are presented. A particular emphasis has been placed on abiotic migration models based on the fugacity concept.

Fate Model Types

Environmental compartments in migration models can be presented as a sparsely populated set of phases (i.e. atmosphere, surface water, underground water, soil, etc.), each phase being homogenous, well mixed and constant in time. A phase is defined as a section of the environment characterized by the uniform chemical compound concentration and homogenous properties (i.e. section of atmosphere including clouds and suspended substances, sea water, surface water, underground water, soil-containing water and air, etc.). If the given description does not sufficiently reflect reality, the model has to be extended by increasing the number of phases, adding heterogeneity in one, two or three dimensions, or introducing temporal variability. It is important to critically evaluate each variant of model complexity, and to apply it only when necessary. As a result of each model extension, more mathematical complexities are introduced, and therefore it becomes necessary to increase the number of parameters.

Table 1. Classification of fate models in reference to the flow of a chemical compound through specific environmental compartments and the possibility of changing conditions in the modeled environment in time.

Fate model type	Model description
Closed system, steady-state conditions	The simplest model type. No input or outflow of chemical occurs within the modeled environment. Mass balance equation describes the partitioning of a given amount of chemical compound among the different phases of a defined control volume. The total amount of chemical compound present in the control volume is equal to the sum of amounts in each phase usually, each separate amount is a product of concentration and compartment-specific partial volumes. Mass balance is an algebraic equation.
Open system, steady-state conditions	Models are extended by adding the "in" and "out" flow components of chemical in the modeled environment, and also the possibility of chemical formation and entering into chemical reactions. However, the conditions in the studied environment do not change in time. The intensities of flow_{in} and flow_{out} for a chemical are equal. Flow intensity is expressed in moles or grams per unit time, while for the open system, the basic unit is mol or ram. Mass balance is a simple algebraic equation.
Open system, non steady-state conditions	Mass balance equation in this case is a differential equation: $\text{d(amount)/dt} = \text{total intensity of flow}_{\text{in}} - \text{total intensity of flow}_{\text{out}}$ The intensities of flow_{in} and flow_{out} are expressed as amount/time, e.g. mol/h or g/h. The equation can be solved under the proper initial or boundary conditions, giving algebraic expression for the concentration as a function of time.

* "Control volume" is a part of the environment delineated by borders within which all transport processes and the total amount of the chemical compound present under the initial conditions, as well as all processes during which a given compound is involved, have been defined [12].

Considering the flow of a chemical compound through specific environmental compartments and the possibility of changing conditions in the modeled environment in time, the fate models can be divided into three main types as described in Table 1 [11].

Processes to which Chemical Compounds are Subjected in the Environment

In order to develop a model, the properties of chosen chemical compound and selected section of the environment have to be investigated; the properties should be analyzed in relation to the expected processes of transport and transformation. Therefore, modeling entails the integration of different processes, to which a specific chemical compound is subjected, into a larger and more complex model structure. Such a structure is presented as mass balance which had been related to the selected environmental compartment.

As Wania and Mackay have suggested [2], the processes analyzed in the model can be divided into four main groups:

1. Identification and classification of ways in which a given compound is introduced into the environment. For example, thinking about emissions, it is possible to identify a discharge of pollutants into the air, inflow of pollutants into the sea or river, leaching from agricultural areas, etc. In the case of modeling migration processes in atmosphere-soil or atmosphere-surface waters systems, introduction in the form of dry and wet deposition can be understood as well as emission.
2. Identification of transport processes (ways in which a given compound is transferred within the environment). Transport processes can be divided into two main groups:
   - diffusion processes; a chemical compound moves in the air or water from the site of higher compound concentration to that of lower concentration. The following processes belong to this group:
     - evaporation of a chemical compound from water into the air, and the opposite process, e.g. condensation,
     - sorption from water onto the suspended matter in the water column, and the opposite process of desorption; absorption of a chemical compound by fish and other live organisms via diffusion in gills and the chemical pathway of oxygen,
     - sorption from atmosphere onto aerosol particles, and the opposite process of desorption,
     - sorption of a chemical compound from water into the benthic sediment, and the opposite process of desorption,
     - diffusion from soil into the air,
     - transport of a chemical compound through the membranes of live organisms, e.g. from the air via lungs into the blood stream, or from the content of intestines via intestinal wall, or from the blood to different internal organs of the body [13].
   - processes related to the flow of medium in which a given chemical compound is present (e.g. air, water, biological material, etc.). The transfer of the chemical compound occurs due to reasons not connected to its presence in the transporting medium. The examples of such processes are: deposition of the chemical compound in rain water or dust, sedimentation of a chemical compound bound to suspended matter from the water column, or the re-suspension processes.
3. Partitioning processes among the phases which determine the amount of a given compound that will be present in various phases, e.g. partitioning between water and air, or between water and fish, etc.
4. Chemical transformation processes which define whether or not and to what degree the studied compound is formed as a result of the reaction. Moreover, they determine the compound's degradation time for a given environmental compartment. The examples of transformation processes are: photolysis, hydrolysis and oxidation.

