Chapter

Introductory Chapter: Development of Assessment Models to Support Pollution Preventive and Control Decisions

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1. Introduction

The continuous increase in human activities affects the environment in notable ways; these effects need to be monitored and controlled when appropriate to ensure the sustainability of our lives. Environmental pollution is one of the major problems that associate these activities; it is initiated when a substance is released into the environment in a way that prevents its natural restoration [1, 2]. These releases could be classified as planned and uncontrolled releases. The first class is a part of routine human activity where discharge is performed after complying with the regulatory requirements, whereas uncontrolled releases associate accidents and nonregulated activities [1]. Uncontrolled releases and historical practices have led to several contamination problems, so restoration or remediation programs are being initiated to control these problems from spreading [2]. Currently, preventing and controlling environmental pollution and restoration of affected environmental systems receive great attention globally. This attention was translated into issuing strengthen regulations and allocating natural and human resources to support pollution prevention and control activities. In this respect, a continuous increase in research efforts was dedicated to investigate new materials and/or systems to evaluate their potential applications in preventing and controlling environmental pollution, that is, wastewater, gaseous, and solid waste management, and in and ex situ remediation projects. **Table 1** lists some pollution control and prevention systems and their classifications in terms of the scientific bases of the used technologies. These investigations are supported with enormous efforts to understand, simulate, predict, and decide on the performance of these materials and systems under predefined conditions using wide range of models. In this context, kinetic models are applied to:

1. assess the formation and/or evolution of the system and its subsystems;
2. assess, control, and optimize the chemical reactions used in different waste treatment technologies;
3. design and optimize the operation of remediation projects; and
4. support the decision-making process at regulatory agencies and operational facilities during different life cycle phases of pollution control and prevention systems, that is, planning, design, licensing, etc.

Technologies classification	Wastewater	Solid waste	Gaseous waste	Remediation In-& ex-situ
Physical	Sedimentation, Floatation.	Segregation, Compression, Shredding	Cyclone, Bag-House, Electrostatic precipitator	Soil washing, Soil vapor extraction
Physico-chemical	Solvent Extraction, Reverses osmosis Ultra & micro Filtration, Sorption/Ion Exchange, Coagulation/ Precipitation.	-	Stripping, Filters, Sorption	Permeable reactive barrier, Electro-Kinetic
Chemical	Advanced oxidation	-	-	Chemical Stabilization
Biological	Tricking filters, Attached growth on granular bio-filters, Activated sludge	Aerobic, Low/High-Anaerobic Digestion	-	Bio-treatment, Ex-situ-slurry biodegradation, Root zone Treatment
Thermal	Evaporation	Incineration	Combustion	Incineration, Vitrification

Table 1.
Technology for preventing and control of environmental pollution

Modeling by definition is an abstract of the real systems, where essential features, event, and process (FEP) that affect the performance of the studied system are presented [3, 4]. Generally, the modeling efforts are divided into research and assessment models. Research (process) models use laboratory and field experiments to identify FEPs that affect a subsystem or more, whereas assessment models link important processes (determined from research model) to predict the overall system performance [5, 6]. **Figure 1** illustrates the integration of research and assessment models, in which the studied subsystems are characterized and the factors that affect their behavior are identified experimentally. Then models are used within the research efforts to interpret, extrapolate/interpolate, and optimize the collected data; the modeling results will be used to evaluate and rank the FEPs that affect the system. In assessment models, important FEPs are linked to identify the problem formulation and basic system description, and then conceptual and computational models are constructed, verified, and used [5–11]. For instance, the quantification of the effect of time on the pollutants migration in terrestrial, aquatic, and/or atmospheric subsystems is usually conducted by measuring the concentration of major pollutants at incremental time at different distances from the source. Experiments are run for specified time determined based on the temporal scale of the study. The collected experimental data are analyzed to quantify the processes that control the migration. This analysis might include the use of simple empirical, semiempirical, or mechanistic mathematical models that allow a clear understanding of the nature of the processes that affect the migration. In terrestrial subsystems, these processes might include percolation, retardation, biodegradation, advection, and hydrodynamic dispersion [8, 11]. In subsequent sections, the development of assessment models to support the decision-making process will be illustrated with special emphasis on the prediction of pollutant migration. In this respect, the iterative nature of the assessment modeling will be overviewed, the conceptual model will be introduced, and some conceptual models that could be used to predict pollutant migration will be illustrated. The selection of

