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A Language to Describe Geographic Physical Processes

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DISSERTATION

A Language to Describe Geographic Physical Processes

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"Modelling is both an art and a science." Richard J. Huggett (1993, p.51) *to those who accompanied me on my way*

Abstract

Geography investigates changes in physical structures and in distributions of objects in space; these structures and distributions are shaped by processes. Models of processes are built in order to understand and analyze the observed changes. Geographic information systems (GIS), helping with space related analyses, play a supportive role for spatial process modeling due to their static nature. The integration of the concepts related to processes in GIS is one of the unsolved issues of geographic information science.

The goal of this research is to better understand requirements of process modeling in order to extend GIS with functionality for process modeling in the long term. The integration of sophisticated process modeling capabilities in GIS that address the specialized methods of different application areas and disciplines is not realistic. An abstraction from details of quantitative process modeling is required to identify generic process modeling functionality.

This research carries out a systematic analysis of mathematical models of geographic processes with a focus on geographic physical processes in order to develop a generic method to describe these processes: a *process description language*. This language consists of:

- a *vocabulary* consisting of mathematical operators to describe the model;
- *composition rules* for combining the terms of the vocabulary to models;
- a *visual user interface* to guide through the modeling procedure.

The approach to the specification of a vocabulary of the process description language focuses on existing knowledge on modeling physical processes with deterministic models. Geographic physical processes are a subgroup of physical processes, which suggests the applicability of physical principles to the modeling of geographic physical processes. The physical principles referred to are conservation principles that specify the behavior of continuous physical processes. An analysis of the mass conservation

equation leads to the vocabulary of the process description language. The foundation of the vocabulary in mathematical equations provides the rules for composing the terms of the vocabulary. The user interface is derived from the general procedure of establishing deterministic process models.

The result of this research is a process description language that provides a possibility to describe process behaviors on a general level and to compose descriptions of process components to models. A user interface guides the user from a conceptualization of a process to equations modeling the process.

The application of the process description language is tested for two geographic physical processes: the spread of a pollutant in a lake and the dispersion of exhaust fumes of a factory. The output of the application of the process description language is the specification of the behavior of a process together with the indication of required parameters, initial and boundary conditions. The resulting models are considered as *sketch models* that provide the required information to simulate the processes. This research provides the basis for the implementation of a process description tool that supports the linkage of process modeling and GIS.

Keywords: geographic physical processes, process modeling, geographic information systems (GIS), process description language, process composition

Kurzfassung

Der Fachbereich Geographie untersucht, wie sich physische Strukturen und Verteilungen von Objekten im Raum verändern. Die Strukturen und Verteilungen werden von Prozessen geformt und beeinflusst. Modelle werden erstellt um die beobachteten Veränderungen zu analysieren und zu verstehen. Geographische Informationssysteme (GIS) werden vielfach für räumliche Analysen verwendet; in Bezug auf die Prozessmodellierung spielen sie auf Grund ihrer statischen Natur nur eine unterstützende Rolle. Die Integration der Konzepte, die mit Prozessen in Zusammenhang stehen, in GIS ist eine der ungelösten Aufgaben der geographischen Informationswissenschaften.

Das Ziel der vorliegenden Arbeit ist es die Anforderungen der Prozessmodellierung besser zu verstehen um langfristig GIS mit Funktionalität zur Prozessmodellierung erweitern zu können. Die Integration von Methoden zur Prozessmodellierung in GIS, die den Anforderungen verschiedenster Anwendungsbereiche gerecht werden, ist nicht realisierbar. Daher muss eine Abstraktion von den Details quantitativer Modellierung durchgeführt und eine allgemeine Methode zur Prozessmodellierung angestrebt werden.

In dieser Forschungsarbeit wird eine systematische Analyse mathematischer Modelle geographischer Prozesse durchgeführt um eine allgemeine Methode zur Beschreibung dieser Prozesse zu definieren; der Fokus ist hierbei auf geographisch physikalischen Prozessen. Die allgemeine Beschreibungsmethode ist eine *Prozessbeschreibungssprache*, die aus drei Komponenten besteht:

- einem *Vokabular*; das sind die mathematischen Operatoren, die ein Modell beschreiben;
- *Regeln zur Zusammensetzung* der Elemente des Vokabulars;
- einer *graphischen Benutzerschnittstelle*, die die Benutzer durch die Modellierung führt.

Die Methode zur Spezifizierung des Vokabulars basiert auf Wissen über die Modellierung physikalischer Prozesse mit deterministischen Modellen. Geographisch physikalische Prozesse sind eine Untergruppe physikalischer Prozesse, was die Anwendung physikalischer Prinzipien in der Modellierung dieser Prozesse ermöglicht. Die physikalischen Prinzipien sind in diesem Zusammenhang Erhaltungssätze, die kontinuierlichen physikalischen Prozessen zu Grunde liegen. Eine Analyse des Massenerhaltungssatzes führt zum Vokabular der Prozessbeschreibungssprache. Die Ableitung des Vokabulars von mathematischen Gleichungen liefert die Regeln zur Zusammensetzung der Elemente des Vokabulars. Die Elemente der Benutzerschnittstelle werden aus der allgemeinen Vorgehensweise bei der Spezifikation von deterministischen Modellen abgeleitet.

Das Resultat dieser Arbeit ist eine Prozessbeschreibungssprache, die es erlaubt das Verhalten von Prozessen auf einer qualitativen Ebene zu beschreiben, und die es ermöglicht Beschreibungen von Prozesskomponenten zu Modellen zusammenzusetzen. Eine Benutzerschnittstelle führt den Nutzer von einer Konzeption des Verhaltens eines Prozesses zu Gleichungen die den Prozess beschreiben.

Die Anwendung der Prozessbeschreibungssprache wird an zwei Beispielen demonstriert: der Ausbreitung von Giftstoffen in einem See und der Ausbreitung von Abgasen eines Fabriksschlots. Das Ergebnis der Anwendung der Prozessbeschreibungssprache ist die Spezifikation der Prozesse zusammen mit benötigten Anfangs- und Randbedingungen sowie Parameterwerten. Die erstellten Modelle werden als Modellentwürfe bezeichnet; diese Modellentwürfe beinhalten die benötigte Information zur Simulation der Prozesse. Diese Arbeit stellt die Basis für die Implementierung einer Prozessbeschreibungsumgebung zur Verfügung, die die Integration von Funktionalität zur Prozessmodellierung und GIS voranbringen kann.

Schlüsselbegriffe: geographisch physikalische Prozesse, Prozessmodellierung, geographische Informationssysteme (GIS), Prozessbeschreibungssprache, Zusammensetzen von Prozessmodellen

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1 Introduction

> "Escaping a static view of the world remains one of the most important challenges of GIS" (Goodchild, 2001, p.6).

The world with all its physical and social structures and distributions of living beings and objects therein is permanently undergoing changes and is the result of past changes. Geographers are investigating these changes of structures and of distributions in space. The key to understanding changes is the understanding of ongoing spatial processes. Geographic information systems (GIS), helping with space related analyses, play a supportive role for spatial process modeling due to their static nature. The integration of process in GIS is one of the unsolved issues of geographic information science (Langran and Chrisman, 1988; Burrough and Frank, 1995; Goodchild, 2001). This chapter introduces the specific goals of this research regarding process modeling and GIS together with the chosen approach, the expected results and contribution, and the target audiences.

1.1 Motivation

The focus of the discipline of geography is on process and the analysis of spatial processes, respectively of spatial patterns created by processes, is a major task in the field of geography (Abler et al., 1977). "Geography is not about collecting facts,. . . , but about understanding the causes – the processes in space and time – that created these facts" (Frank, 2000, p.100).

A process is a continuous operation or a sequence of operations in space and time; processes are evoked by different mechanisms and lead to a recognizable pattern (Getis and Boots, 1978; Coffey, 1981). Spatial or geographic processes are processes that fall into the research interest of geography. Geographic processes can either be social processes such as the movement of people, urbanization, flow of ideas, etc. or physical processes. Examples for geographic physical processes are hill slope erosion, water runoff, spreading of a pollutant in a lake, and groundwater flow.

Model building is the primary tool for analyzing the effects of processes. Specialized modeling tools are developed in disciplines such as ecology, physics, biology, and meteorology. The models built in these disciplines are becoming more and more sophisticated, realistic, and complex. Space is recognized as an important part of process models (Neuhauser, 2001).

Geography contributes theoretical foundations of geographic information systems (GIS); GIS help at analyzing and representing spatial phenomena. The functionality provided by GIS does not reflect, however, the importance of processes and process modeling in geography. A possible explanation lies in the origin of GIS: GIS have been developed originally for exploiting location in space as a unifying organizing principle of data sets. GIS applications focus on locating objects in space, displaying objects in relation to their surroundings, querying recorded attribute information of objects, and performing navigational tasks. Typical tasks performed with GIS are making maps, entering data, selecting items, displaying maps, and classifying attribute data (Albrecht, 1998). These tasks are generally fulfilled based on a single snapshot of reality (Worboys, 2005).

Providing a single snapshot of reality is not sufficient for studying processes, because the concept of process is inseparably connected to time. The predominantly static nature of current GIS restricts the usefulness of this software for questions of interest in geography related to the representation and the analysis of spatial processes (Kavouras, 2001; Miller and Wentz, 2003). GIS provide little support for the actual modeling of spatial processes and the simulation of the processes. The application of GIS in the field of modeling is mainly directed towards managing data sets and visualizing results of process simulations. Some specific process models have been integrated into certain GIS. GRASS GIS, for example, provides tools for hydrologic modeling, wildfire modeling, and landscape structure modeling.

The extension of GIS with time is a current topic in the GIScience community. Various aspects of this issue are investigated: temporal GIS, moving objects, representation of events in GIS, the extension of spatial data models etc. Research on time and GIS primarily deals with changes of discrete objects. The results of these efforts are not directly applicable to the modeling of natural processes, because these phenomena are continuous.

The ability to handle time is not the only requirement for successful process modeling. Processes are generally described with mathematical constructs or equations that model the behavior of the process. The evaluation of the equations allows the simulation of a process. The core functionality of GIS does not foresee neither the mathematical description of processes nor the interfacing of GIS and process modeling tools.

The potential of GIS regarding the spatial aspects of process modeling and analysis is not yet exploited. Process modeling capabilities in GIS could, for example, improve the understanding of the processes that generated structures appearing in spatial data collections; in addition, the influence of variations in space on process behaviors could be studied in detail. The focus of the geoinformation community is on the location of change caused by processes in addition to information on the amount of change (Câmara, 2008).