The level of complexity related to environmental modeling according to processes to which chemical compounds are subjected in the environment can be schematically demonstrated taking consideration of both migration pathways and a chemical's fates in environmental compartments [8, 14] (Fig. 1).

Model Development

The process of model development can be described in the form of seven major steps, presented in Fig. 2.

Defining Modeled Area

The part of the environment studied within the concept of the model is called the modeled area. The modeled area description comprises the definition of its borders, i.e. physical borders that separate it from its surroundings and a description of the existing relations inside the area, as well as the relationships that characterize interactions with the surrounding area outside the borders of the modeled area [1]. The definition of the modeled area must contain temporal and spatial components, and the choice and characterization of the processes underway in the system.

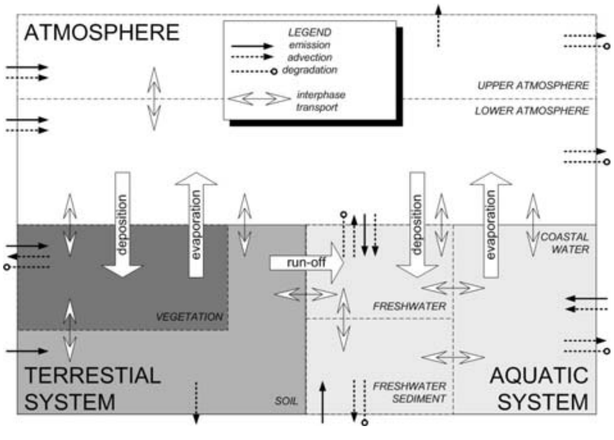

Fig. 1. Migration pathways and transformation possibilities in environmental compartments.

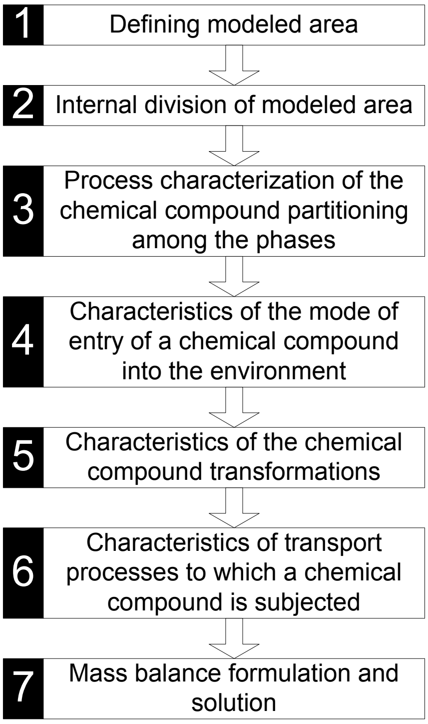

Fig. 2. Migration models development procedure.

Internal Division of Modeled Area

The division may coincide with the phase boundaries or cross over inside the phase. Internal division of modeled area results in subsystem formation. Subsystem boundaries should be chosen so that the conditions within the entire subsystem volume are in equilibrium, i.e. the chemical compound concentration is uniform in the entire volume. When the mass transport across the phase boundaries (e.g. between soil and air) is very fast we can assume that both phases constitute one subsystem, and therefore one mass balance equation can be formulated for the two phases. For the slowly reached equilibrium, a division into two subsystems along the phase boundary should be introduced. When the phase is well mixed and the concentration gradient does not occur in various locations then the phase boundaries should be treated as subsystem boundaries. Sometimes the division into subsystems should be applied inside one phase. Such a situation takes place in the case of an insufficiently mixed phase which displays, for example, vertical or horizontal stratification, and temperature and/or concentration gradient (e.g. thermocline in lakes, halocline in seas and atmospheric inversion).

Process Characterization of Chemical Compound Partitioning Among the Phases

At this stage of model development the following issue should be addressed: for a given concentration of the studied compound in one phase, what will be the compound's concentration in another phase that has remained in contact with the first one for the time period sufficient for reaching equilibrium. To this end, the behavior of chemical compounds under laboratory conditions, at controlled temperature and in the presence of constant pure phases has to be analyzed. Next, data on partitioning among phases should be transformed into environmental conditions that are defined in a more complex and less precise way, and under which phases have variable composition and properties [11].

