PROTECTION OF THE ENVIRONMENT: POLLUTION SPREAD – MATHEMATICAL MODELS AND OPTIMIZATION

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Summary

It is clear that there is a growing need for modeling the spread of a pollutant in the geosphere and the biosphere. However, the underlying mechanics are seldom completely understood, and environmental decision making still relies mainly on case

studies. As a consequence, it is important to use sound mathematical principles in devising and using a model attempting to simulate the fate of one or more chemicals through the environment. This chapter tries to give an overview over standard issues of mathematical models for pollution spread. Moreover, interconnections with decision support processes are shown which might greatly increase the effectiveness of the corresponding environmental decision making processes.

1. General Modeling Methods

There are basically two different principles in use for modeling. The widely used *deductive principle* starts with the underlying laws of nature, be they physical, chemical, or biological, as incorporated in the corresponding theories, and tries to apply these theories on the task at hand. The result is usual a mathematical description of the processes involved in terms of one or more formulae, e.g. equations. These equations are usually too complicated to be solved manually, except perhaps in peculiar circumstances, and therefore the help of a computer is needed to model the system in question. This approach has been successfully used for centuries in physics. This principle is also called the mechanistic method or the process-oriented method. In contrast to this, the *empiric* or inductive principle starts with a hypothesis about the quantitative behavior of the system under consideration and tries to fit measured (i.e. observed) parameters to this hypothesis. After the fitting process, conclusions with respect to the qualitative behavior of the system can be drawn. This method is often used if the total system is too complex or not well enough understood to allow an application of the deductive principle. Sometimes, this method is also called the statistical method.

Both methods have their merits, and it is seldom the case that a real-world problem can be solved by sticking meticulously to one of these approaches. Hybrid approaches of any flavor might also be used. Nevertheless, it can be argued that the deductive principle leads to more insight than the empiric approach, and that the results gained by its use are in general more precise. We therefore focus in what follows on the deductive principle for modeling.

1.1. Pollutant Transport

Pollutant transport, one of the main focuses of simulations for environmental decision making, can roughly be classified into the following categories:

Advection: This is the passive transport of pollutant in a medium in which a flow exists. Examples include the movement of sulphur dioxide in the atmosphere due to wind, the downstream flow of a pollutant in a river, etc.

Convection: The passive transport of pollutant in a medium in which density differences exist. The density differences will exist mainly due to temperature differences. As an example, consider the rise of a hot smoke plume from a fire into the atmosphere. The smoke, being hotter than the surrounding air, is less dense and rises due to convection.

Dispersion: This effect is responsible for local mixing of the pollutant due to turbulence in the medium. Dispersion can only happen when a flow in the medium exists, and is therefore inherently coupled with advection.

Diffusion: The local mixing of the pollutant due to Brownian motion of the pollutant particles. In contrast to dispersion, diffusion is a property of the pollutant, and not of the medium.

Phase Transfer: Here, a pollutant enters a different phase (and possibly a different medium), i.e. from liquid to gaseous phase by evaporation or vice versa due to precipitation.

Chemical Processes: These can be biological processes or non-biological ones. For example, eating polluted food can induce a chemical transformation of the pollutant inside the body.

Biological Processes: Here, living beings participate actively in the transport of pollution. This can, for example, happen when migration processes or food-webs are considered in the model.
Not all of these processes need to be considered for all types of models. For example, chemically inert materials like heavy metals sometimes do not need specific considerations with respect to their chemical transformations. On the other hand, their health effects with respect to enzymatic reactions might be important. Moreover, advection and convection can be conveniently treated as mathematically equivalent.

No matter what kind of processes are modeled, from the above list it should be clear that a successful, realistic model of pollutant transport in the environment needs a breakdown of the complete system (i.e. the environment) into subsystems with corresponding submodels. Models not using this modeling paradigm are usually not able to capture the dynamic movement of pollution through the ecosphere and geosphere.

Example 1: Consider the case in which one wants to model the effect of airborne pollution released by a waste incinerator on land-based ecosystems. A typical list of subsystems might include

- the atmosphere,
- land-based ecosystems,
- individuals, and
- individual organs.