The integration of sophisticated process modeling capabilities in GIS that address the specialized methods of all the different application areas and disciplines is impossible. Instead, GIS need to be complemented with a general ability to represent processes. This thesis conducts a systematic analysis of mathematical models of geographic processes with a focus on geographic physical processes and develops a generic method to describe these processes: a *process description language*. The language consists of a vocabulary whose elements can be composed; it, therefore, supports the construction of complex models from simple components. Extending GIS with functionality for describing processes shows areas of improvement regarding process modeling on the GIS side and thereby lays the foundation for a process-enriched GIS.

1.2 Focus on Geographic Physical Processes

Processes can be classified into discrete and continuous processes, respectively into social and physical processes. These kinds of processes differ in fundamental properties. Physical processes are continuous and adhere to physical laws such as conservation laws, which is not always true for social processes. This thesis puts the focus on physical processes that are of interest in geography, namely, *geographic physical processes*. This focus is acceptable due to an emphasis of environmental process models in conjunction with GIS (Bivand and Lucas, 2000).

Consider the following example of a geographic physical process: a pollutant spreading in a lake. Assume that the contaminant is added to the water of the lake by throwing a toxic liquid overboard of a boat. Subsequently, the contaminant spreads continuously until it is diluted in the water. The process of the distribution of the contaminant follows physical laws. The process changes the quality of the water in the lake. A model of this process may answer the following questions (c.f. Thomas and Huggett, 1980):

- where are the areas that are most affected by the contaminant?
- how is the contaminant distributed across the lake after a certain time period?

Geographic physical processes are a subgroup of physical processes. Therefore, physical laws that underlie models of physical processes can also be used for modeling geographic physical processes. For building a simple model of this example process, I assume that the following two physical principles hold: a) the law of mass conservation, i.e., the amount of pollutant in the system remains unchanged once it has been added, and b) the flow of the pollutant is dominated by diffusion, which causes the pollutant to spread from areas of higher to areas of lower contaminant concentrations in the lake. These and similar characteristics of processes can be expressed in mathematical languages.

An example of a mathematical language used for formulating deterministic mathematical models of physical processes is partial differential equations (PDEs). Fundamental for the description of a process with partial differential equations is that the quantity of interest is described by continuous functions (Bastian, 2008). Models based on these equations describe the change in the concentration or density of the quantity of interest in a system. They are, therefore, suitable for answering the questions regarding the distribution of the pollutant in a lake posed in the context of the example process.

1.3 Research Hypothesis and Goals

The uncountable number of spatial processes, the different vocabularies used in disciplines working with processes, and the variety of possible conceptualizations of processes in models cause a confusion regarding the specific process modeling functionality to be integrated in GIS. This thesis aims at identifying generic process modeling functionality that can be included in GIS. First steps towards a GIS with process handling capabilities are:

- a possibility to describe process behaviors,

- a possibility to compose descriptions of process components to models.

The specific goal addressed in this thesis is the development of a generic method to describe and compose process models; I call this generic method a *process description language*. The hypothesis guiding this research is: *A language can be provided that assigns a model equation to geographic physical processes in order to describe the general behavior of these processes.*

The process description language needs a foundation in formal tools, i.e., mathematical models of physical processes, to provide a comprehensive vocabulary for modeling geographic physical processes qualitatively. I aim at a vocabulary of the language that consists of terms for describing *prototypical process behaviors* identified by an analysis of conservation principles of physical processes.

The description of processes with the process description language remains on an abstract or qualitative level and focuses on capturing the general behavior of a process; the resulting models can be seen as *sketch models* of processes. This thesis is not directed towards improving models of spatial processes. Disciplines such as ecology, biology, climatology, etc. have highly detailed and advanced quantitative models of their processes of interest. These models provide a detailed description considering numerous possible influences that allow an exact numeric prediction of a process.

I do not intend to extend GIS with sophisticated functionality for analyzing spatial processes quantitatively. The idea of a monolithic GIS that suits a large variety of purposes seems out-dated in times of web-service architectures. In addition highly developed tools exist for handling the quantitative analysis and modeling of processes, e.g., FlexPDE, MATLAB, or FEFLOW.

The process description language is developed for geographic physical processes, which are considered a good start for such a language. Extensions of the gathered insights to modeling social processes are left for future work.

1.4 Approach

Geographic physical processes can be modeled based on the same principles as physical processes, because they are a subgroup of physical processes. A type of models for describing the behavior of physical processes is deterministic models. These models describe the transport of mass, energy, or momentum in a system. The formulation of a deterministic model requires to define the system of interest, state variables, and transport laws. Partial differential equations (PDEs) are a mathematical language frequently used for expressing deterministic models of physical processes.

The modeling of geographic physical processes based on deterministic models requires a *process description language*. This language consists of:

- a *vocabulary* consisting of mathematical operators to describe the model;
- *composition rules* for connecting the terms of the vocabulary to models;
- a *visual user interface* to guide through the modeling procedure.

The approach towards the language's vocabulary is based upon the following claim: PDEs that describe the general behaviors of geographic physical processes can be derived from conservation principles of physical processes. An analysis of a general (mass) conservation equation considering variations in flow laws and other terms in the conservation equation leads to commonly used linear partial differential equations. Each of these PDEs refers to a type of process with certain characteristics. The identified equations are considered prototypical process equations that provide the foundation of a vocabulary of a process description language. The process description language is, therefore, a tool for specifying mathematical models of processes.

The terms of prototypical process equations that compose mathematical process models are state variables, flow terms, and source or sink terms. The rules for the composition of these terms are given by characteristics of mathematical models written as PDEs: the terms are composed by addition.

PDEs provide a model of processes in a highly aggregated form; selecting a specific equation for modeling a certain process requires knowledge about PDEs. To increase the usability of the process description language a user interface is introduced that guides a user through the procedure of specifying a sketch model of a process of interest. The development of the user interface is closely linked to the general procedure of process modeling and a conceptualization of processes based on block models. Block models allow the specification of process behavior based on flows affecting a specific block in the system of interest.

Two application examples are provided for assessing the suitability of the sketch models established by using the process description language. The examples show that the vocabulary is appropriate for modeling geographic physical processes and how the process description language supports the composition of process components to models. The established sketch models of the example processes are transferred to a process simulation tool; this step shows that the sketch models comprise the required pieces of information for a quantitative analysis of processes.

1.5 Expected Results and Contribution

The expected outcome of this research is a language to describe models of geographic physical processes. The general behavior of the processes is in the foreground of the models resulting from the application of the process description language. The language's generality applies useful across disciplines. The process models are formulated with differential equations, which provide the basis for a quantitative analysis of the process' behavior. The user of the process description language is supported during the modeling procedure by a user interface.

The definition of this process language is based on the idea of using partial differential equations in a qualitative study of geographic physical processes. The construction of a language based on mathematical models assures the composability of the identified elements of the language's vocabulary; simple parts are used to compose complex wholes. On the one hand, the process description language allows the representation of a large number of geographic physical processes; on the other hand, a large variety of geographic physical processes and their specifics can be mapped to a manageable set of prototypical process behaviors that capture the general behavior of the processes.

The process description language achieves the specification of the behavior of the processes and the data required in models together in one environment; the data provide initial and boundary conditions, and parameter values. The output of the process description language can be used for simulating the processes and serve as input for existing spatial modeling tools.

1.6 Intended Audiences

This work is placed at the interface between the communities of geography, GIS and process modeling. The intended target audiences are in particular:

- Geographic information scientists: The enhancement of GIS with capabilities to handle processes is a current topic in the field of geographic information science. The present work presents a language for the description of generic geographic physical processes. This language allows the specification of required data sets and the general behavior of process at one place, which is a step towards a process-enriched GIS.

- Geographers: The focus of this work is on geographic physical processes that fall into the field of physical geography. The presented process description language provides a basic method to establish models of general process behaviors. Possible analyses of resulting process models may be of interest to geographers.
- Implementers of geographic information systems: The proposed set of prototypical process behaviors is intended to serve as a basis for the extension of GIS with basic functionality for modeling geographic physical processes. Implementers of a next generation GIS are provided with a comprehensive set of process behaviors for this purpose. In addition, the discussion of process modeling in the context of GIS shows which aspects of GIS need to be improved for making process modeling work.
- Modelers of spatial processes: Modelers of spatial processes could contribute simple specifications of processes and support the assessment of the suitability of the process description language for the description of geographic physical processes. Even though the process description language may not serve their sophisticated requirements of model building, model builders could profit by GIS that are extended with basic functionality to handle processes.

1.7 Organization of the Thesis

The development of a process description language is placed at the interface of three disciplines: geography, process modeling and GIS; the relation of this thesis to these disciplines is discussed in the first two chapters. The first part of chapter 2 introduces concepts of geographic processes with an emphasis of geographic physical processes. Modeling approaches and modeling tools are reviewed in the second part of chapter 2. Chapter 3 looks at previous work in the GIS field dealing with the integration of process models and GIS, the extension on GIS with time, and approaches to integrate processes in GIS.

Mathematical models of physical processes formulated with partial differential and difference equations are the formal tool used for the development of the process description language. Foundations of physical process modeling and of mathematical languages are introduced in chapter 4.

The idea of the process description language is outlined in chapter 5. The process description language is based on mathematical models and consists of a vocabulary and rules for composing the terms of the vocabulary. It is offered to the user through a graphical user interface.

The derivation of a vocabulary of the process description language based on an analysis of conservation laws is given in chapter 6. The vocabulary consists of prototypical process equations. Three main groups of equations are determined, namely transport equations, steady-state equations, and wave equations. The qualitative characteristics of these mathematical models and the phenomena they describe are discussed in detail.

Chapter 7 shows the application of the process description language for two examples: a simple example referring to the spread of a chemical in standing waters and an example modeling the diffusion of exhaust fumes of a factory. The establishment of sketch models for these processes is shown by using the user interface of the process description language.

The sketch models of the example processes presented in the previous chapter are implemented for simulation in the modeling software FlexPDE in chapter 8. The step of implementing the sketch models created with the process description language completes the cycle of using the language to come from a textual description of a geographic physical process to a basic simulation of the process of interest. Subsequently a possible framework for the development of a process description tool is outlined.

Chapter 9 concludes this thesis by summarizing and assessing the research on the process description language. The achieved results open directions for future work on the topic of extending GIS for process modeling functionality.

2 Concepts of Spatial Process Modeling

Processes are continuous operations or sequences of operations; they may lead to recognizable structures or have predictable effects (Getis and Boots, 1978; Coffey, 1981). Processes can be initiated by different kinds of forces such as physical, social or political forces (Getis and Boots, 1978). Detecting the mechanisms or forces behind processes helps to understand phenomena taking place. The major tool for analyzing process behaviors is process modeling. Some examples for processes with varying characteristics analyzed in different fields of studies are given below.