Characteristics of the Mode of Entry of a Chemical Compound into the Environment

The amount of the compound and the way in which it is emitted into the environment should be determined. This means that the set of answers for exemplary questions should be known: Is a particular compound discharged directly into water or atmosphere? Does the production approximate the emission, as is the case for the majority of pesticides? Does emission equal the production minus appropriate coefficient, as for the hydrocarbons or PCBs?

Characteristics of Chemical Compound Transformations

Chemical transformations are the processes which change the molecular structure of substances. It should be established which reactions result in the formation of the analyzed compound, what the resulting amount is, and how long it takes. Moreover, the degradation time and the amount of the degraded compound should be determined for a given environmental compartment.

Characteristics of Transport Processes to which a Chemical Compound is Subjected

It should be determined how fast the analyzed compound will migrate from one phase to another. To this end, it should be established how and with what rate the studied chemical compound undergoes transport processes.

Mass Balance Formulation and Solution

In order to formulate mass balance equations, one or several separated, specific subsystems that are called "control volumes" should be isolated [15]. Control volumes are interconnected via internal transport processes [11]. For each control volume, mass flow among the control volumes and the surroundings outside the borders of modeled area as well as between the pairs of adjacent control volumes has to be determined. The boundaries of control volume can be delimitated, for example, by the atmospheric layer above the analyzed area, marine sediments in the entire sea at a given depth, or natural boundaries of a water body such as lake, i.e. water level and bottom profile. Control volume should be preferably entirely homogenous, which means that the concentration of a given chemical compound should be nearly uniform throughout the volume. In the case of insufficient vertical circulation, temperature, chemical compound concentration and other parameters related to water in a lake or sea may have varying values at different depths and for various water bodies. The differences might be large enough to require that the lake or sea is divided into n levels, which will result in n separated control volumes, or several separated water bodies [11].

There are many ways to divide a modeled area and to delineate control volumes. Depending on the requirements, the most suitable boundaries should be chosen; the internal interactions within the modeled area (i.e. between different control volumes) and interaction between the modeled area and its surroundings should also be defined. However, the model ought to be as simple as possible. Each added level of complexity requires a higher number of equations and the determination of larger number of parameters. Depending on how the modeled area has been defined, various boundary conditions are required, and different processes undergoing inside the control volumes have to be included. The examples of boundary conditions are: flow of pollutants across the interface (e.g. interface between the atmosphere and lake), or pollutant concentration in riverine discharge, or pollutant concentration in a parcel of air moving over a certain area of the lake [15].

The next step in defining control volumes is the formulation of mass balances for each such volume and chemical compound; in each case, the resulting mass of chemical compound equals the sum of all incoming mass minus the sum of all outgoing mass [15]. When the mass change (M) is constant over time, the mass balance can be described by the following formula:

$$\Delta M = \Delta M_{\text{transport}} + \Delta M_{\text{chemical reactions}} = \\ = (M_{\text{in}} - M_{\text{out}}) + (M_{\text{formation}} - M_{\text{degradation}}) \qquad (1)$$

where:

- ΔM is a change in chemical compound in a control volume over a given time;
- M_{in} is the mass of chemical compound flowing into control volume from outside;
- M_{out} is the mass of chemical compound outflowing from control volume;
- $M_{\text{formation}}$ is the mass of chemical compound that is formed inside control volume;
- $M_{\text{degradation}}$ is the mass of chemical compound that undergoes chemical transformations [1].

When the chemical compound mass change inside control volume varies with time, the following differential equation can be used:

$$dM_i/dt = I_i - O_i + P_i - R_i \qquad (2)$$

where:

- M_i is the mass of chemical compound "i" in control volume;
- I_i, O_i, P_i, and R_i are, respectively, the sum of the rates of inflow, outflow and internal formation of mass as well as internal degradation processes of the chemical "i" in control volume [1].

If the amount of chemical compound present in the control volume remains constant in time, the left and right sides of equations (1) and (2) equal 0. Such conditions are an example of the steady-state system. The assumptions of the steady-state system often simplify the analysis of the problem. The steady-state conditions should not be assumed if system conditions change significantly in time. Then the mass balance equation for the system varying in time should be applied [16]. When one condition is unknown for a given mass balance, control volume can be used to calculate this unknown, e.g. to calculate the transported or involved in chemical reactions amounts of pollutant that are difficult to measure physically [16].