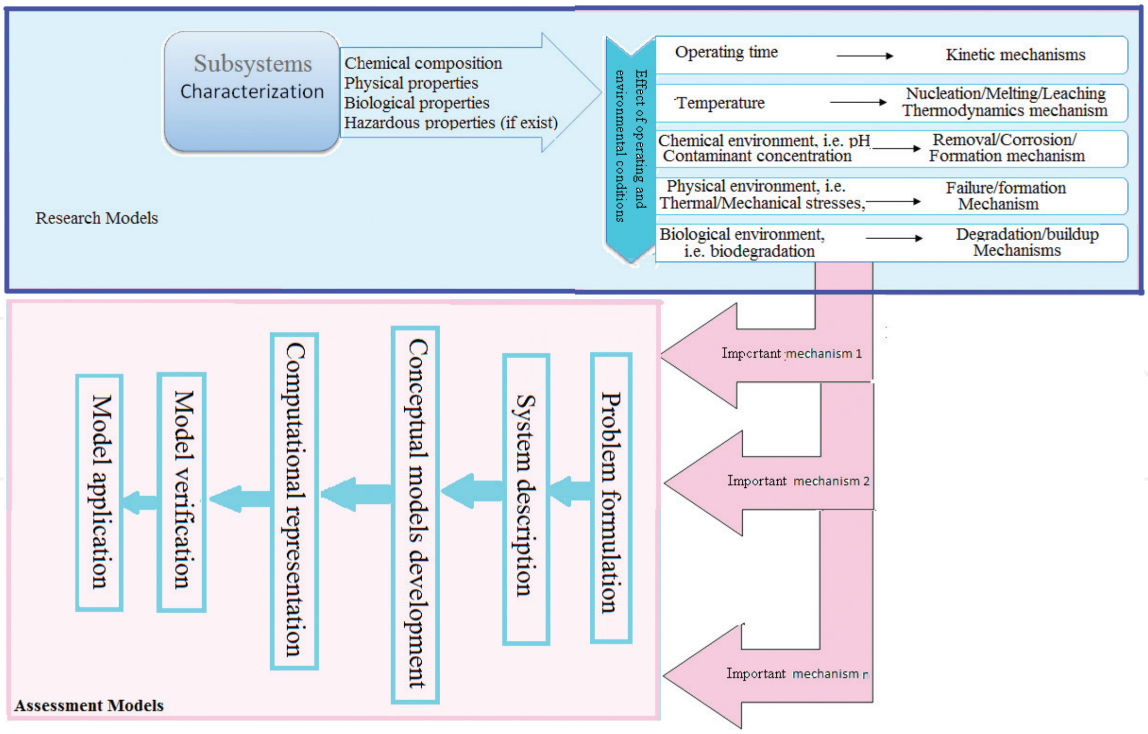

Figure 1.
Integration of research and assessment models in studying a system.

computational models will be presented, where some simple models that could be used to estimate the migration in terrestrial subsystems will be summarized.

2. Iterative nature of the assessment modeling

Assessment models are used to support the decision-making process during different life cycle stages of any pollution prevention and/or control system, for example, sitting waste management facility and designing remediation program. Their outputs should provide assurance that the systems will be sited, designed, operated, etc., in a manner that compiles with the safety requirement issued by the regulatory body. Assessment modeling starts with problem formulation and basic system description based on available system information. During problem formulation, the assessment objectives and audiences, regulatory framework, system boundaries, spatial and temporal scales, stage of project development, critical receptors (affected groups), adopted assessment approaches, nature of assumptions, data availability, level of accuracy, cost, and uncertainty treatment should be clarified [4]. The level of the assessment complexity is largely dependent on the national regulations and state of project development. Assessment modeling is an iterative process, where basic system data are used to develop a simple model that contains all essential FEPs derived based on basic system description. The model is then verified using system-specific data to check its prediction adequacy. If adequate simulation results are obtained, the model will be applied; otherwise more system-specific data should be collected to help in improving the model predictions. **Figure 2** illustrates the iterative nature of the modeling process and its relation with the system-specific data, in which the developed model complexity or simplicity is determined based on the stage of development of the studied system and the availability of system-specific data [11, 12]. The developed model, in each iterative stage, is produced from multi-step process that includes the development of conceptual and computational models (mathematical model and the tool that solves the mathematical model) [5–9].