- The formation of rock is related to physical characteristics of the earth; it is caused by physical forces, takes place on a temporal scale of thousands of years, and is analyzed in the field of geomorphology.
- The migration of people is related to individuals; it is caused by social, economic, etc. forces, takes place on a temporal scale of months or years, and is studied in human geography.
- The growing of a plant is initiated by biological and chemical processes; the process takes place on a temporal scale of days, and is of interest in the field of biology.
- The switching-on of a light bulb requires electricity and takes place because a wire starts to glow; the process happens on a time scale of milliseconds and falls into the studies of physics.

Geographic processes and more specifically geographic physical processes are topic of this thesis. A general classification of processes into discrete and continuous respectively social and physical processes is reviewed in section 2.1. The subsequent discussion of processes and their models in this chapter is grounded on two main research areas: geography providing information on the concepts behind spatial processes (section 2.2) and process modeling contributing knowledge required for effectively describing and analyzing processes (section 2.3).

2.1 A General Classification of Processes

Processes differ in the temporal and spatial scales on which they take place, the objects or individuals affected by the processes, change being discrete or continuous, the forces triggering a process etc. The differentiation between continuous and discrete change leads to a fundamental classification into continuous and discrete processes (Sowa, 2000).

In case of a continuous process changes are incremental and take place without breaks. Sowa (2000) distinguishes between continuous processes with a starting point (initiation), an ending point (cessation), and processes without specific starting and ending points (continuation) (c.f. Figure 2.1). In case of discrete processes changes take place in discrete steps, which are referred to as *events*. Events are followed by *states*, which are periods of no change according to Sowa (2000).

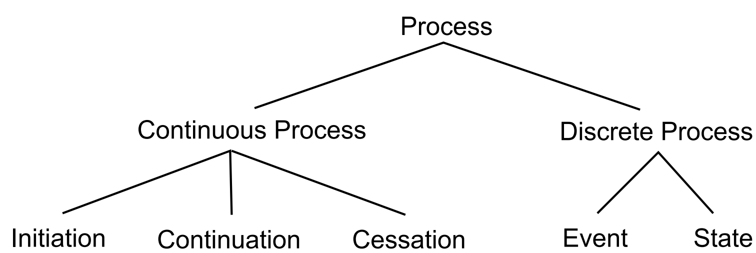


Figure 2.1: Continuous vs. discrete processes (Sowa, 2000).

The differentiation of social and physical processes is related to the differentiation of discrete and continuous processes. Physical processes are governed by physical laws and establish the physical reality; they are continuous processes. Hayes (1985) found in his work on naive physics that people intuitively consider the physical world, which consists of physical processes, as continuous; he mentions the concept of scale changes as one of the sources of this intuition. Social processes are governed by social, i.e. legal, rules. Social processes involving individuals are mostly discrete like a change in the marital status; in some cases they can, however, be conceptualized as continuous processes when looking at, e.g., the migration of a group of individuals.

The fundamental difference between physical and social processes can be explained by the differentiation between information causation and material causation (Frank, 2007). If a computerized or human information processing unit at one place is the cause of a physical spatial process at a possibly distant other place, we speak of *information causation*. Information causation is not limited to spatial or temporal neighborhood: a decision by a single person in a *center of power* can be transmitted to another person and have devastating effects at a very distant location or at a later moment in time. Information causation is also referred to as causation at a distance. An example would be a person speaking causing the listening person to take a vase and throw it against the wall. In the case of information causation, the energy transmitted from one unit to the other is not necessarily corresponding to the energy used in a resulting action. This makes the modeling and prediction of processes in the social domain difficult.

In the case of *material causation* the energy transmitted from one unit to the next corresponds to the gain of energy in the receiving unit. This conservation of energy or some other property like mass or momentum is a common principle of physical processes. Influences of physical processes are restricted to the neighborhood, which means that they are local processes.

2.2 Geographic Processes and Related Concepts

"The main constituents of Geography are space, relations in space, and changes in space"(Morrill, 1970, as cited in Kavouras, 2001, p.50). Processes that are of interest in geography, *geographic* or *spatial* processes, are "mechanisms which produce the spatial structures of distributions" (Abler et al., 1977, p.60). Getis and Boots generally describe spatial processes "as tendencies for elements to come together in space (agglomeration) or to spread in space (diffusion)" (1978, p.1).

"The term geographic might be said to refer to features and phenomena at or near the surface of the Earth" (Goodchild, 2001, p.1). Geography focuses on spatial objects of size somewhere between 10 cm and 10.000 km and processes where change is noticeable in minutes to 10.000 years. Processes are considered geographic if their frequency in time and space falls into this frequency interval typical for geography. Table 2.1 gives examples for geographic structures and processes of interest in the fields of human or social geography (cf. Abler et al., 1977) and of interest in physical geography (cf. Briggs and Smithson, 1993).

A geographic process discussed intensively in theoretical and in practical terms

Geographic social processes	Geographic physical processes
movements of people and goods	water runoff
flow of information	infiltration of water
growth of cities	drainage to groundwater
urbanization	flux of pesticides
land use patterns	hillslope erosion
distributions of services	sediment transport and deposition
diffusion of innovations	channel flow
spread of diseases	heat flow

Table 2.1: Examples of geographic social and physical processes.

is diffusion of elements such as people, diseases, and innovations. Haggett (2001) refers to two main types of diffusion: expansion diffusion and relocation diffusion. In the case of expansion diffusion the quantity being diffused remains in the originating area, which does not happen in the case of relocation diffusion. Expansion diffusion can be further divided into contagious diffusion and hierarchic diffusion. Contagious diffusion refers to diffusion showing a wave-like behavior; like a contagious disease it requires contact between involved elements. Hierarchic diffusion describes diffusion of, for example, an idea that diffuses first among places on the same hierarchy level before reaching places at lower hierarchy levels. The types of diffusion phenomena mentioned by Haggett (2001) are visible in an analysis of demographic processes by Getis and Boots (1978).

Some additional examples for research of diffusion phenomena: Torsten Hägerstrand analyzed in his work of 1953 *Innovation Diffusion as a Spatial Process* the diffusion of agricultural innovations in Sweden (Haggett, 2001). Getis and Boots (1978) analyzed change of patterns caused by spatial and demographic processes, which include diffusion processes. The movement of people in space was modeled by Tobler (1981). Beckmann (1970) studied diffusion of economic change. The expansion of a city is an example of spread given in Abler et al. (1977). Epidemic waves are an example for the successful use of diffusion models in applied geography (Haggett, 2001).

Despite the interest of geography in social processes, I restrict my work to geographic processes that are part of the physical domain, i.e., geographic physical processes. Applications in the context of integrating geographic information systems (GIS) and process models show an emphasis of environmental, i.e., physical processes. The physics applying to the spectrum of processes of interest in geography is Newtonian physics; quantum physics and relativistic effects can be excluded (Goodchild, 2001). I consider physical processes that are of interest in geography a good start for developing a process description language for GIS.

The restriction to strictly local and continuous processes that adhere to physical laws seems to be acceptable in geography; Tobler's first law of geography says: "everything is related to everything else, but near things are more related than distant things" (Tobler, 1970, p.236). Miller states in a discussion of Tober's first law and spatial analysis: "I also suggest that relations among near entities do not imply a simple, sterile geography; complex geographic processes and structures can emerge from local interactions" (Miller, 2004, p.284).

Consider the example of a contaminant spreading in a lake introduced in section 1.2. The event of adding the contaminant to the water is followed by the process of spread of the pollutant, which is caused by physical forces. The lake provides the spatial structure in which the process takes place and which is affected by the process. This short description of the process referred to a series of concepts: space, time, scale, structure, object, event, change, force, etc. The following subsections discuss some of these concepts and the foundations of the view on geographic physical processes taken in this thesis.

2.2.1 Space and Time

"Our daily experience indicates that there is only one physical space in which we and all other things exist" (Frank, 1998, p.42). The views on the objective reality can, however, be different. Spaces in geography are differentiated according to scales (Kuipers and Levitt, 1978; Zubin, 1989; Montello, 1993), algebraic structures that describe, e.g., perceptual and cognitive spaces (Couclelis and Gale, 1986) or geometric representations used.

From a philosophical point of view the absolute and the relative space concept are distinguished. Absolute space was propagated in Newton's and Kant's works; the relative space concept was used by Leibniz (Blaut, 1961; Meentemeyer, 1989; Couclelis, 1992; Sui and Maggio, 1999). Absolute space conceptualizes space as empty space, the Void, with permanent objects being placed in the space as in a container (Blaut, 1961; Meentemeyer, 1989; Sui and Maggio, 1999). Location in space, the georeference, is an attribute of an object (Winter, 1998; Galton, 2004). The interactions between the objects are defined by distance and connectivity relationships based on Euclidean geometry. Absolute space together with Euclidean geometry are the prevailing spatial concepts used in GIS. The Euclidean model is useful for applications in cartography and navigation and also for management of extensive databases (Miller and Wentz, 2003).

Relative space, the opposing view on space, does not exist without objects and processes. In this space concept, space is created by the relationships between objects; it allows the expression of processes (Blaut, 1961; Couclelis, 1992; Sui and Maggio, 1999). Other geometric models than Euclidean geometry might be better suitable for analyses in the framework of relative space (Miller and Wentz, 2003). Câmara et al. (2000) mention spatial interaction models and location-allocation models as examples for applications based on the relative space framework. Measurement based systems make use of the relative space concept (c.f. Buyong et al., 1991; Leung et al., 2004). Another example application is the field of qualitative spatial reasoning, which exploits spatial relations such as, for example, far, near, north, south, east, and west without using quantitative calculations (Frank, 1992, 1996; Freksa, 1992; Sharma et al., 1994; Kuipers, 1994).

Abler et al. (1977) state clearly that the questions concerning spatial distributions posed by geographers require relative conceptualizations of space. This demand is picked up again by more recent research on space concepts conducted by Batty (2005) and Miller and Wentz (2003). These authors indicate the importance of the exploration of alternative conceptualizations and geometries of space for advancing the fields of GIS and spatial analysis. Despite these demands, the framework for investigating processes in this thesis builds on the absolute view on space and Euclidean geometry.

In the GIS-community the discussion about conceptualizations of space is a discussion about object-based and field-based approaches (Couclelis, 1992; Winter, 1998; Galton, 2004). Both approaches are generally considered in a given coordinate framework. Therefore, absolute space provides the fundamental framework for both views. Objects are zero-dimensional points, one-dimensional lines or two-dimensional areas, discrete, countable, and carrying location as an attribute (Longley et al., 1991; Winter, 1998). The field-based view of space captures the continuous properties of the real world, which is useful for describing terrain, rivers, oceans, etc. Representing space as fields means to measure variables that describe properties of space (Longley et al., 1991; Winter, 1998).