Of course, this list of subsystems is not exhaustive. The geosphere has been deliberately skipped. Likewise, no attention has been paid to the aquatic distribution of pollutants, to the corresponding water-based ecosystems, the simulation of the effects of a pollutant on cells, etc. □

1.2. Modeling Recommendations

The following recommendations which can be made with respect to environmental modeling are cited from [17].

- *The purpose and the scope of the study have to be fixed a priori*. Especially, the part of the environment under consideration and the time scale has to be fixed. The same principle applies to the level of detail of the study and to the pollutants considered.
- *The underlying processes have to be identified*. To tackle this problem, the list of transport processes from the earlier section might be helpful.
- *The corresponding mathematical equations have to be formulated*. Usually, the equations that one searches for are ordinary or partial differential equations, see Section 3 and 4. At this stage of the modeling process, expert help might be particularly useful.
- *The corresponding data has to be acquired*. Note that in many cases data is not directly available and needs to be estimated from other sources. This leads to parameter estimation problems.
- *The model structure has to be verified*. Citing from [14], "verification of the model structure means testing of the underlying process description. This is done by using experimental data…" Verification is a test of the internal logic of the model.
- *The model structure has to be calibrated*. Calibration is the fitting of model parameters using measurements, usually obtained during a verification process. This is necessary since parameters are not known to their exact values and all models are simplifications of reality. Calibration will usually be done by a (semi-)automatic optimization process, and is a problem in its own right.
- *A sensitivity analysis has to be done*. Models whose variables are overly sensitive to certain parameters are prone to numerical difficulties and can be classified as ill-posed. In such a case, a reformulation of the model might be necessary.
- *The model has to be validated*. This is the comparison between independent measurements and the results of a model. Note that this is conceptually different from verification. Moreover, validation is only possible with respect to an independent data set at hand.
- *An uncertainty analysis has to be done*. Since input data usually contains stochastic errors, it is important to know how stable the computed results are with respect to variances in the input data.
- *The model has to be documented*. This is evident. Otherwise, the work done will be lost.

Note that it is quite unlikely that the procedure outlined above will yield good results right after the first step. Usually, several iterations and backtracking steps are needed to fulfill all the demands expressed in the list. For example, if the verification step fails, the equations found might have to be modified, and data has to be gathered again. Modeling is an iterative process.

Moreover, since almost all simulations have to be done on a computer, it is inevitable that the model will be implemented as software. With respect to this, the usual engineering principles for software development and documentation apply. For

example, software should be developed in a modular way to ease debugging and maintenance, etc. This applies especially to the numerical computations which will lie at the heart of the software code. They can be prone to numerical difficulties and particularly hard to debug. Unfortunately, this is often neglected during the implementation phase. For example, it is not true that an analytic solution of an equation should always be used when it is known. Numerical approximations can be equally precise and less time consuming to compute.

Note that, as soon as a model has been developed, the actual application of it is relatively cheap, no matter how often it is applied. It makes therefore sense to put a rather large amount of effort into modeling.

Example 1: (continued cf. [4]) A possible breakdown of the modeling system needed to track the fate of the pollutant emitted by the waste incinerator into sub-models and modules is the following.

- The *meteorological preprocessor*, which uses observational meteorological data to compute all the meteorological parameters needed for the time period of interest in the spatial domain considered,
- the *air dispersion model*, in which the distribution of the pollutant in the atmosphere is simulated,
- the *ecosystem dispersion model*, which simulates the fate of the pollutant in the ecosystems considered, through different trophic levels, through food chains, etc.,
- the *chemokinetic model*, in which the concentration of the pollutant in different organs of different individuals, living in the abovementioned ecosystems, is traced,
- the *cytodynamic multistage model*, which simulates the effects of the pollution on different cell populations in the organs of the individual life forms considered,
- the *effect quantification module*, agglomerating the cytodynamic effects on the individuals to an effect at the population level, and finally
- the *optimization module*, which minimizes this effect by optimizing the decision variables specified.