Basic Notions used in Migration Models Based on the Fugacity Concept

Fugacity f

The behavior and migration of chemical compounds in the environment can be described in different ways. It has been proven that the approach based on the fugacity concept is convenient in application. The migration of a chemical compound into environmental compartments and its concentration in specific media result from the compound's fugacity and emission values, compartment-specific partition coefficients and the properties of the environment. By using fugacity, the behavior of organic pollutants in the environment can be described particularly well. As a result, the simplified equations with regard to partitioning of a chemical compound among the phases, transport and chemical transformations as well as the development of a coherent model are obtained [15, 17]. Therefore models based on the fugacity concept are the dominant type of environmental migration models.

Fugacity is a thermodynamic term connected to chemical potential; it characterizes the tendency of a chemical compound for migrating from a given phase [11]. Fugacity is expressed in units of pressure and is used as an equilibrium criterion, e.g. environmental phases which are in the equilibrium as regards composition have equal fugacity values, but not necessarily equal concentrations. Systems tend to equalize the fugacities, i.e. molecules diffuse from the phase of high fugacity to that of low fugacity [15].

Z Value

Many variables involved in a various model's equations can be expressed in terms of capacity by multiplication of a particular variable by specific factor or coefficient called "proportionality constant value." For example, temperature may be related to the amount of heat per unit volume ($\text{cal}\cdot\text{m}^{-3}$) via a constant which results in the term called heat capacity ($\text{cal}\cdot\text{m}^{-3}\cdot[°\text{C}]^{-1}$). Similarly, fugacity can be connected to concentration by means of a similar constant, e.g. Z value, called fugacity capacity and expressed in $\text{mol}\cdot\text{m}^{3}\cdot\text{atm}^{-1}$. The relationship can be described by equation [18]:

$$C=Z\cdot f \qquad (3)$$

Z value depends on temperature, pressure and physicochemical properties of a given chemical compound and the medium in which this compound is present. At high dilution, a relation between fugacity and concentration is usually linear. Z value describes in a quantitative way a chemical compound's volatility or escaping tendency from an investigated medium.

For a given fugacity and small Z value, the concentration is low and therefore only a small amount of the chemical compound influences its propensity for migrating from a given phase. Concentration of the chemical compound will be higher where Z value is higher [18]. Chemical compounds tend to accumulate in phases with high Z values. High concentration of the chemical compound can also be achieved when fugacity is not large. In summary, if Z values for a chemical compound can be determined for each modeled phase in the environment then it is also possible to calculate how the chemical will partition among phases. The methods of Z value calculation for the chemical compounds present in various phases are summarized in Table 2.

Table 2. Characterization of major types of phases and adequate Z value equations.

Phase	**Z value equation**
Pure chemical substance (in solid or liquid phase) [18]	$Z= 1(P^{S}v)^{-1}$ (4) where: P^{S} – chemical's partial pressure v - molar volume of particular chemical compound ($m^3 \cdot gmol^{-1}$)
Gaseous phase (e.g. atmosphere)	in general, fugacity equals the partial pressure of gas (P) therefore by using the ideal gas law the following relationship can be obtained: $Z= C\cdot f^{1} = 1\cdot R^{-1}T^{-1}$ (5) In gaseous phase Z is not dependent on physicochemical properties of the chemical compound, and it usually equals about 40 $gmol\cdot m^3\cdot atm^{-1}$ [18]
Liquid phase (i.e. aquatic ecosysystems: sea water, river water, underground water, etc.)	fugacity is usually connected to concentration by means of the Henry's Law constant (H): $P=H\cdot C$ (6) Therefore Z value equals: $Z=l\cdot H^{-1}$ (7) The Henry's Law constant can be calculated from the ratio of vapor pressure of pure substance to solubility [18].
Sorptive phases	if a sorption coefficient Kp expresses the ratio of the compound concentration in sorbent to its concentration in water (in $g\cdot m^{-3}$ or ppm), and the concentration of adsorbed substance equals S (in $g\cdot m^{-3}$) [18] then: $Z\ 10^{-6}K_p\cdot S\cdot H^{-1}$ (8)
Biota (plant and animal life in the environment will be called biota in further part of this work)	Fat content in a given biota equals B (volume fraction). It has been assumed that parameter B also expresses the octanol content in a given biota. Z value for a biota (ZB) equals: $Z_B= B\cdot Z_O$ (9) hence: $Z_O= K_{ow}\cdot Z_w$ (10) where $Z_w= 1\cdot H^{-1}$ (11) hence: $Z_O\ K_{ow}\cdot H^{-1}$ (12) and $Z_B= BK_{ow}\cdot H^{-1}$ (13) where: K_{ow} is octanol-water partition coefficient [18].