The object-based and field-based concepts are in a strong relation with representations of space in GIS. The two groups of representations available in GIS are vector and raster representations. These representations "are dual to each other with regard to space bounding and space filling" (Winter, 1998, p.1). The relationship between concepts and representations is not a one-to-one relationship; both kinds of representations can be used for object- and field-based conceptualizations (Winter, 1998). Couclelis (1992) discusses which representation to use for what kind of system and states that ideally, a hybrid representation should be chosen. Several accounts for a unification of representations of spatial data and a development of hybrid representations exist (Winter, 1998; Câmara et al., 2000; Goodchild et al., 2007).

Spatial conceptualizations are complemented with conceptualizations of time. Research on geographic representations supposes a strong relation between space and time (cf. Egenhofer and Golledge, 1998; Goodchild et al., 2007). Absolute space is related to absolute time, whereas relative space is connected to relative time (Blaut, 1961). Various time concepts exist that are relevant, for example, in database related research: time can be cyclic, linear, continuous, discrete, etc. (Snodgrass, 1992; Medak, 2008). Types of times in GIS are reviewed in Frank (1998).

2.2.2 Scale, Structure and Process

The temporal and spatial scales, on which the behavior of a process is observed, influence the conclusions that are drawn about the process' characteristics. A light bulb seems to start glowing immediately after pushing the switch; the change is experienced as a sudden change - a discrete event. Investigating the physical process causing the light bulb to glow in detail shows that there is a continuous transition between the states of no light emission and light emission. Scale, therefore, influences which aspects of a phenomenon are seen as discrete or continuous. Changing the level of detail of an investigation can change the applicable tools for modeling a phenomenon; e.g., the behavior of individuals can be modeled differently than the behavior of groups of people. Rule like statements for expressing the behavior of people in mathematical models are easier to establish for groups of people than individuals (Thomas and Huggett, 1980).

Processes on different scales take place in parallel in natural systems (Benenson and Torrens, 2004). The interaction of heterogeneous processes is a problem addressed in process modeling (Batty et al., 1999; Mitasova and Brown, 2001; Pullar, 2002). However, not all processes taking place influence each other. The landscape, which is subject of change of the slow process of landscape formation, is appearing static in relation to a hiker walking up a hill, flowers growing on the hillslope, and the stone rolling down the hill. These three examples of processes are not directly influenced by the slow process of landscape formation. The landscape is seen as a structure in which the faster processes take place (Coffey, 1981).

Spatial structure refers to the relative location of objects to each other and of a single object in relation to all objects of a distribution (Abler et al., 1977). There is a strong interdependence between spatial structure and spatial process, because these two concepts are essentially the same (Blaut, 1961; Abler et al., 1977). "What we call spatial processes are mechanisms which produce the spatial structures of distributions. Reference to spatial process is inescapable in any explanation of spatial structure" (Abler et al., 1977, p.60). What makes us differentiate structure and process is the speed or frequency of change we perceive in objects. As said above structures like a landscape are subjects of very slow processes or of processes that do nothing; what we see are states having a certain structure. Dynamic processes happen on a faster temporal scale, which makes us see the change. According to Abler et al. (1977) the separation between structure and process explains the relationship between events and experiences from their causes. This separation allows geographers to use processes for explaining structure or structure for explaining processes (Abler et al., 1977).

2.3 Modeling Spatial Processes

"Environmental processes in real world are three dimensional, time dependent and complex, frequently involving non-linearity, stochastic components, and feedback loops over multiple space-time scales" (Bivand and Lucas, 2000, p.5). This statement on environmental processes applies to other kinds of processes as well; processes in general are complex subjects. When we want to analyze the effects of processes, we need models of the processes. Models abstract from the details of the infinitely complex world and provide us with a manageable representation of parts of reality. They serve the purposes of describing a part of reality, predicting the effects of processes and phenomena, or evaluating alternative scenarios for planning purposes (Lowry, 1965).

The procedure of model building generally includes the following steps: formulating the model, fitting the model with variables and parameters and testing the model (Lowry, 1965). The formulation of a model requires a decision on "what processes should be considered in which scale in terms of space, time or complexity" (Seppelt, 2002, p.269). Simplifications of reality are always taking place during the process of model building and always have to take place to create a manageable representation of reality. The art of model building is to conceptualize a process in such a way that meaningful conclusions can be drawn from the developed model.

A possible simplification of process models is the disregard of space and space-related properties of a process. Models from, for example, the area of mathematical ecology describe the interaction of predators and preys generally without including space (Neuhauser, 2001). Space is, however, recognized as important for making the models more realistic and account for the heterogeneity of the environment (Sklar and Constanza, 1991; Epstein and Axtell, 1996; Richter, 2008).

Fitting a model with variables and parameter values leads to a central problem of models of natural phenomena: the acquisition of input data for the models in the required spatial and temporal resolution (Wickenkamp et al., 1996; Mitasova and Brown, 2001; Richter and Seppelt, 2002). Another practical problem is the evaluation of nonlinear parameter values, which causes problems in modeling frameworks concerning the efficiency and stability of the quantitative analysis.

In summary, the choice of a modeling approach depends on the kind of process, the purpose of the model, the available data, and the existing knowledge on the process. The following sections introduce types of models used in geography (section 2.3.1) and modeling software supporting mathematical modeling of processes (section 2.3.2).

2.3.1 Types of Models in Geography

The quantitative revolution in geography, which took place in the 1950ies and 1960ies, brought models as new tools to geography. Many of the mathematical models of that time were based on the idea of General System Theory (Baker and Boots, 2005). General System Theory, which was introduced by Bertalanffy (1973), studies the elements of systems and their interactions and exploits analogies between various application areas. The new tools made geography move from making descriptions of reality to stating emperical laws regarding geographic phenomena[1]. Models of that time often remained theoretical and untested. Nowadays, geographical models have to be tested against large, real data sets; this explains the importance of spatial statistics in today's quantitative geography (Baker and Boots, 2005).

A general classification of models used in geography is given by Thomas and Huggett (1980). They differentiate three types of models: scale models, conceptual

[1] Wikipedia, Quantitative Revolution, 2009

models, and mathematical models. The following review of these models is based on Thomas and Huggett (1980). Scale models or iconic models are to scale models of reality; e.g., a model railway. Scale models that include some abstraction from reality, are analog models; a map is an example for an analog model.

Conceptual models try to discover how a system functions by identifying the system's components and their relationships. The system *city*, for example, can be understood as individuals and institutions and the interrelations between these two. These two components and the principle of supply and demand create flow of people, goods, money, and information. An example for a conceptual model of physical geography is a drainage basin: components of a drainage basin are, e.g., soil, vegetation, groundwater, and streams. "These units are linked together by flows of energy, minerals, and water which gradually change the composition and form of the landscape" (Thomas and Huggett, 1980, p.3).

Translating conceptual models into a mathematical language creates mathematical models, which are used in this thesis. Mathematical models differ from the previously mentioned models, because they have the ability to numerically predict states of a system. Mathematical models are equal to computational models implemented in a machine-readable language mentioned by Goodchild (2001). Thomas and Huggett (1980) discuss two big groups of mathematical models: deterministic and probabilistic models. In the field of geography, deterministic models are mainly, but not exclusively, applied in physical geography, where a system can be described based on physical laws. These models predict the behavior of a system exactly. Examples are models based on storage and flow, spatial interaction models, and spatial allocation models. Other geographic processes, like the spread of a disease, exhibit a chance-like nature and are better modeled with probabilistic methods. Probabilistic models are, for example, models investigating spatial autocorrelation and geographical decision models. The result produced by deterministic models is always the same for a specific set of initial values; this is not the case for probabilistic models. Probabilistic models represent results as probability distributions rather than unique values.

Besides the differentiation between deterministic and probabilistic mathematical models, mathematical models can be further specified according to the following properties[2]:

- Linear vs. nonlinear models: a linear mathematical model is characterized by the exclusive use of linear operators. If nonlinear operators occur in a math-

[2] Wikipedia, Mathematical model, 2009

ematical model, the model is said to be nonlinear. Nonlinear models, which often refer to chaos and irreversibility, are in general more difficult to analyze.

- Static vs. dynamic models: The difference between static and dynamic models refers to the consideration of time; time is not present in static models.
- Lumped vs. distributed parameter models: In a homogeneous model, the parameters are considered to remain unchanged throughout the system; the parameters are then called lumped parameters. In the case the model is heterogeneous and the parameters change in the system, the model uses distributed parameters.

A conceptualization used in the context of deterministic models is stock and flow components in systems. A stock or storage component refers to the concentration or density of a quantity being investigated; the available concentration or density of the quantity is affected by flows in the system. The relation between storage and flow elements is described in storage equations, which are of interest for modeling geographic physical processes in this research.

Other kinds of models used in social geography are geometric, demographic, and network models (Sklar and Constanza, 1991). Geometric models establish a geometric paradigm based on distance and space (Sklar and Constanza, 1991); examples are Thünen models. Sklar and Constanza (1991) summarize various models describing flow, location of settlements, etc. under the heading of demographic models (c.f. Getis and Boots, 1978). Network models are complex gravity models that describe among others transportation problems and commodity flows.

Subcategories of computational models used in modern geography are cellular automata and agent based models (Hornsby, 1996). These two kinds of models are methods to explore or reproduce spatial structures that stem from individual behavior. They are, for example, used for modeling urban phenomena (Batty et al., 1999; Benenson and Torrens, 2004).

2.3.2 Process Modeling Software

The focus of mathematical modeling is generally on creating realistic, quantitative models that are useful for prediction purposes. The models are supposed to lead to reliable numeric results (Wickenkamp et al., 1996). The model equations of mathematical models, therefore, need to be solved and evaluated. Tools supporting modelers at developing deterministic models are, for example, STELLA, FEFLOW, MATLAB, and FlexPDE.

STELLA[3] is a modeling tool for describing the relations between stock and flow components of systems. The components of a system of interest can be graphically composed. The mathematical foundation is provided by differential equations. Partial differential equations cannot be incorporated in a STELLA model; the modeling of processes depending on space and time is, therefore, not possible with STELLA (Pullar, 2002).

FEFLOW[4] is a modeling tool based on finite elements for modeling processes of water flow and mass transport through porous media. It offers the possibility to integrate GIS data as input data and suits the needs of quantitative modeling of physical processes.

MATLAB[5] is a tool used for evaluating mathematical models of different kinds. The application of MATLAB to environmental modeling is elaborated by Holzbecher (2007).

FlexPDE[6] is a solution tool for partial differential equations based on finite element methods. It is applicable to problems with one, two, or three spatial dimensions. This software tool is used exemplarily for simulating the sketch models of geographic physical processes in chapter 8.

A discipline dealing with the modeling of highly complex phenomena and the continuing development of models and modeling environments is ecology (Maxwell and Constanza, 1997; Rizzoli et al., 1998). Three examples for modeling tools from the field of ecology are the SIMILE modeling environment, the spatial modeling environment (SME), and the 5D environment.