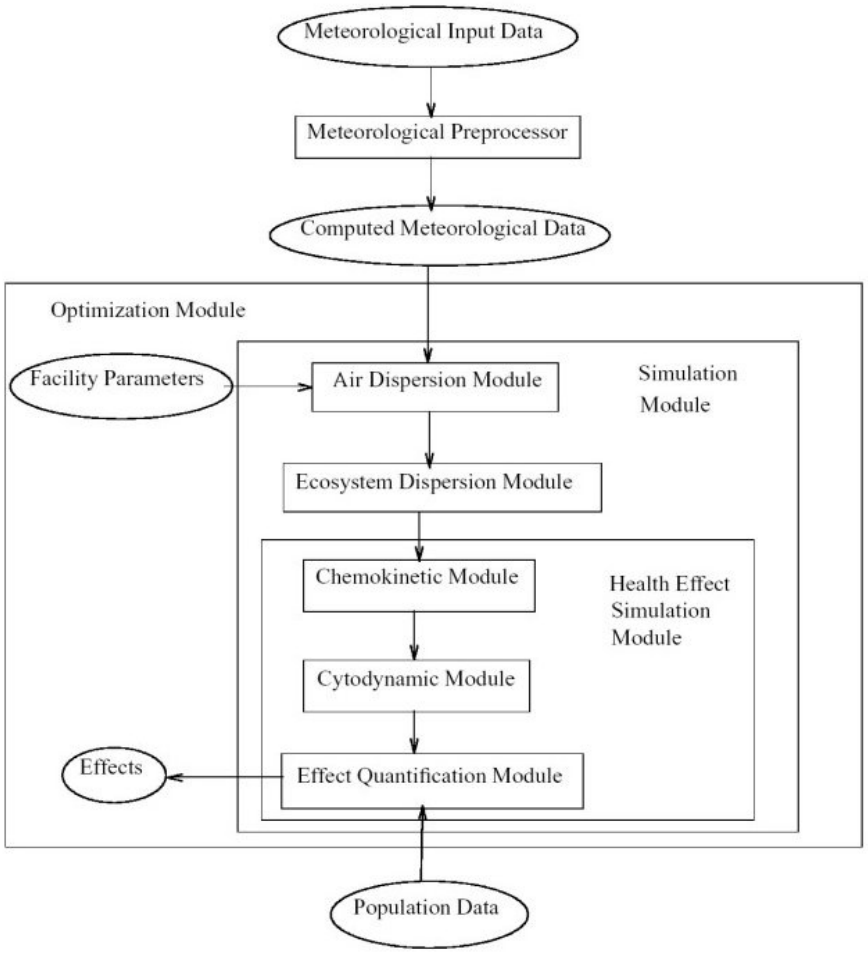

Figure 1: Submodules and data flow in Example 1.

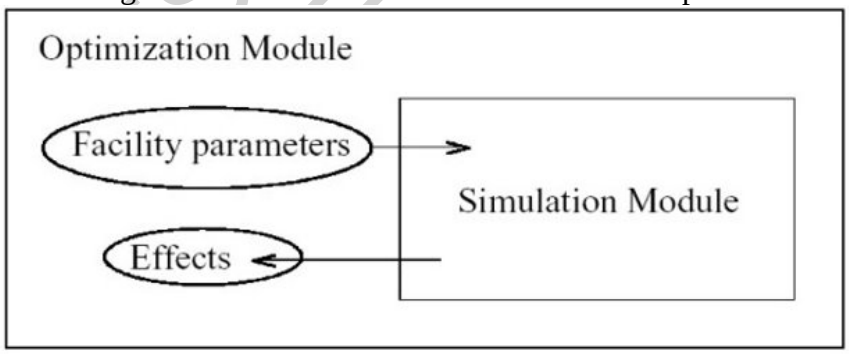

Figure 2: General structure of an environmental decision aiding software.

Note that the meteorological conditions of the atmosphere are independent of the fate of the pollutant and of the location of the facility, but not vice versa. It makes therefore sense to calculate the meteorological variables needed over the time period of interest beforehand and use this data in subsequent simulation runs inside the optimization module.

The corresponding data flow between the submodules is depicted in Figure 1.

2. Optimization

Up to now, the decision process with respect to environmental issues and health concerns was mainly based on simulations of different decisions. However, the need for an automated optimization process incorporating detailed estimates of effects of the pollution has recently been acknowledged by the European Environmental Agency [10, 3]. Unfortunately, up to now only few attempts have been made to integrate the decision process into a general optimization procedure, thereby automatically minimizing a measure of risk. Models used up to now have either been rather simplistic, or have resorted to stochastic optimization techniques, methods which are known for their notoriously slow behavior.