D value

In equations describing the environmental behavior of chemical compounds the product of flow intensity of medium, in which the chemical is present, and Z value (G·Z) is used very often. Because of this the product G·Z has been substituted by D value:

$$G\cdot Z=D \tag{14}$$

For example, two environmental subsystems can be considered, e.g. phase 1 and phase 2. If the volumes of the two phases are V_1 and V_2, respectively, and chemical compound concentrations in the two phases are C_1 and C_2, then the respective fugacity values will be $f_1=C_1\cdot Z_1^{-1}$ and $f_2=C_2\cdot Z_2^{-1}$. The transfer intensity of chemical compound between phases can be described by the following equation:

$$N=D_{12}\cdot(f_1-f_2) \tag{15}$$

D value is expressed in $mol\cdot hPa^{-1}$ and depends on factors such as the interfacial area between phases and diffusion rate. Evaporation can be used here as an example:

$$D=K_{OG}\cdot a\cdot R^{-1}T^{-1} \tag{16}$$

...where K_{OG} stands for total mass transfer coefficient ($m\cdot year^{-1}$) and "a" is interface area (m^2) [18]. Processes that proceed with high rates have high D values [11].

Classification and Examples of Environmental Migration Models for Chemical Compounds

Risk Evaluation Models

Emission of chemical compounds into the environment may incur damage to the environment and human health. Therefore it is necessary to evaluate and control the potential risk for humans and the environment with regard to the use of some chemical compounds, in particular to those who are about to be introduced to the environment for the first time. For example, *EUSES* program (*The European Union System for the Evaluation of Substances*) can be used for risk assessment [19]. *EUSES*, available at http://ecb.jrc.it/euses/ (software and documentation free of charge) has been used to evaluate the risk to humans and the environment associated with the introduction of novel substances into the environment and further use of the chemical compounds that are already present in the environment. It is a valuable tool used in preparation of the above-mentioned risk assessments and decision-making process by various scientific and administrative institutions, and the decision makers in the field of environmental protection. Models can supplement or substitute the environmental monitoring data and play an important role during the environmental impact assessment prior to the introduction of novel chemical compounds [11]. In many cases hazards for living organism health (including humans) or environmental damage could be limited if toxicity, persistence or bioaccumulation properties are assessed before chemical compound fabrication, application and introduction to environmental components. For example, bioaccumulation can be estimated by calculating the bioconcentration factor at equilibrium, which is a product of the fatty tissue content in a given organism and octanol-water partition coefficient.

More detailed calculations in relation to bioavailability, metabolism and bioconcentration can be performed by using *Fish* and *Foodweb* models [11] (both available at http://www.trentu.ca/academic/aminss/envmodel/models/ free of charge). Persistence in the environment can be calculated by means of *Level III* model [20] or an even simpler *Level II* model [21] (also available at http://www.trentu.ca/academic/aminss/envmodel/models/). *Level II* is a steady-state model, constant over time, and based on the fugacity concept and mass balance. It is a multiphase model comprising four environmental compartments, i.e. water, atmosphere, soil and sediment. *Level III* represents the real environment better because it includes transport processes between various compartments, constant over time, and based on the fugacity concept and mass balance. *Level III* model contains the same four environmental compartments as those in *Level II* model [22]. The equilibrium state inside each compartment has been assumed, but such an assumption has not been made for between the compartments. Transport processes of chemical compounds among and within environmental compartments, and degradation processes in the model are expressed by means of transport equations. The critical input data are environmental parameters, physicochemical properties and half-life time values of chemical compounds, and emissions of chemicals into the environment [21]. The concentrations of chemical compounds in specific environmental compartments, interface transport rate, transfer intensity based on medium flow, degradation rate and a chemical's persistence in the environment can be calculated from the model.

Migration Potential of a Chemical Compound

A significant issue to be considered when introducing novel substances into the environment is their propensity for long-distance transfer [23, 24]. Similarly to persistence, the chemical's propensity for long distance transfer in the environment cannot be measured, but it can be estimated with the help of a model. Transfer with air masses constitutes a very large share of long distance transport of chemical compounds. Oceans and rivers can also play a significant role in the long distance transfer of a chemical compound. Even the migration of fauna may become a significant factor in the transfer of chemical compounds.

Abiotic Models

Modeling can be applied to areas of varying surface size. Local scale models cover the smallest areas such as lakes or parts of a lake, etc. Models may comprise only a section of one environmental compartment, e.g. soil only.

Regional models are the next size up in class and may comprise a river mouth area, drainage basin of a sea, entire country or a continent. Global models have the widest range and are used for studying the cycling of chosen pollutants on the intercontinental scale. Examples of the application of migration models for chemical compounds in different environmental compartments and areas of various sizes are presented below. The model described by Mackay et al. [25] and Juntunen and Bidleman [26] is an example of the migration model used for describing the transfer rate of chemical compounds between air and water. The surface area and depth of the water compartment has been defined in this model. Moreover, it was assumed that water is well mixed throughout its entire volume, and suspended matter onto which chemical compounds can be adsorbed is included. The air phase is treated similarly to the water phase. The model contains the description of physicochemical properties of some chemical compounds which serve as an example, but there is a possibility to add other substances that are a subject of interest for a given user.