The spatial modeling environment (SME) addresses the needs of collaborative model development in the domain of ecology (Maxwell and Constanza, 1997). SME consists of various components such as graphical modules related, e.g., to STELLA and a modular modeling language, which aims at providing a modeling standard.

The SIMILE modeling environment is based on STELLA models and focuses therefore on differential equations (Muetzelfeldt and Massheder, 2003). The representation of PDEs is not possible with this modeling language.

The 5D environment is a spatial modeling system developed by a group of ecolo-

[3]http://www.iseesystems.com/softwares/Education/StellaSoftware.aspx
[4]http://www.feflow.info/
[5]http://www.mathworks.co.uk/products/matlab/
[6]http://www.pdesolutions.com/

gists, hydrologists, mathematicians, and programmers (Mazzoleni et al., 2006). This modeling environment furthers insights gained in the development of SIMIILE; it offers an interface to the specification and integration of spatial models considering issues of input data specification, visualization, and model construction.

2.4 Summary

Spatial processes create distributions of objects in space. The analysis of processes and structures created by processes has a long tradition in geography. The primary tools for analyzing processes are models of the processes. This chapter introduced geographic processes together with related concepts and general principles of process modeling.

The specific processes of interest for this thesis are geographic physical processes; these are continuous processes that adhere to physical laws and are of interest in the field of geography. Examples of geographic physical processes are flux of pesticides, water runoff, and spread of exhaust fumes. The modeling approach chosen to describe these processes is deterministic mathematical modeling.

3 Geographic Information Systems and Spatial Processes

The focus of geography is on process and process models are built to analyze the processes of interest. Space and spatial data play an important role in today's process modeling in general. Câmara (2008) puts it as follows: "We do not only want to know how much changes, but where the changes happen". Geographic information systems (GIS) that help with analyses of space related phenomena, do not reflect the interest in processes of geography and other disciplines (Burrough and Frank, 1995; Sui and Maggio, 1999; Miller and Wentz, 2003; Mazzoleni et al., 2006). GIS are tools for the management, analysis, and visualization of spatial data (Burrough and McDonnell, 1998); they are not process modeling tools. Kavouras (2001, p.50) recognizes in GIS a "...lack of a concrete theoretical foundation, which among others, has not found acceptable ways to represent generically data, processes, and data on flows and interactions associated with socio-economic applications". Therefore, the use of GIS during model building is restricted to tasks such as data management, integration of data from various sources, provision of Digital Elevation Models (DEMs), visualization of simulation results, and simple spatial analyses (buffers, overlays) (Sui and Maggio, 1999; Mitasova and Brown, 2001; Satti and Jacobs, 2004; Batty, 2005; Fedra, 2006).

Three limitations of GIS are discussed in the context of process modeling. These limitations of GIS refer to the missing capabilities to represent time, to deal with mathematical constructs, and to handle multidimensionality.

- Time: GIS are relying on a map metaphor, which suggests that the environment is static (Burrough and Frank, 1995; Sui and Maggio, 1999; Kavouras, 2001). They have problems with the representation of time and do not provide sufficient functionality for querying spatio-temporal processes or analytical capabilities for analyzing spatio-temporal processes (cf. Langran and Chrisman, 1988; Hornsby and Egenhofer, 1997; Sui and Maggio, 1999; Pang and Shi, 2002;

Fedra, 2006). Their static nature hinders the modeling of spatio-temporal phenomena and the analysis of these phenomena (Langran and Chrisman, 1988; Wu, 1999; Kavouras, 2001; Miller and Wentz, 2003).

- Mathematical capabilities: GIS and the programming languages available in GIS do not provide sufficient analytical capabilities for solving mathematical formulas. The ability to represent a matrix in GIS could be useful for describing the relationships between elements of a dynamic phenomenon and flows between these elements (Miller and Wentz, 2003).

- Multidimensionality: GIS in general lack functionality for 3-dimensional and 4-dimensional descriptions of processes; only the integration of simple 2-dimensional process models is possible (Van Deursen, 1995; Bernard and Kuhn, 2000). An exception is GRASS GIS that incorporates a model for three dimensional groundwater flow. GIS data structures are 2D, which causes a loss of information when importing 4D simulation results of a process into the system for their visualization and analysis (Bernard and Kuhn, 2000).

Takeyama and Couclelis (1997, p.90) see the benefits of including process models in GIS in the integration of "new kinds of phenomena and behaviors such as design, learning and gaming". Pang and Shi (2002, p.342) say that the inclusion of process models in GIS allows GIS users to study the "spatial and temporal relations (e.g., overlap, proximity, before, after) between different processes over time". In my opinion, extending GIS for time and process related functionality serves two general purposes:

1. A GIS with capabilities to deal with time and process has potential for enhanced spatial respectively spatio-temporal analyses. GIS could become a tool for understanding better the processes leading to patterns apparent in spatial data.

2. The integration of GIS and process models makes models spatially explicit (Satti and Jacobs, 2004) and reduces problems regarding the data exchange. The interoperation between specialized modeling tools and GIS could be improved if GIS had some understanding of the process concept.

The limitations of GIS regarding time and process have been approached from different points of views. The following review of these approaches focuses on temporal GIS (section 3.1), the integration of GIS and process modeling tools (section 3.2), and process representations in GIS (section 3.3).

3.1 The Evolution of Temporal GIS

Sinton (1978) identified patterns of generalizations of observations. The three required attributes of an observation are theme, location, and time. Either of these attributes is kept constant, controlled, or measured. In the case of a map or a snapshot, time is the constant attribute and either location or theme is the controlled respectively measured attributes. Temporal GIS requires time to be a controlled or measured attribute to make analyses of spatial data considering temporal aspects possible (cf. Shaw and Xin, 2003).

"A TGIS [temporal geographic information system] must be able to monitor and analyze successive states of spatial entities, and also be equipped to study dependencies between linked entities" Wang et al. (2004, p.770). Examples for queries handled by a temporal GIS are (Langran and Chrisman, 1988):

- How has the usage of this plot of land changed between 1960 and today?
- Has a storm occurred in that area in a certain time period before the landslide occurred?
- Has this town been constantly growing over the last 20 years?

The topic of information systems that can manage space and time together requires the extension of temporal databases for space or the inclusion of temporal data in spatial data models. The queries mentioned above pose problems to conventional databases, because these databases store only one state of the world - one snapshot - and queries referring to previous states cannot be answered (Snodgrass, 1992). The development of a temporal GIS requires a data model that defines the structure and temporal relations among objects together with operations (Snodgrass, 1992). These operations are given by temporal query languages (Snodgrass, 1992), which makes temporal data models and temporal query languages two important research topics. An example for work on query languages in the field of GIS is given by Yuan and McIntosh (2002). The demand for extending GIS with temporal query languages comes after the work on extending GIS with query languages for space (Frank, 1982); eventually both kinds of query languages need to be integrated.

A fundamental distinction of approaches to integrating time in GIS and databases is the differentiation into object- and field-based approaches. Object-based approaches deal with moving objects like taxis or people and field-based approaches describe the change of fields, which, for example, refers to change in the environment (Galton and

Worboys, 2005). The subsequent discussion of time in GIS focuses on object-based approaches.

Güting et al. (2000) differentiate between discretely moving objects and continuously moving objects. Discretely moving objects are for instance land parcels; changes concerning these objects can be captured by updates of a database (Güting et al., 2000). Continuously moving objects cannot be integrated in a database that easily, because not every single state can be stored in a database (Güting et al., 2000); cars are an example for continuously moving objects. Two ways to represent time exist: change-based and time-based approaches (Al-Taha and Barrera, 1990 as cited in Hornsby and Egenhofer, 1997). In the change-based approach changes in objects are recorded, whereas in a time-based approach time is stored as an attribute of an object.

Changes of objects and semantics of change were investigated in the GIS field (Claramunt and Thériault, 1996; Hornsby and Egenhofer, 1997, 2000; Mountrakis et al., 2002; Medak, 2008). Hornsby and Egenhofer (1997), for example, developed typologies of changes in object states. An object preserves its identity and operations for single objects (e.g., destruct, create) and multiple objects (e.g., merge, combine) are defined. In addition, properties of objects can be manipulated. This leads to a *change description language*, which allows the visual combination of operators for describing the semantics of object change over time (Hornsby and Egenhofer, 1997).

Worboys (2005) moves from an object-oriented to an event-oriented approach. He differentiates between *things* and *happenings* and argues that happenings should be treated as equally important as things in GIS. For the event-oriented approach to be useful “representations, query languages, and techniques for reasoning” (Worboys, 2005, p.2) need to be developed. Worboy’s approach to representing occurrences is the construction of algebraic theories. As an introductory example for the application of his approach, he describes the motion of a vehicle. The paper also contains a conceptual description of how the theory can be used to model geographic phenomena.

Change-based or time-based models can record when, what and where changes in objects happened, which is not enough to represent the logical sequence of changes implied in spatial processes. These models do not explain why changes happened (Pang and Shi, 2002; Brown et al., 2005). Despite the importance of these approaches for addressing the limitations of GIS regarding time representation, the insights gained from these approaches are not directly applicable to process modeling.

3.2 Integration of GIS and Process Modeling Tools

Model builders need the analytical functionality and the capabilities to represent processes of process modeling tools and the capabilities of GIS to process and to visualize spatial data. The technical integration of these two kinds of tools is the logical consequence of the needs of model builders. Different levels of integration are differentiated that are shown in Figure 3.1; the levels of integration are loose coupling, tight coupling, embedded modeling in GIS, modeling tools integrating GIS functionality (Sui and Maggio, 1999). The different levels of integrating GIS and modeling functionality are briefly discussed subsequently; further reviews of the advantages and disadvantages of these approaches are discussed in the literature (Abel et al., 1997; Hornsby and Egenhofer, 1997; Sui and Maggio, 1999; Bivand and Lucas, 2000; Mitasova and Mitas, 2002; Richter, 2008).

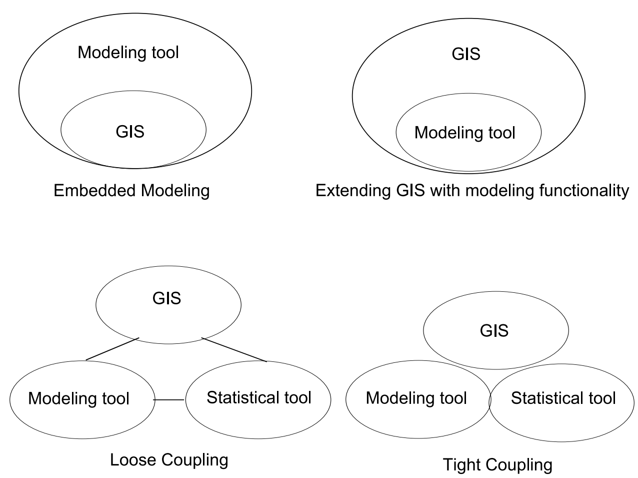


Figure 3.1: For types of coupling as discussed in Sui and Maggio (1999).