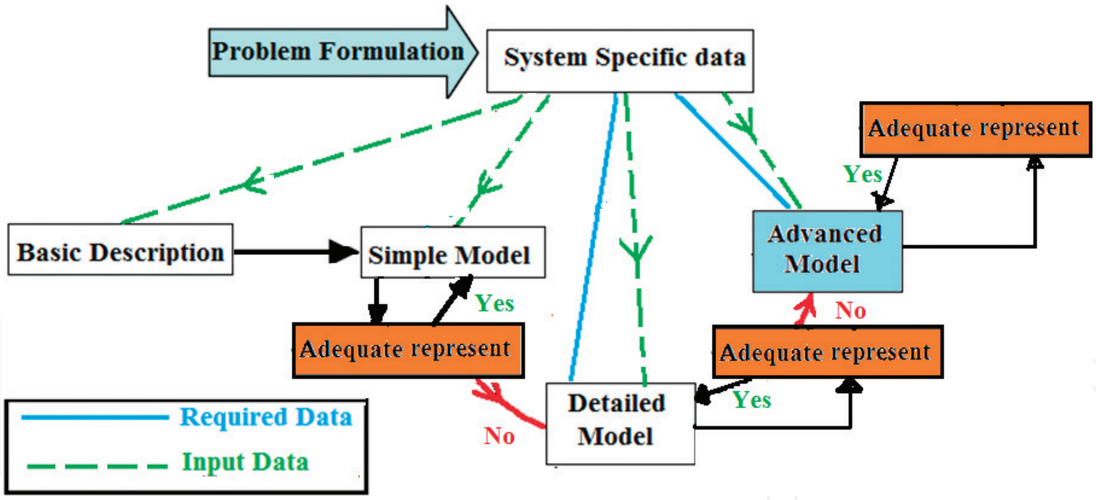

Figure 2.
Iterative nature of the modeling process and its relation with system-specific data.

3. Development of conceptual model for pollutant migration assessments

Conceptual model is defined as "A simplified representation of how the real system is believed to behave based on a qualitative analysis of field data" [11]. The development of a conceptual model starts with a clear determination of available information and knowledge gaps about the system. Subsequently, essential FEPs and their interactions in each subsystem are identified, and assumptions that were made to include or exclude any of these FEPs are highlighted based on the results of the research models [11]. Finally, flowcharts are used to describe the graphical relationship between different processes in different physical subsystems. It should be noted that the conceptual model could be imperfect if over- or under-simplification of the studied system were used, where over-simplification can lead to ineffective model with large uncertainties and under-simplification can lead to complex model that raises the project costs. Imperfect conceptual model could be resulted from incomplete problem identification/assessment context, wrong assumptions in developing the conceptual model, and poor identification of the important processes.

Conceptual models are usually constructed based on source-pathway-receptor analysis, where pollution sources are defined by investigating the driving forces and duration of the releases for each pollutant, the routes of pollutant transport between different physical subsystems are determined, and receptor exposure mechanisms and duration are identified [9, 13, 14]. Below are some examples that illustrate the construction of conceptual model for pollutant migration into different subsystems that could be developed to support the pollutant control and prevention decision-making process.