Soil surface models are an important model type, particularly in the field of soil science. The processes that govern the cycling of chemical compounds in soil, such as evaporation, degradation rate, leaching by water, soil recovery rate to the acceptable level of contamination were described and presented as a migration model by Cousins et al. [27, 28]. From among migration models that include soil surface, there are the ones described by Jury, Spencer and Farmer [29-32], and Mackay and Stiver [33]. By using them one can predict, for example, pesticide concentration in river water after rainfall over the arable land located in a river basin.

Another migration model, namely *Soil* [11] (available at http://www.trentu.ca/academic/aminss/envmodel/models/ftp/soilx.exe), assumes that the soil matrix consists of four phases, e.g. air, water, and organic and inorganic matter. It has been assumed that organic matter contains 56% of organic carbon. The surface area and depth of soil has been defined which allows the calculation of volume and mass of soil components. The amount of chemical compound present in soil is expressed in $kg \cdot ha^{-1}$. The rate of each process and its share in the removal of a compound from soil can be calculated by applying this model. The model can be used to calculate potential evaporation or contamination of groundwater. In *Soil* model only the processes occurring in the direction from soil to air have been included while transport in the opposite direction was omitted. A more complex model (available at http://www.trentu.ca/academic/aminss/envmodel/models/ftp/soilf.exe), is *SoilFug* [34, 35]. It allows to investigate the dependency of pesticide leaching from soil on rainfall intensity, and to predict the rate and efficiency of pesticide loss and degradation in agricultural areas.

The next model type has been developed in order to study interactions and processes that occur at the sediment-water interface [36, 37]. By using these models, one can calculate, among other things, accumulation and loss of contaminant from sediment in lakes, and concentrations of chemical compounds in organisms that live/feed in areas rich in benthos. Such models may become helpful for determining which transport processes are most significant under given circumstances and moreover, in estimation of the time expectancy which is necessary for sediment reversion (allowable pollution level) in the case of a “hot-spot” pollution event. In *Sediment* model (available at http://www.trentu.ca/academic/aminss/envmodel/models/ftp/Sedt2install.exe) [11] the surface and depth of water phase has been defined, and the assumption was made that water is well mixed in its entire volume. Water contains suspended matter, which consists of organic and inorganic matter. Sediment has the same surface as water, and it also has a specified depth and percent content of soil and water. It has been assumed that sediment is well mixed. The fat content in organisms living in water and sediment has been defined in order to facilitate bioconcentration calculations. Among the transport and chemical transformation processes included in the model are: sediment formation, resuspension, degradation in sediment, diffusive exchange between the water column and pore water in sediment, and reactions in sediment. In addition, irrigation processes can also be included, e.g. infiltration of groundwater into the sediment.

As a result of combining models of air-water and sediment-water exchange [36, 37] and adding chemical reactions and flows, migration models for a lake have been created of which *QWASI* [38] is an example (available at http://www.trentu.ca/academic/aminss/envmodel/models/ftp/QWASI300install.exe). *QWASI* describes the migration of chemical compounds in a complex aquatic system (water, sediment, suspended matter and air). Appropriate flow equations for a chemical compound being transferred in medium, based on diffusion and degradation processes, were used. The model allows the analysis of seasonal variability of the behavior and migration of chemical compounds in dependency on temperature and flow. It is also possible to add new values of parameters that influence this variability. The response time of the system can also be studied.

A *QWASI* model was used multiple times for different areas [38], and modified for many chemical compounds and various aquatic ecosystems. It was applied, among others, by Woodfine et al. [38] to model the transport of metals. After substantial modifications of *QWASI* two models have been developed, i.e. *CoZMo-POP* [8, 39] and *POPcycling* (both available at http://www.scar.utoronto.ca/~wania/downloads/ after authorization) [40, 41]. They are multiphase, non-steady state models based on mass balance that describe long-term migration and behavior of persistent organic pollutants (POPs) in coastal and river mouth environment (*CoZMo-POP*), and in the Baltic Sea (*POPcycling*). The main focus has been placed on a quantitative approach to environmental migration routes of POPs. The model also describes the release level of POPs and seasonal variability of their emission from soil and vegetation into air and freshwater. Based on those models, the predictions can be made about POP concentrations in air, water, sediment and forest. Simulations can be performed under various boundary conditions, i.e. for different assumptions regarding emission, inflow of air masses, etc. In both models, a key role is played by a two-way exchange and circulation of POPs between the atmosphere and the land and water surfaces as well as one-way outflow of contaminants from soil into freshwater, and next to the sea or lake. The processes resulting in the loss of POPs during transport in the air and water, e.g. degradation and deposition in atmosphere, and degradation, sedimentation and evaporation from river water have been incorporated into the models.