Applications of Loose Coupling

Loose coupling connects GIS and modeling tools through data exchange. Every software tool is used independently from the other for specific tasks. Problems occur related to the exchange of data sets and related to the quality of the analysis of spatial relationships.

Examples of applications based on this approach are: Richter (2008) modeled the dispersal of populations and genetic information by combining GIS and partial differential equations; Richter and Seppelt (2002) modeled the dispersal of pollen; Mitasova and Brown (2001) analyzed processes like surface water flow and erosion.

Applications of Tight Coupling

Tight coupling refers to the integration of software through a common interface. In the case that GIS are used as the interface for modeling, models are implemented in GIS programming languages like Python (Mazzoleni et al., 2006). This works only for simpler models, because the programming languages of a GIS do not provide the analytical capabilities required for solving mathematical formulas.

An early example of integrating a dynamic model in a GIS is described in Wickenkamp et al. (1996). For modeling a groundwater system they used an approach based on the conceptualization of processes as stocks and flows. The results were represented in temporal snapshots. The GIS contributed to the spatial representation of results from different study areas, which facilitated planning actions.

Satti and Jacobs (2004) integrated an Agricultural Field Scale Irrigation Requirements Simulation (AFSIRS) and a database management system within ArcGIS. This proceeding established a GIS-based Water Resources and Agricultural Permitting and Planning System (GWRAPPS), which allows the quantification of required irrigation water for farms and regions. They use the database management system to overcome the shortcomings of GIS in dealing with temporal data. The integration of the model in a GIS makes the model spatially explicit rather than a lumped parameter model, which assumes homogeneous distributions of soils, crops, etc. The GIS serves as the user interface to the modeling system and is used for data preprocessing, data visualization and analysis of results.

Wu (1999) proposes to use GIS as a simulation platform for exploring complex spatio-temporal phenomena; the example he uses is the simulation of polycentric urban development. For his simulation he integrates raster GIS and cellular automata. GIS serve again the purposes of data management, analysis, and visualization.

Applications of Embedded Modeling

Embedded modeling in GIS aims at integrating modeling functionality in the GIS environment. One of the first examples of a model built within a raster GIS environment is the Limburg Soil Erosion Model (LISEM) (De Roo et al., 1996). It was built with PCRaster, a GIS based upon Map Algebra (cf. section 3.3). The advantages of integrating modeling functionality in GIS are related to the integration and management of data, the usability of the model, and the abstraction from implementation details (De Roo et al., 1996).

Hofierka et al. (2002) present models of landscape processes in the open source GIS GRASS. The process they model is "shallow surface water flow and sediment transport, including net erosion and deposition" (Hofierka et al., 2002, p.3). They implemented a method to solve partial differential equations in GRASS GIS. The GRASS GIS version 6.3.0 provides a series of implemented models especially hydrological models. The specification of a model in GRASS GIS works via a user interface that requires the user to specify sources of particular parameters and input data.

A dynamic modeling environment based on cell spaces is TerraME (Carneiro et al., 2008). Its strength is the incorporation of spaces with varying characteristics in cellular automata models, agent-based models, and network models (INPE, 2009). TerraME has been tested in applications of land use and land cover change modeling (Carneiro et al., 2008).

Modeling Systems Containing GIS Functionality

Required GIS functionality can also be integrated into specialized modeling software. This approach is chosen in case of complex models that require only a limited amount of spatial analysis functionality. Ecology is an example for a discipline working on models in specialized modeling software that include GIS functionality. The review of modeling tools in section 2.3.2 already mentioned tools including GIS functionality such as the 5D environment and the Spatial Modeling Environment (SME).

Batty et al. (1999) built modeling software for cellular automata models of urban regions. This software provides the flexibility for modeling their projects they could not find in GIS. The modeling software includes some GIS functionality, but is directed towards dynamic modeling and simulation. In simulations of urban dynamics a wide range of parameters can be included and combined, which allows the analysis of many different models. These models also differ in scale, when the dimensions of the spatial system are varied.

Conclusion

I draw the following conclusions from the above review of applications working on the integration of GIS and process modeling tools: GIS functionality is important for model building, because spatial data are part of models describing processes occurring in space and GIS are designed for dealing with spatial data. The named applications focus on a specific process and its modeling rather than on finding solutions for model building including space in general. In addition, the improvement of GIS itself is not addressed in the applications except for the applications of embedded modeling. The resulting *solutions* for integrating GIS and process modeling tools are, therefore, specific to *a* GIS, *a* process modeling tool, and *a* process.

3.3 Extensions of GIS Focusing on Processes

Applications of embedded modeling discussed in the previous section were the LISEM model and models in GRASS GIS. These two examples indicated that some process models were successfully integrated in GIS. This section reviews approaches towards extending GIS with process modeling capabilities providing the basis for modeling processes in GIS in general.

An approach that is at the interface between work in the area of temporal GIS and processes in GIS is the work on complex spatial phenomena by Yuan (2001). Complex spatial phenomena, like rainstorms or wildfires, need a modeling approach that allows to describe their object as well as field characteristics. A wildfire has field-based properties, showing the distribution of the fire in space, and object-based properties like splitting, merging and incarnation. Yuan (2001) proposes to represent these phenomena as a hierarchy of events, processes, and states. The process, in her understanding, explains *how* the phenomenon takes place. By means of the example of rainstorms, Yuan shows how this hierarchical structure can be integrated in a GIS. Her approach allows queries, concerning the number of rainstorms in a certain area, the paths taken by rainstorms, the duration of the rainstorms, etc. In addition, spatio-temporal relationships between the rainstorms and other objects can be queried.

PCRaster (Van Deursen, 1995), Geo-Algebra (Takeyama and Couclelis, 1997), and a modeling framework incorporating a map algebra programming language (Pullar, 2002) build on the idea of Map Algebra and extend it for processes. Map Algebra was established by Tomlin (1990) and provides a generic language for *cartographic* *modeling*, i.e. the analysis and manipulation of raster maps. The strength of Map Algebra is that it defines a set of general functions that can be combined to allow for complex analyses.

PCRaster [1] is one of the first attempts to integrate process models in a GIS environment (Van Deursen, 1995). This environmental process modeling tool extends the idea of Map Algebra with functionality for dynamic modeling. Dynamic modeling functionality needs to be capable of dealing with continuous phenomena such as diffusion, dispersion, motion, and transformation (Van Deursen, 1995). PCRaster is a GIS script language, which is aimed at providing generic functionality for modeling dynamic environmental phenomena. In order to determine the necessary functionality of PCRaster, concrete models were studied. PCRaster does not provide a formalism for the definition of the necessary process components. The implementation of PCRaster and environmental models was done by **?**.

The objective of Takeyama and Couclelis (1997) is to extend the analytical capabilities of GIS for purposes such as design, learning, and gaming by their Geo-Algebra. They recognize the difficulties of modeling processes in GIS related to the different approaches to represent information and mathematical models in GIS and in other modeling tools. The Geo-Algebra allows the description of map dynamics as map equations; map equations relate to the way in which map data are analyzed in Map Algebra. Geo-Algebra also allows the formulation of cellular automata models in GIS. They integrate functionality for "spatial data manipulation and mathematical process modeling" by connecting Map Algebra and cellular automata models (Takeyama and Couclelis, 1997, p.86).

Pullar (2002)developed MapScript, which is a programming language based on Map Algebra that uses fields for representing landscape processes. He extended Map Algebra with functionality for "computing gradients, fluxes, and flows across space" (Pullar, 2003, p.269); this additional functionality is necessary when modeling landscape processes that frequently involve surface flows. MapScript is one component of a proposed process modeling framework, which allows the combination of different modules and their analysis in a raster-based GIS (IDRISI). A key strategy used in this modeling framework is the separation of complex processes into sub processes: a storm event, for example, is composed of modules for "rainfall, loss rate, infiltration, runoff, and visualization" (Pullar, 2003, p.273). Every sub-process is a separate module in the modeling framework, which contributes to the comprehensibility of the

[1] The PCRaster software is available online: http://pcraster.geo.uu.nl/.

modeling of complex process.

The further development of MapScript led to the Vector Map Algebra (VMA) of Wang and Pullar (2005). The VMA is a data structure that is based on vector fields, which are continuous surfaces that show density distributions or potential distributions. The authors state that most physical and landscape processes, the processes they are interested in, can be modeled with vector fields and operations on vector fields. Their idea is to integrate vector fields in GIS based on the ability of GIS to handle scalar fields, i.e. raster data. Their approach allows the modeling of dynamic spatial processes, which is currently impossible because of the inability of GIS to represent and describe changes in state variables across landscape surfaces (Pang and Shi, 2002; Wang and Pullar, 2005).

De Vasconcelos et al. (2002) developed a raster based GIS approach, which integrates functionality for modeling and simulating spatio-temporal phenomena based on theory developed by Zeigler (1976). The Dynamic GIS (DGIS) framework achieves the simulation of the phenomena based on existing spatial data structures. The selection of a discrete-event model is required for simulating a specific phenomenon in the DGIS framework. The discrete-event based approach does not exclude models based on differential equations, because Zeigler et al. (2000) showed a homomorphism between these representations.

Pang and Shi (2002) use a Voronoi model for describing the interaction between processes. Vector or raster data models are not applied, because they "...cannot dynamically maintain topological relations between real world objects" (Pang and Shi, 2002, p.324).The Voronoi structure can represent point, line and area objects and maintains their adjacency relationships by the boundaries of the Voronoi regions. Spatial movement is integrated by the operations switch, insert and delete. An example given in Pang and Shi (2002) describes the effect of a moving air mass on soil patches in a *flow path*, i.e., a set of neighboring patches. In the case of the process of air masses moving over soil patches, there are three processes involved: movement of air masses, changes in soil in the flow path, changes in wind direction. They also show that their process-based model is able to represent the interaction between spatial processes on different scales.

Reitsma worked on a data structure called *nen* (node, edge, node) for advancing themodeling of spatial processes(Reitsma, 2004; Reitsma and Albrecht, 2005). Her objective is to put the process concept first and to store the processes that cause changes in the states of systems explicitly. Her *nen* approach includes rules, spatial extent and attributes of point processes; these pieces of information describe what happens between one state and the next state. She implemented FLUX, a modeling environment based on an open source agent based modeling tool. The examples she presents are the different kinds of processes that take place after rainfall on a hill: Hortonian overland flow, infiltration, percolation, surface ponding, and groundwater flow. Snapshots of the system at different times show which processes are currently active in the region studied. This result is a qualitative account of kinds of processes and interactions of processes that are taking place after rainfall. Her approach allows asking new queries concerning state or change of processes and interactions among processes, which offers new possibilities for the analysis of processes.

