Environmental Modeling

Module 1: Introduction

Prabhas K. Yadav, PhD

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The content of the module: Introduction

Model and Modelling

Model is a simplification of reality that is constructed to gain insights into select attributes of a physical, biological, economic, or social system.

Modelling can be defined as the process of application of fundamental knowledge or experience to simulate or describe the performance of a **real system** to achieve certain goals.

Modeling has long been an integral component in organizing, synthesizing, and rationalizing observations of and measurements from real systems and in understanding their causes and effects.

Why Environmental Modelling?

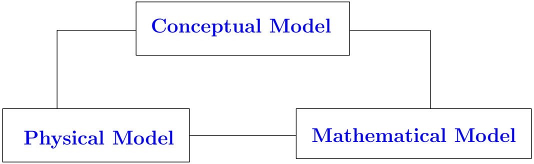
1. **Better understanding** of and glean insight into environmental processes and their influence on the fate and transport of contaminants in the environment.
2. **To determine** short- and long-term chemical concentrations in the various compartments of the ecosphere for use in regulatory enforcement and in the assessment of exposures, impacts, and risks of existing as well as proposed chemicals
3. **Hypothesis testing** relating to processes, pollution control alternatives, etc.
4. **To simulate** complex systems at real, compressed, or expanded time horizons that may be too dangerous, too expensive, or too elaborate to study under real conditions.
5. **To implement** in the design, operation, and optimization of reactors, processes, pollution control alternatives, etc.

Why Environmental Modelling?

6. **To generate data** for post-processing, such as statistical analysis, visualization, and animation, for better understanding, communication, and dissemination of scientific information
7. **For satisfying** regulatory and statutory requirements relating to environmental emissions, discharges, transfers, and releases of controlled pollutants
8. **Use in environmental impact assessment** of proposed new activities that are currently nonexistent

Types of model

Most common modeling approaches in the environmental area can be classified into three basic types:



Mathematical modelling forms the foundation for use of computer in modelling.

While the three types of modeling are quite different from one another, they complement each other well.

Next we discuss each types of the model.

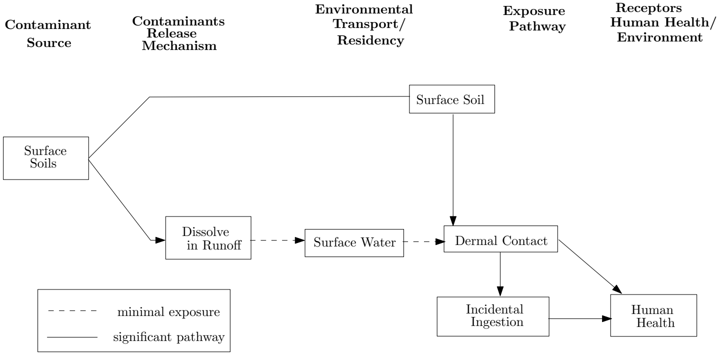
Conceptual model

1. **A picture** of the system processes (e.g. Maps of places, ideas, relationships; Flow charts, graphs; Hypotheses, theories)
2. **Qualitative**, usually based on schematic figures/maps -the first step in any successful modelling efforts
3. Represent important system:
   i model components
   ii processes
   iii interaction

Use of conceptual models:

1. As an initial step
2. For hypothesis testing
3. For mathematical model development
4. As a framework

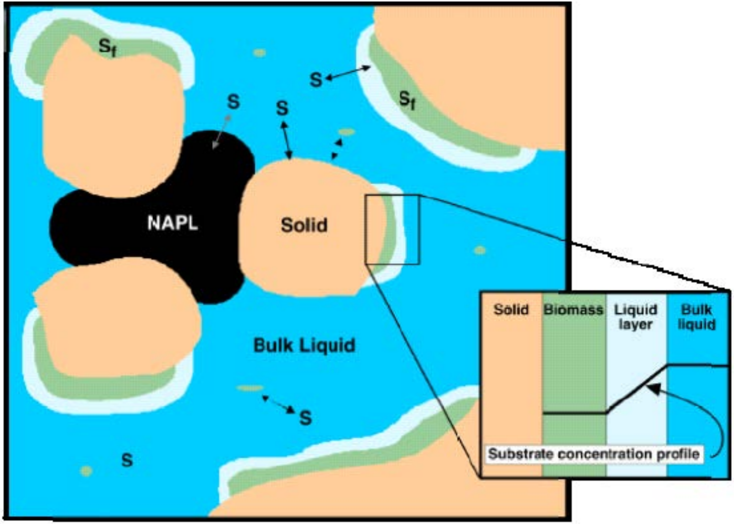
An example of conceptual model



A conceptual Model for the Movement of Contaminant(s) Bound to Surface Soils to a Person