To characterize the extent of the contamination problems due to contaminant spill, there is a need to collect samples from potentially affected subsystems, that is, groundwater, surface water, air, and soil and subsoil. Sampling procedure should consider both the main pollutants and subsystem properties, for example, pollutant concentrations in different subsystems, water pH, velocity, wind velocity, etc. Characterization results will be analyzed within the research modeling efforts, and the results of this analysis will determine the complexity of the model. Based on these results, homogenous or nonhomogenous subsurface may be considered to estimate pollutant percolation and sorption, and the elimination or inclusion of biodegradation and aquifer recharge as sink or source for pollutants in the subsurface and surface water will be determined. In this case, different terrestrial and atmospheric exposure pathways to receptors, downstream the contamination source, were identified as main exposure routes. **Figure 3** illustrates the main processes that can lead to pollutant migration or attenuation from a contaminant spill into different subsystems. The pollutants are assumed to be transported by percolation, surface runoff, and evaporation, and attenuation is assumed to occur as

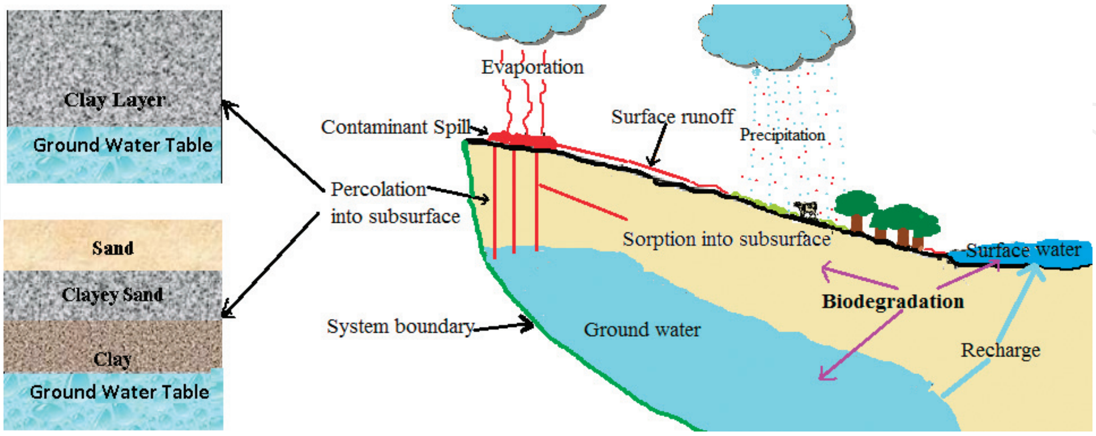

Figure 3.
Conceptual model to predict pollutant migration/attenuation from the source term into the surrounding environment.

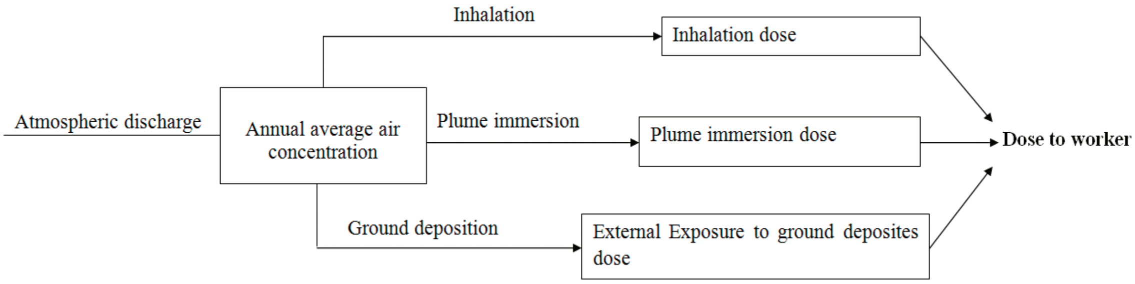

Figure 4.
Conceptual model to quantify the effect of continuous atmospheric discharge on the worker [14].