In contrast to the applications discussed in the previous section, the approaches presented here focus on providing a general inclusion of processes rather than discussing the integration of a single process in GIS. The above reviewed approaches to integrate processes in GIS all focus on environmental processes, which are physical processes; the use of field-based data structures in the approaches prevails. These data structures are either connected to Map Algebra or to operations on vector fields and partial differential equations.

3.4 Summary

GIS have limitations regarding the modeling and the analysis of spatial processes. A number of approaches related to the integration of time and process in GIS have been discussed in this chapter. I differentiated approaches that are dealing with time in GIS, with the integration of GIS and process modeling tools, and with process modeling in GIS.

The differences in the conceptualizations of space, time, and dynamics in GIS and process modeling tools cannot be overcome by any of the presented levels of integration. Raper and Livingstone (1995, p.253) argue that “the next step should be the fusion of models and spatial representations within new object-oriented environments and *not* the integration of incompatible systems which force representational compromises”. Sui and Maggio (1999) and Albrecht (2008) propose the development of spatio-temporal specifications or high-level common ontologies between GIS and process models as the future direction of space-related process modeling (cf. Hornsby and Egenhofer, 1997; Reitsma and Albrecht, 2005). The present research aims at identifying generic process modeling functionality for a potential extension of GIS.

4 Deterministic Models of Physical Processes

The kinds of models for describing the specifics of processes used in this thesis are deterministic mathematical models formulated as differential equations, respectively, difference equations. Differential and difference equations are mathematical languages that are suitable for expressing the principles underlying the behavior of physical processes. This chapter introduces foundations of physical process models (section 4.1) and the mathematical languages used (section 4.2).

4.1 Foundations of Deterministic Process Models

> "Natura non facit saltus."
> Carl von Linné, Philosophia Botanica (Stockholm, 1751)[1].

The general behavior of a physical process adheres to physical laws and is characterized by the transport of mass and energy typical for physical systems (Abel et al., 1997). Formulating these characteristics in a mathematical language leads to a mathematical model of the process. A "mathematical model is an equation, or set of equations, whose solution describes the physical behavior of a related physical system" (Logan, 2004, p.1).

The fact that quantities such as mass, energy, or momentum are conserved in closed natural systems is fundamental for the development of deterministic physical process models. Because of the conservation principle, change in a quantity of interest in a region can be specified by amounts of the quantity going in or out or being destroyed or created in that region. Models based on this physical principle describe the change in the concentration or density of the quantity of interest in a system over time.

An example for the conservation principle is the conservation of mechanical energy: In a mechanical system, the sum of the kinetic and potential energy of the system at

[1] Wikipedia, Natura non facit saltus, 2009

the final state ($E_{kin,F}$, $E_{pot,F}$) corresponds to the sum of the kinetic and potential energy in the system at the initial state ($E_{kin,I}$, $E_{pot,I}$). When a ball is rolling down a slope the potential energy the ball has on top of the slope is transformed into kinetic energy when the ball rolls down. The total amount of energy in the system is, however, constant over time:

$$E_{kin,F} + E_{pot,F} = E_{kin,I} + E_{pot,I} \; .$$

The view on physical processes in a model can follow the Eulerian or the Lagrangian view, which corresponds to looking at either change or movement (Brown et al., 2005). "The Eulerian view describes the processes that influence properties (e.g., temperature) at fixed locations, and thus is a description of change. The Lagrangian perspective, on the other hand, tracks the changing location of particles through space and, therefore, is a description of movement" (Brown et al., 2005, p.28). The view on physical processes taken here is the Eulerian view.

The establishment of a deterministic model requires the identification of an equation or set of equations that describes the phenomenon of interest. A conceptualization of a process based on stock or storage and flow elements supports the derivation of a model of a process. In this approach to process modeling *storage equations* or *continuity equations* are established; storage equations contain the description of the state variable or state variables, which refer to the quantities whose change is of interest. Storage equations describing the behavior of the process at the system's boundary have to take the boundary conditions into account. The changes in state variables are caused by flows, i.e., inflow and outflow of the quantity in a certain region and sources or sinks of the quantity (Thomas and Huggett, 1980). Storage equations are a conceptual representation of the fundamental conservation principles in a physical system.

An example for a phenomenon being conceptualized based on storage and flow elements is the following: The state variable of interest is the amount of litter available over time. Inflow of litter is caused by leaf fall and timber fall; outflow of litter is due to litter decomposition and translocation of litter to soil (cf. Thomas and Huggett, 1980). Based on the identification of these storage and flow elements a simple model of the process can be built.

As said before, the identification of the quantity of interest and the flows that cause this quantity to change are the core of a deterministic process model. A complete description of a model, however, requires the specification of additional model components that provide information on the system of interest, its boundaries, the initial distribution of quantities, and parameter values.

The domain in which a process takes place can be considered as *continuous* or *discrete* (Thomas and Huggett, 1980). In a continuous representation of a domain values of a quantity can be derived for any possible location. A discrete view on a domain splits a domain into regular or irregular regions, e.g., cells or blocks; the blocks are then homogeneous units for specifying the values of a quantity. The specification of storage equations for the blocks that represent a domain leads to *block models*. These models are used for supporting the conceptualization of a process of interest in this thesis.

The procedure of process modeling resulting in a complete description of a process with a deterministic model consists of the following steps (Thomas and Huggett, 1980):

1. State the problem of interest;
2. Describe the system in which the process takes place including the system's physical components, boundaries, and spatial configuration;
3. Specify the system components, i.e. state variables of interest;
4. Derive storage equations describing the change of the state variables;
5. Specify the flows causing changes of the state variables;
6. State initial conditions, boundary conditions, and parameter values.
7. Solve the equations for the given conditions to show the change in the system over time;
8. Test the model by comparing predicted values with observations of the phenomenon;
9. Adapt the model if necessary.

A mathematical model of a physical process can be expressed in different mathematical languages. I use partial differential equations and difference equations for formulating mathematical models of geographic physical processes (section 4.2).

4.2 Mathematical Languages Used

Differential equations and partial differential equations are used for modeling phenomena in a variety of disciplines such as physics, engineering, biology, economics, etc. They fall into the category of deterministic mathematical models and are generally used to describe dynamic and distributed parameter models. Difference equations are the discrete counterpart of continuous differential equations; a differential equation can always be expressed as difference equation and vice versa. The following sections introduce differential equations, partial differential equations, and difference equations. Section 4.2.4 specifies the operators occurring in mathematical models formulated with difference equations and partial differential equations.

4.2.1 Ordinary Differential Equations

A differential equation is an equation of "an unknown function of one or several variables that relates the values of the function itself and of its derivatives of various orders"[2]. Ordinary differential equations (ODEs) depend on one independent variable and contain derivatives with respect to this variable only. The general form of an ordinary differential equation is (for F being a function in n+1 variables and y' representing a derivative of the function to the independent variable x) (Baron and Kirschenhofer, 1989):

$$F(x, y, y\prime, y\prime\prime, \ldots, y^{(n)}) = 0\ .$$

Fundamental for the description of a process with a differential equation is that the quantity of interest is described by continuous functions (Bastian, 2008). The application of differential equations requires, therefore, that densities or concentrations of a quantity can be meaningfully determined. For this reason, these equations are less suitable for answering questions regarding individual objects, their interactions and behaviors, especially if the independent variable represents space. Differential equations are not an option for building a model of the behavior of a single car driver in a street network; however, the approximation of traffic flow as densities makes a model with differential equations possible (**?**). The characteristics of physical processes and their adherence to material causation make them describable by differential equations (Frank, 2007).

[2]Wikipedia, Differential Equation, 2009

Differential equations are classified by linearity and order. Equations can be linear or non-linear depending on the use of linear operators in the equations; if, for example, a derivative of the unknown function is multiplied by the function itself, the equation is non-linear. The order corresponds to the highest derivative used in the equation.

An example for a model formulated with an ordinary differential equation is the Malthus model that describes population growth. The Malthus model contains the population *F=F(t)*, time *t*, and a growth rate r (Logan, 2004). The model specifies that "the time rate of change of the population F=F(t) is proportional to the population" (Logan, 2004, p.2):

$$\frac{dF}{dt} = r * F,\ t > 0\,.$$

The Malthus model contains time as single independent variable. It derives conclusions about the growth of the object *population*; the model does not directly contain information on what happens to a particular individual of the population.

4.2.2 Partial Differential Equations

Unlike the Malthus model of population growth, which depends solely on time, phenomena may depend on more than one independent variable like time and space. In these cases partial derivatives of the independent variables can be required for describing the change of a variable of interest (Logan, 2004). The kinds of differential equations needed for describing these phenomena are partial differential equations (PDEs). The phenomena of physical geography fall into this category, because either several spatial dimensions or space and time are required for modeling them. The general form of a PDE in one spatial dimension x and time t includes partial derivatives of the unknown function y to both independent variables (Logan, 2004):

$$F(x, t, y, y_x, y_t, y_{xx}, y_{xt}, \ldots) = 0\,.$$

PDEs are a powerful language for the description of the behavior of physical processes founded on conservation laws (cf. Frank, 2001; Logan, 2004; Holzbecher, 2007; Markowich, 2007). A PDE is widely applicable, because "it can be read as a statement about how a process evolves without specifying the formula defining the process"[3]. Because of this property, the same PDE can be used for modeling the behavior of processes that seem very different (cf. Beckmann, 1970).

[3]Encyclopædia Britannica Online, Partial Differential Equation; April 2007

A problem expressed with PDEs is well-posed "if (i) it has a solution, (ii) the solution is unique, and (iii) the solution depends continuously on the initial and/or boundary data (stability)" (Logan, 2004, p.70). The specification of a PDE problem, therefore, requires information on initial distributions of the variables of interest and information on how the process behaves at the boundaries of the problem domain for being complete.

PDE problems are grouped into non-linear and linear PDE problems. Non-linear PDEs have complex characteristics and their solution is often challenging. The starting point of this thesis is well-known, linear PDEs of at most second order. The presented approach may, however, by extended to non-linear PDEs as well.

Linear PDEs of second order are classified into equations modeling wave-like, diffusion-like, and steady-state phenomena. This classification of equations is based on the type the equations have - hyperbolic, parabolic, or elliptic (Logan, 2004). This classification allows some theoretical insights that are useful for the solution of PDE problems. Hyperbolic and parabolic equations referring to wave-like and diffusion-like processes are evolution equations that show the change of a variable of interest over time. These equations lead to initial boundary value problems, which means that initial values and boundary values have to be supplied for solving these problems. Elliptic equations do not contain a time-dependent term and model, therefore, steady-state or equilibrium equations. These equations fall into the category of boundary value problems and require only the specification of boundary values.