Click here for more details

An another example of conceptual model

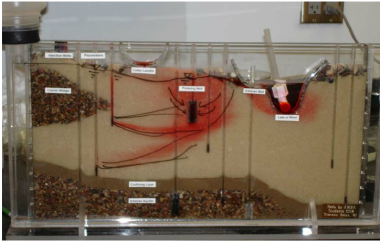


Subsurface Biodegradation Process

Physical model

Small scale physical representations which retain certain key features of larger natural system, e.g., *Laboratory simulation* of the processes and systems under investigation, e.g. to explore the behaviour of the system or test the mathematical models.

Few Examples of Physical Model



Contamination in aquifer
Check details here

A physical model of a Weir
Check details here

Mathematical model

Mathematical equations that translate a *conceptual* understanding of a system or process into *quantitative* terms– the most common modelling tool

Various levels from very simple algebraic models to lumped parameter models composed of ordinary differential equations to dynamic spatially distributed models described by partial differential equations are defined.

An example of a mathematical model equations

Lotka–Volterra equations, also known as the predatorprey equations. More details here

$$\frac{dx}{dt} = \alpha x - \beta xy$$

$$\frac{dy}{dt} = \delta xy - \gamma y$$

Where,

i x is the number of prey (for example, rabbits);

ii y is the number of some predator (for example, foxes);

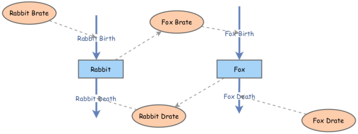
iii $\frac{dx}{dt}$ and $\frac{dy}{dt}$ represent the growth rates of the two populations over time;

iv t represents time; and α, β, γ, δ are positive real parameters describing the interaction of the two species.

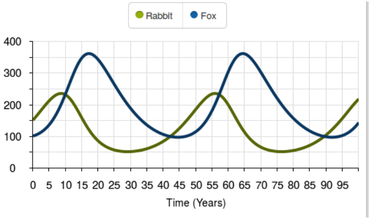
Mathematical Model

Solving the Predictor-Prey Dynamics

More foxes will decrease the population of rabbit, which will effect the birth rate of fox.



Conceptual model with mathematical input (check here)



The model output

The result for 100 years suggest that populations of fox and rabbit are cyclic.

Mathematical model- variables and output relationship

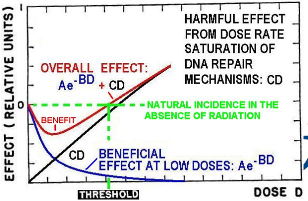
Mathematically, or rather symbolically the variable and output are represented as:

$$y = f(x_1, x_2, \ldots, x_n)$$

In the above equation:

Independent variables or also **system input** are x_i, few e.g. cause, stimulus, forcing functions
Dependent variable or also **system output** is y, few e.g. effect, response, state variables

An example of cause-effect relation:
More detail here



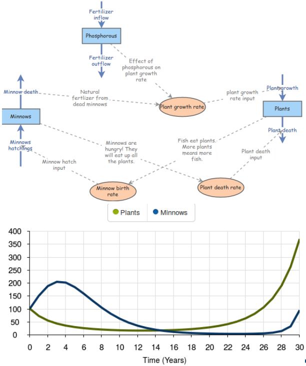
Fundamental use of mathematical models

Mathematical model are fundamentally used for:

1. For Diagnosis e.g. What are cause of algal growth in a lake?

Algae bloom in Lake Erie, USA (more details here).

2. For Prediction e.g. How will it effect the lake quality?



more detail here

Categories of Mathematical Models

The following classification are generally found in literature:

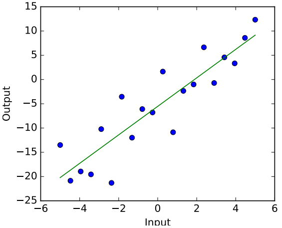
Type	
Empirical Based on data analysis	**Mechanistic** Based on mathematical theory
Time Factor	
Static or steady-state Time independent	**Dynamic** Time dependent
Data uncertainty and Variability	
Deterministic Do not address data variability	**Stochastic** Address variability/uncertainty

Empirical versus Mechanistic Model

Empirical Model

Empirical model are based on statistical relationships between parameters of interest and other variables.
The relationships are usually defined by regression and correlation analyses.

An example:



In this model:

Output = 2.94*Input - 5.53

In the example *Input* can be concentration and *Output* can be water quality indicator.
What are 2.94 and -5.53?
How do you say the model is good?
You may want to learn how the plot is created from here.