But the general strategy of the task is clear: after a simulation module has been developed for simulating the environmental effects and the health effects for a given choice of parameters which characterize the environmental policy, an optimization module to be developed can handle the task of finding optimal choices for the describing parameter values (compare Figure 2). Since the cause-effect relationships of pollution and human health are quite complicated and dynamic, it has to be expected that only in this way an optimal strategy for pollution control can be developed. Of course, all parts of the cause-effect chain need to be considered.

However, it is quite obvious that a more detailed consideration of the task at hand is necessary. To this end, two main questions need to be asked and answered in the development process.

- What are the parameters of the decision process that can be controlled by the decision makers?
- How can the effects on the environment and on the health of certain individuals be quantified?

The first question asks for the decision (or external) variables, the second focuses on the state variables of the model. While there are no definite answers to these questions, we can give at least an example how such answers might look like

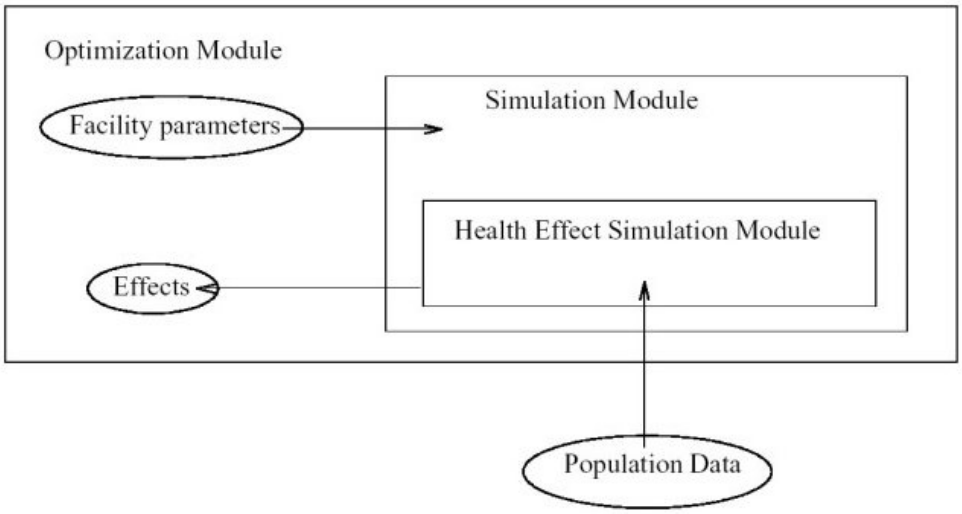

Figure 3: General structure of an environmental decision aiding software system, including the simulation of health effects.

Example 1: (continued): Typical answers to these questions might look as follows: the decision makers are concerned with the location of a waste incinerator. The actual question of the need of such a facility has already been answered positively. As such, only the location plays a role, which can be conveniently expressed as two real-valued variables $(y_1, y_2) \in \mathbb{R}^2$. Moreover, the height of the smoke stack and the width of the opening are open for optimization. As such, there are four real-valued decision variables. Of course, all of them might be subject to quite restrictive constraints. As a trivial example, both height and width of the stack need to be strictly positive. Other, more complicated constraints have to be expected in real-life scenarios.

With respect to the second question, a well-established measure for individual carcinogenic effects within a certain organ or tissue of a person is the number of malignant cells appearing within a certain time period. Likewise, a measure for cytotoxic effects is the number of cells which have died during a fixed time period. Note, however, that detrimental effects due to toxicity not leading to the death of certain cells can not be accounted for in this scheme. Since we are dealing with low-toxic doses, actual outbreaks of symptoms are not an issue here.

Taking now the position of a postulated central authority (i.e. a governmental health care official), *the total sum of all health effects over all individual has to be minimized*. The same analysis holds with respect to environmental issues.

The refined structure of a typical software system is depicted in Figure 3.