Another example of a model for chemical compound migration in the lake ecosystem was reported by Reed-Andersen et al. [42]. By using this model, one can analyze the decrease in phosphorus concentration – and the related lowered eutrophication level – resulting from different scenarios of phosphorus emission. The following scenarios can be considered: the increased flow of phosphorus from algae to consumers; the application of alum; and modified management of coastal zone which should result in the decreased phosphorus discharge and reduction of inorganic fertilizer load in the catchment area. Phosphorus load in the lake and its catchment area comes from the dry and wet deposition and from groundwater. Additional loads are due to fertilizing of arable land. The outflow of phosphorus encompasses the harvest, feeding of animals on the cultivated plants, water drainage, sedimentation, and feeding by fishes. Phosphorus may also be released from the sediment into the water column, and from aquatic organisms into the water and sediment.

Modeling of migration and behavior of mercury in lake and forest ecosystems have been described by Meili et al. [43]. The research was conducted in southern Sweden. By using the model, it is possible to estimate, among others, a critical level of air contamination that becomes a risk to sensitive environmental components.

Cabaret model (available at http://nest.su.se/MNODE/Methods/cabaret.htm with documentation) is used to investigate the circulation of nutrients in coastal marine environment. With the help of the model, it is possible to calculate salinity and mass balance for water and nutrients in onephase and multiphase aquatic systems. In the model there is a possibility to select the length of season which would allow the elucidation of the investigated system [44].

With the help of migration models, the nutrient mass balance in an agricultural system can also be described, e.g. the model of methane emission from rice fields [45]. This particular model is focused on crop management that would stimulate the growth and development of rice. The model includes decomposition of organic matter in soil and roots of plants presently cultivated, and interactions between methane and oxygen in soil. The impact of applying different crop management strategies on methane production from rice fields can be estimated. It is also possible to evaluate the influence of soil composition (the presence of competing electron acceptors) as well as the use of organic and inorganic fertilizers on methane emission. By using this model, one can explain seasonal variability of methane emission. Calculations can be performed at regional as well as country scales.

The model described by Holysh et al. [46] can serve as an example of migration model for chemical compounds in rivers. It was developed from the modified *QWASI* model by solving the differential equation that describe concentrations in water as a function of river length. The chemical compound migration between water and sediment at a steady rate was also included in the model; it is also possible to calculate, among other things, half-life time of chemical compounds in a river. Another migration model for chemical compounds in rivers is *MONERIS* (*MOdeling Nutrient Emissions in River Systems*) [47, 48] (MONERIS user manual available at http://www.icpdr.org/icpdr-pages/item20080506172727.htm). By using *MONERIS*, different scenarios of "changing human activities vs. changing emission and thus, indirectly, assessment of contamination levels in river" can be created. This model has also been adapted to quantitative estimation of heavy metals emission from point and diffuse sources in the catchment area.

By using *MONERIS*, one can prepare various scenarios of emissions and their impact regarding heavy metals. The basic input data for the model are emissions and water quality data for a given river, GIS data for the catchment, digital maps, and statistical information about land use, wastewater treatment plants, soil types, etc.

GloboPOP [49] (available at http://www.scar.utoronto.ca/~wania/downloads/) is the global scale migration model for contaminants. With the help of the model, it is possible to elucidate migration and processes to which chemical compounds are subjected. Depending on the needs, the user can use the values of environmental parameters defined in the model (e.g. surface area of arable land or oceans) or he/she can modify them. The chemical compounds described in the model or other, previously characterized by the user substances can be modeled. Other parameters that can be changed are, for example, the size and time of emission, simulated period, etc. *GloboPOP* model has been modified, and the results obtained with its help were published by Wania and Daly [49].

Different scenarios of the intercontinental scale emission, migration and behavior of DDT and α-HCH have also been investigated my means of *ECHAM4* [50] (description available at http://www.mpimet.mpg.de/en/wissenschaft/modelle/echam.html) which is a four-phase dynamic model; the transfer of contaminants occurs via atmospheric transport only. Soil, vegetation and ocean surfaces are treated as two-dimensional layers. Research on permeation of radon from soil into houses, due to the difference between indoor and outdoor pressure, may be conducted with the help of the migration model described by Andersen [51]. This model allows following the migration of chemical compounds from soil into the air, and of radon in porous media. It can also be used for calculating radon flow from the surface of the earth and the intensity of radon vaporization from building materials, for example, from cement. Processes such as the formation and radioactive decay of radon, its diffusive transport and transport processes based on the flow of radon-containing medium can also be included in the model. Many parameters may vary in time, while those related to transport (diffusion and permeability) may be anisotropic.