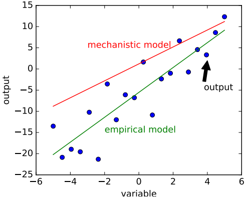
Empirical versus Mechanistic Model

Mechanistic Model

Mechanistic Model rely on *mathematical equations* to describe the chemical, physical and biological processes governing the system

In general system is predicted using:

1. applying scientific principles such as the conservation of mass, momentum and energy.
2. Mechanistic models include kinetic, thermodynamic equilibrium and mass transport models.
3. Parameter estimates (i.e. chemical reaction rates, mass transfer coefficients) have a critical role in mechanistic modelling.



More on figure can be found here.

Static and Dynamic Models

A dynamic model accounts for time-dependent changes in the state of the system.

A static (or steady-state) model calculates the system in equilibrium, and thus is time-invariant.

Dynamic models typically are represented by differential equations.

Example:
More details on this can be found here and here

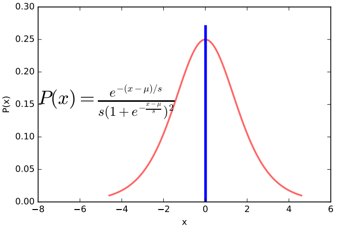
Deterministic and Stochastic Models

In **deterministic model** each component and input is determined exactly by mathematical equations.

Stochastic models are mathematical models which contains random (stochastic) components or inputs.

Model output variables are known only in terms of probability distributions from stochastic modelling.

Example logistic distribution



More details on this figure can be found here. For plot check here.

Application of Environmental Modelling

Environmental Medium	Issues	Uses of Models
Atmosphere	Hazardous air pollutants; air emissions; toxic release; acid rain; smog; CFCs; particulates; health concerns; global warming	Concentration profiles; exposure; design and analysis of control processes and equipment; evaluation of management actions; environmental impact assessment of new projects; compliance with regulations
Surface Water	Wastewater treatment plant discharges; industrial discharges; agricultural/urban runoff; storm water discharges; potable water sources; eutrophication; food chain	Fate and transport of pollutants; concentration plumes; design and analysis of control processes and equipment; waste load allocations; evaluation of management actions; environmental impact assessment of new projects; compliance with regulations
Groundwater	Leaking underground storage tanks; land application of solid and hazardous wastes; leachates from landfills and agriculture; injection; potable water source	Fate and transport of pollutants; concentration plumes; design and analysis of remedial actions; drawdowns; evaluation of management actions; compliance with regulations

Example of Lake Water Quality Modelling

Use Lake Models to Ask:

1. What is the lakes present water quality?
2. **Development**:
   2.1 What was the lakes water quality before development?
   2.2 How will future watershed development affect water quality?
3. **Nutrients**:
   3.1 What are the most important sources of nutrients to the lake?
   3.2 What level of nutrient loading can the lake tolerate before it develops algae problems?
4. **Nutrient management**:
   4.1 How much must nutrients be reduced to eliminate nuisance algal blooms?
   4.2 How long will it take for lake water quality to improve once controls are in place?
   4.3 How successful will restoration be, based on water quality management goals?
   4.4 Are proposed lake management goals realistic and cost effective?

Steps in Environmental Modelling

Environment modelling includes the following steps:

Developing Conceptual Models → Developing Mathematical Models → Calibrating and Verifying Models → Sensitivity and Uncertainity Analysis

1. **Developing Conceptual Models**
   1.1 Define the problem
   1.2 Define the evaluative environment
   1.3 Define the relevant **contaminant properties** and characteristics
   1.4 Define the relevant fate and transport phenomena
   1.5 Define the **state** of the system
2. **Developing Mathematical Models**
   2.1 Clearly define a control volume
   2.2 Consider which transport phenomena control contaminant inputs and outputs across the model boundaries
   2.3 Consider reaction kinetics within the control volume
   2.4 Develop mathematical model

Steps in Environmental Modelling

3. **Calibrating and Verifying Models**
   3.1 Compare field data to model results
   3.2 Calibrate the model by tuning model input parameters to obtain a close fit to field data
   3.3 Develop performance criteria with which to judge the model
   3.4 Verify the model by testing the calibrated model with a second, independent set of field data
4. **Sensitivity and Uncertainty Analysis**
   4.1 **Sensitivity analysis**: determination of the effect of a small change in model input parameters on the model results
   4.2 **Uncertainty analysis**: determination of the uncertainty in the model results due to uncertainty in the model input parameters