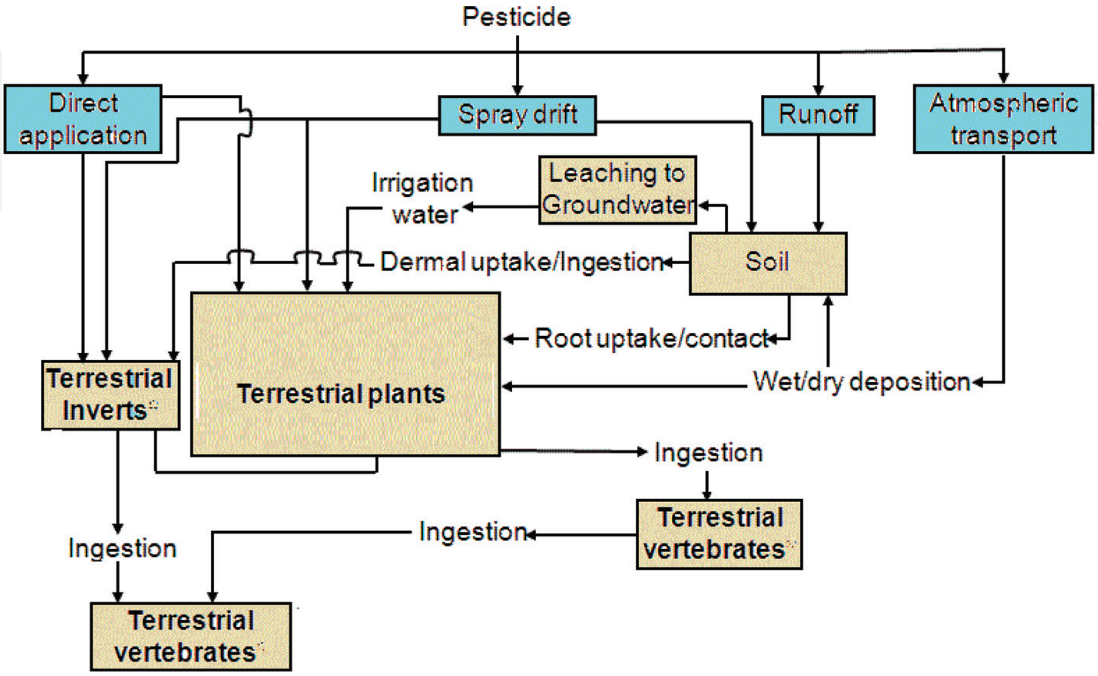

Figure 5.
Conceptual model to quantify the effect of pesticide application on the environment [15].

a result of sorption into the subsurface and biodegradation within surface water, groundwater, and geosphere.

To determine the worker dose in a radioactive waste incinerator facility during the planning phase for transition from batch to continuous operation, a conceptual model was constructed [14]. The pollutants are assumed to be transported through the air via advective-diffusive process, and the exposure means were determined to include inhalation of gaseous pollutants (which is the main exposure mean in that study), direct dermal exposure, and ingestion of contaminated water (**Figure 4**).

Generic conceptual model to quantify the effect of pesticide application on the environment is suggested by US EPA (**Figure 5**) [15]. The model represents terrestrial exposure pathways, where the pollutants (pesticide) are transported through the atmospheric and aquatic subsystems and were assumed to affect terrestrial receptors, that is, plants, invertebrates, and vertebrates. The exposure means included inhalation, dermal exposure, and ingestion with a detailed characterization of the dietary routes.

4. Computational representation of the conceptual model

The development of the computational model that represents accurately the conceptual model is a crucial task, where the accuracy of the obtained results will be used to judge if the modeling effort is enough to represent the system or there will be a need to acquire field data and develop an updated model (**Figure 2**). For a simple conceptual model, a simple empirical model could be used, as the site-specific information is available and a more realistic model could be used [13]. The type of the mathematical representation of the conceptual model is defined during the problem formulation, and the selection of the appropriate model is bounded by [4, 11]:

1. System dimensions: decision should be made if one, two, and three dimensions will be used to represent the system.

2. Nature of the boundary conditions: Source terms release assumptions should identify if the release is constant or variable throughout the time and space.