Migration models are also used for estimating the efficiency of wastewater treatment plants [52]. By using models it can be calculated how much of the chemical compound will vaporize, degrade, and remain in the sediment and treated wastewater.

Biotic Models

An important type of migration model describing the processes of bioaccumulation and bioconcentration are models for predicting pollutant bioaccumulation in live organisms, in particular in fatty tissue of fishes [53-55]. With their help one can estimate the potential risk of pollutant bioaccumulation and bioconcentration in fish and other organisms, and particularly in birds and humans consuming fish. The uptake of pollutants from the aquatic environment by fish occurs through trophic chain via ingestion of food, and through gills via passing water. The excretion of pollutants from the body of a fish occurs through gills by fecal ejection, in the processes of spawning and metabolism, and by dilution via fish growth. The listed processes are included in the model in the form of equations. The models for pollutant bioaccumulation in fish are very useful for elucidating how the differences in values of octanol-water partition coefficient and metabolic half-life time influence bioaccumulation. Modeling studies have shown the important role of food intake in the uptake of pollutants.

Specific types of migration models which are the extended models of bioaccumulation in fish, are the models of pollutant migration in trophic chains [56, 57]. By using this model type, one can estimate not only bioaccumulation and bioconcentration at consecutive trophic levels but also, for example, the influence of changes in the trophic chain structure on the chemical compound concentration in the organisms at the top trophic level. The above-mentioned issues are important because, among others, the consumption of fish by humans is frequently the main mode of entry of hydrophobic chemicals into the human body. In practice, such models are multiphase and include a one-way flow between phases. Consecutive links in the model are, for example, water, phytoplankton, zooplankton, invertebrates, small fish and finally large fish. Each link is a consecutive level of the model while the preceding link constitutes food for the following one.

Food chain models that encompass many species are often developed by applying a general equation for bioaccumulation to each of these species via the use of proper parameters. The final set of equations for n organisms has n unknown fugacity values; the equations are solved sequentially by starting at the lowest trophic level and proceeding to the largest animals. Another approach is to arrange the equations in the form of a matrix followed by solving it [11].

The succesive group of migration models describes uptake of chemical compounds by plants [58-60]. These models allow calculating an uptake of organic pollutants by flora. The assimilation of chemical compounds may occur from the air, water and soil. There is a problem associated with these models, namely that the uptake processes of chemical compounds are poorly researched and understood. The uptake of pollutants by plants has also been incorporated into many models that describe the environment in a comprehensive way. *CoZMoPOP* [8, 39] and *POPcycling* [40, 41] are the examples of models which include the plant aspect. The plant aspect has been added to models because flora differs significantly in respect to the characteristics of pollutant exchanges with soil and air as compared to those among water, sediment, soil and air. (The methods of incorporating flora into migration models have been described in detail by Cousins and Mackay [61].) Other interesting examples of practical use of mathematical models describing migration of chemical compounds are pharmacokinetic models [62, 63].

Animals are treated as a set of interconnected elements in which the basic exchange occurs through blood flowing among all of them. The model may also include the impact from pollutants present in the air and food, and impact via skin exposure. Next, the dynamics of chemical compound transfer in venial and arterial blood to and from different organs and tissue types are calculated. Chemical compound loss may occur via metabolism and excretion in urine, feces and sweat. In the case of mammals, such loss may also take place during lactation, while in birds, reptiles and amphibians during egg laying. Models are widely used for determining drug activities in a human body and the optimal drug dose to achieve the set target. This model type has also been applied to assess the occupational exposure (continuous or instantaneous) to a toxic compound, e.g. solvent, fuel vapor, etc. With the help of the models it is possible to calculate the chemical compound concentration in blood, tissues and internal organs, response time and flows, and also to establish a relationship between the chemical compound concentrations in the environment and in the tissues of organs.

Summary

Models have become an indispensable tool for environmental management and legal regulatory measures on emissions of chemical compounds to the environment. The use of models has allowed the elucidation of many previously unsolved scientific issues. Moreover, they are a tool that is handy and flexible enough to be adapted to other conditions by means of modification and improvement. By using models, one can reconstruct processes to which chemical compounds had been subjected in the past, and perform simulations of those processes in the future as well as predict future cycling of the chemicals through different ecosystems on both global and regional scale and for various time intervals.

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