2.1. The Effect Function

Suppose that one is able to calculate or approximate the time- and space-dependent pollutant concentration in certain ecotrophic levels, individual beings, or organs of different beings. How this can be done will be outlined in later sections. Moreover, suppose additionally that one is also able to calculate or approximate the effect of the pollution. This is usually done in terms of toxicity and carcinogenicity, i.e. effects on the cell level are quantified. What remains is to find an agglomeration of the different effects on the different levels into one value. The minimization of *all* the quantified effects simultaneously is evidently a multicriteria problem for which the knowledge of some approximation of the efficient set would be of great use. However, the high computational demands to compute such an approximation as well as methodological difficulties will usually force the modeler to globalize all the different effects by way of a utility function. However, the ever increasing computational power might change this observation soon. The choice of such a utility is nontrivial, and it does not seem to be clear what effect a corresponding choice has on the solutions of the resulting single-criterion optimization problem. Often, a weighing function is used to globalize all the different effects. Unfortunately, some of the efficient points of the abovementioned multicriteria problem will be missed in this way [5]. Another possibility would be to use agglomeration with the weighted max-norm. With such a utility function one would be

able to calculate all efficient points [7], at least in principle. If this approach is computationally feasible for realistic environmental management problems remains to be seen.

Usually, pollutant concentrations are time- and space-dependent. It is therefore clear that the effect function is time- and space-dependent, too. Denoting by $\lambda \in \mathbb{R}^n$ the vector of decision variables one can define after a proper choice of the utility function (which might be time- or space-dependent, too!) an overall utility function

$$U : \mathbb{R}^3 \times \mathbb{R} \times \mathbb{R}^n \to \mathbb{R},$$

such that $U(x,t,\lambda)$ measures the overall effect of the pollution at the point $x \in \mathbb{R}^3$ and at the time $t \in \mathbb{R}$. Of course, this effect depends on the decision variables λ.

Example 1: (continued): In the waste incinerator case discussed above, one might use $\lambda = (y_1, y_2, w, h)^\top \in \mathbb{R}^4$ as the vector of decision variables. The vector $(y_1, y_2) \in G$ represents the location of the pollutant emitter, while $w \geq 0$ is the width of the "smokestack" and $h \geq 0$ is its height.

In the formulation above, a full three-dimensional model has been used. But often, the space variables *x* will be two-dimensional instead.

The agglomeration of effects over a time interval $[0,T], T > 0$, can be done in many ways. One possible method is the time integral of the utility:

$$e(x,\lambda) := \int_0^T U(x,t,\lambda)\,\mathrm{d}t.$$

With this, $e(x,\lambda)$ measures the overall effect of pollution at the point $x \in \mathbb{R}^3$ when the decision λ has been taken. This approach has the advantage that the integration commutes with the use of a linear utility function. Other important and convenient agglomeration functions over time are weighted *p*-norms, i.e.

$$e(x,\lambda) := \left(\int_0^T \left| \omega(t) U(x,t,\lambda) \right|^p \mathrm{d}t \right)^{1/p}$$

$(1 \leq p < +\infty)$ or

$$e(x,\lambda) = \sup_{t \in [0,T]} \left| \omega(t) U(x,t,\lambda) \right|,$$

where $\omega : [0,T] \to \mathbb{R}$ is a weighting function with $\omega(t) > 0$ almost everywhere. This can easily be generalized to semi-norms in which $\omega(t) = 0$ may hold on a subset of $[0,T]$ with nonzero measure, but $\omega(t) > 0$ elsewhere. When interpreting *e* as a sampling

function, this means that some points (in time) are left unsampled. The corresponding agglomeration functions include

$$e(x,\lambda) = U(x,T,\lambda),$$

i.e., only the effect at the end of the time interval considered is accounted for.

Since there are too many different time agglomeration functions which are reasonable in different circumstances, no general proposal can be made.

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Biographical Sketch

Joerg Fliege obtained PhD in mathematics from the University of Dortmund in 1997. After a visit to the Mathematical Sciences Research Institute in Berkeley, California, he spent one year on a "Research in Brussels" project entitled "Dispersion Simulation for Modelling Polluting Facilities". His research interests include vector optimization, locational analysis, and interior point methods for nonlinear problems. His teaching at the University of Dortmund includes lectures in nonlinear programming and interior-point methods as well as mathematics courses for engineers.

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