3. Steady state or time variant model: the system behavior is changing with time or fixed.

4. Uncertainty management: probabilistic or deterministic approaches.

5. Homogenous and nonhomogenous system.

6. Type of flow and transport process: the flow occurs via intergranular or fissure flow, and the transport is governed by advection or hydrodynamic dispersion.

During the development of a mathematical representation, the studied system is usually divided into a subsystem. For the conceptual model presented in **Figure 3**, the system could be divided into source subsystem which describes the mobilization of the pollutant from the source, terrestrial migration, atmospheric transport, and receptors subsystems. **Table 2** shows some simple models that could be used to develop a mathematical representation of pollutant migration in terrestrial compartment [5, 16–20]. This table presents models that could be used to estimate both

Model use	Parameters	Model
Infiltration rate in homogenous soil, (q, m/d)	Soil sorptivity (S, m/d$^{0.5}$), Soil dependent constant (A)	$q(t) = \frac{1}{2}St^{-0.5} + A$
Flow rate in homogenous soil, (q, m/d)	Hydraulic gradient (i), Hydraulic conductivity (k, m/d)	$q = ki$
Flow rate in non-homogenous soil (q, m/d)	Dimensionless time (t*), Dimensionless depth (z*), Change in volumetric water content as the wetting front passes layer n (δθ, m^3 /m^3), Potential head while the wetting front passes through layer n, (H$_n$, m)	$q = \left(\frac{0.5\left[t^*-2z^*+\sqrt{(t^*-2z^*)}+8t^*\right]+1}{0.5\left[t^*-2z^*+\sqrt{(t^*-2z^*)}+8t^*\right]+z}\right)^*kn$ $t^* = \frac{k_n t}{\delta\theta\left(H_n+\sum_{i=1}^{n-1} Z_i\right)} \quad z^* = \frac{k_n}{\left(H_n+\sum_{i=1}^{n-1} z_i\right)} \sum_{i=1}^{n-1} \frac{z_i}{k_i}$
Pollutant Travel time, (t, d)	Vadose zone thickness (d, m), Porosity (n).	$t = dn/q$
Water average velocity (v, m/d)		$v = Ki/n$
Hydrodynamic dispersion (Dl, m^2/d)	Effluent pore volume (u), Distance (L, m), Mean pore water velocity (v, m/d).	$D_i = \frac{vL}{8}\left(\frac{U-1}{\sqrt{U}}\Big\vert_{0.84} - \frac{U-1}{\sqrt{U}}\Big\vert_{0.16}\right)^2$
Distribution coefficient (kd) of element (i) assuming linear isotherm	Concentration in the solution (C, ppm) at initial (i) and final (e) state, Solution volume (V, l), Soil weight (m, g)	$K_{di} = \left(\frac{C_{ii}-C_{ei}}{C_{ii}}\right)\left(\frac{V}{m}\right) \times 1000$
Retardation coefficient (Rf) in vadose zone	Soil density (ρ, kg/m^3), Soil porosity (ε).	$R_f = 1 + \frac{\rho(1-\varepsilon)}{\theta} K_{di}$
Retardation factor assuming Freundlich isotherm	Freundlich constant indicative of the relative sorption capacity (n) and (Kf, mg/g)	$R_f = 1 + \frac{\rho K_f}{\theta n} C^{\left(\frac{1-n}{n}\right)}$
Retardation factor assuming D-R	Maximum sorbed as calculated by D-R isotherm (qm, mg/g), Energy of sorption estimated by D–R model (E, kJ/mol), Gas constant (R,8.314 J/mol K), Absolute temperature (T, K)	$R_f = 1 + \frac{\rho RT q_m E^2}{\theta} \exp\left(\frac{RTln\left(1+1/_c\right)^2}{2E^2}\right)$ $\ln\left(\frac{C+1}{C}\right)\left(\frac{C}{C+1}\right)\left(\frac{1}{C}\right)$

Table 2.
Mathematical models used to assess the migration in soil subsurface [5, 16–20].

flow (infiltration/flow rate, travel time, and average water velocity) and transport parameters (hydrodynamic dispersion, distribution, and retardation coefficient) for homogenous and nonhomogenous soil under saturated and vadose conditions.

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