When using differential equations for modeling, an important issue is the solution of the equations to get quantitative results from the model. Two main approaches to solving (partial) differential equations exist, namely analytical and numerical methods. Analytical solutions are difficult to achieve for a series of partial differential equations, because these equations can be very complex. Numerical methods generally approximate the continuous equations with discrete representations such as difference equations (section 4.2.3). Some methods for numerically solving PDEs named in Press et al. (1986) are: finite difference method, finite element method, Monte Carlo method, spectral method, and Fourier transform method. Computational issues and numerical analyses of PDEs for environmental models are extensively discussed in, e.g., Holzbecher (2007). In this thesis the solution of PDE problems is outsourced to existing software for numerically solving PDEs (FlexPDE, cf. chapter 8).

4.2.3 Difference Equations

Difference equations are a related mathematical model to partial differential equations. These two representations of processes are exchangeable. A model expressed with differential equations can be transformed in a model formulated with difference equations and vice versa. A previous account of the connection between PDEs and difference equations has been given in Hofer and Frank (2008).

Difference equations are discrete representations of continuous partial differential equations that are used in solution approaches such as finite difference methods. They approximate the continuous equations. Difference equations represent the behavior of a process, i.e. the change of a quantity over time, for discrete time steps t1, t2, t3 etc. by establishing a relationship between successive values of the quantity:

$$x_n = F(x_{n-1}, x_{n-2}, ..., x_1, x_0)\,.$$

Difference equations are chosen to provide the mathematical formulation of storage equations derived from block models in this thesis; the block models are based on a conceptualization of a process with stock and flow elements (cf. section 4.1). In a block model the behavior of a process regarding the conservation of a property and the related flows is specified with storage equations for each block or cell in the system; storage equations for blocks at the boundaries of the system of interest have to consider given boundary conditions.

4.2.4 Operators Used in the Equations

Partial differential equations and difference equations are composed from a short list of operators. These operators describe the physical foundations of a process in an aggregated way, which leads to the wide applicability of PDE models mentioned in section 4.2.2.

The following list of operators and terms are required for formulating difference equations that describe block models; the explanations are based on Thomas and Huggett (1980). Figure 4.1 shows a grid representing prototypical cells in a discrete representation of a domain; the explanations of the terms are related to this two-dimensional grid for clarity. The definitions of the terms can of course be expanded to more than two dimensions.

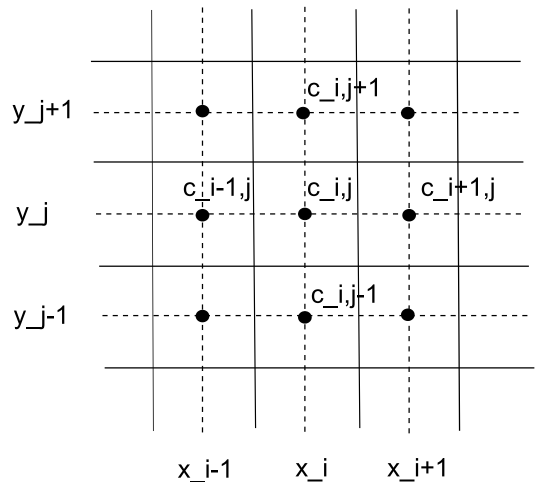


Figure 4.1: Grid representing the center of cells in a problem domain.

- State variable $c = c(x, y, z, t)$: The state variable $c(x, y, z, t)$, or simply c, is the quantity that is of interest in a certain model. The state variable generally refers to the concentration of a quantity; the units of the term are [mass/volume]. The state variable is described by a function in four independent variables in case of a model in three spatial dimensions and the time dimension. In respect to Figure 4.1, the state variable depends on two spatial dimensions $c(x, y)$. A node in the grid of Figure 4.1, e.g. $c_{i,j}$, represents the center of a cell surrounding this node indicated by the dashed line and specifies the value of the state variable in this cell.

- A difference Δc: this term denominates the difference between the values of the state variable c at the beginning and the end of a temporal or spatial interval. A spatial difference, for example in x-direction, is defined as: $\Delta c = c_{i+1,j} - c_{i,j}$; the value of c closer to the origin of the x-axis is subtracted from the value of c to the right of this value in positive x-direction. (A temporal difference is calculated by subtracting the value of c at the beginning of an interval t_1 from the value at the end of an interval t_2: $\Delta c = c_{t_2} - c_{t_1}$.)

- Gradient $grad\, c = \frac{\Delta c}{\Delta x}$: the gradient or *slope* gives the *rate of change* of c over an interval such as Δx. It is calculated by dividing the *difference* of values of c by the size of the interval: $\frac{\Delta c}{\Delta x} = \frac{c_{i+1,j} - c_{i,j}}{\Delta x}$. The gradient is positive when the values of c increase in positive x-direction and negative when they decrease in positive x-direction; the gradient is zero when there is no difference between the values of c. The gradient can be determined in the same manner as exemplarily shown above for all spatial and temporal dimensions involved in a model.

- Second order derivative $\frac{\Delta^2 c}{\Delta x^2}$: The second order derivative is the gradient of two gradients divided by the interval over which the gradients are determined (Δx); it specifies the *change* of the rate of change of c or *curvature*, e.g., at the node $c_{i,j}$: $\frac{\Delta^2 c}{\Delta x^2} = \frac{\frac{c_{i+1,j}-c_{i,j}}{\Delta x} - \frac{c_{i,j}-c_{i-1,j}}{\Delta x}}{\Delta x} = \frac{c_{i+1,j,k}-2c_{i,j,k}+c_{i-1,j,k}}{\Delta x^2}$. The curvature can be positive, negative, and zero. Concave slopes have positive curvature and convex slopes negative curvature; straight slopes have zero curvature (Thomas and Huggett, 1980). As with the gradient, the second order derivative can be determined for all spatial and temporal dimensions involved in a model.

These operators used in difference equations have equivalents in the notation of (partial) differential equations. The intervals involved in the definition of the terms for nodes on a grid are made smaller and smaller until they are infinitesimally small. The application of the limit leads to differential expressions that provide continuous definitions of the terms.

In the context of continuous PDEs two concepts of fields are employed for the specification of the mathematical operators: *scalar fields* and *vector fields*. In a scalar field a scalar is linked to every point in a space; the scalar can, for example, specify temperature or air pressure. In a vector field a vector is associated with every point in space; a vector field is a continuous surface that shows density distributions or potential distributions. Four operators are related to these continuous surfaces: gradient, divergence, curl and Laplace operator. In addition to the state variable, which has the same definition as given above, the operators and concepts used in partial differential equations are (cf. Kemp, 1992; Wang and Pullar, 2005):

- The sign ∂ represents a partial derivative of a term; it can be understood as a difference over a infinitesimal interval.

- The nabla operator ∇ is a vector consisting of the partial derivatives in one, two or three spatial dimensions. The nabla operator for three spatial dimensions is: $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)^T$.

- Gradient *grad*: Applying the nabla operator to a scalar field f, gives the gradient: $grad(f) = \nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right)^T = \frac{\partial f}{\partial x} e_x + \frac{\partial f}{\partial y} e_y + \frac{\partial f}{\partial z} e_z$ with e_x, e_y, e_z

denoting the unit vectors. The gradient of a scalar field results in a vector field in which the vectors point in the direction of the greatest increase; the length of the vectors indicate the rate of change. The gradient can, for example, be used to calculate the slope of the Earth's topography (Kemp, 1992).

- Divergence *div*: Applying the nabla operator to a vector field $V = V(x,y,z)$ gives the divergence of the vector field, which is a scalar field: $div(V) = \nabla \cdot V = \frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z}$. The divergence expresses for every point the tendency of particles to approach the point or move away from the point; it therefore indicates if the vector field contains sources or sinks.

- Curl: Curl is defined for three-dimensional vector fields and describes the rotation at every point in the vector field. It is calculated by the cross-product of the nabla operator with a three-dimensional vector field: $curl(V) = \nabla \times V$. The curl operator is not applied in this thesis.

- Laplace operator $\triangle$: The Laplace operator is a differential operator of second order. The product of divergence and gradient is the Laplace operator for scalar fields, which results in a scalar field. The product of gradient and divergence gives the Laplace operator for vector fields (Kemp, 1992). The definition of the Laplace operator for scalar fields is: $\triangle = div(grad\, f) = \nabla^2 f = \nabla \cdot \nabla f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$. This operator occurs, for example, in models of wave propagation and heat flow.

4.3 Summary

The mathematical languages used for establishing process models in this thesis are partial differential equations and their discrete counterparts - difference equations. These equations describe the behavior of continuous physical processes based on conservation principles. The implied conceptualization of processes is to describe change in concentrations of a quantity by flows of the quantity in a closed system. This view on processes is field-based and objects or events are not specifically considered; it follows the Eulerian view on processes, which describes change. Spatial and temporal scale is implicitly contained in a description of a process by the units of parameters and possibly by the size of blocks defined for difference equations.

5 A Process Description Language

The goals of this thesis are to identify a method to describe process behaviors and to compose descriptions of process components to models. Geographic physical processes are a subgroup of physical processes, which allows the reuse of principles of deterministic process modeling as briefly introduced in chapter 4. The proposed method to establish deterministic models of geographic physical processes is a *process description language*. The process description language consists of the following components (cf. section 1.4):

- a *vocabulary* consisting of mathematical operators to describe the model;
- *composition rules* for connecting the terms of the vocabulary to models;
- a *visual user interface* to guide through the modeling procedure.

This chapter discusses the motivation for developing a process description language (section 5.1) and the approaches to deriving a vocabulary, composition rules, and a user interface of the proposed language (section 5.2).

5.1 Arguments for a Process Description Language

Geographic physical processes are generally studied in the field of physical geography. Water, sediment, precipitation, wind, soil, nutrients, etc. play a vital role in these processes. Terms describing actions that are repeatedly mentioned in this field are: dispersion, deposition, accumulation, translocation, extrusion, interception, weathering, evaporation, etc. (Briggs and Smithson, 1993). The realistic quantitative representation of a process in a specific model is the prevailing subject of modeling these processes. Questions answered with models of geographic physical processes are for example: "How does the depth of overland flow vary in a catchment? How is sulfur dioxide distributed in urban air? How does the concentration of suspended sediment vary in a lake?" (Thomas and Huggett, 1980, p.95).

Models of geographic physical processes are directed towards the detailed description of the specific process at hand. A series of conceptualizations of processes are possible that differ in detail, model type, etc. Consequently, a large set of models of geographic physical processes exists. Approaches dealing with the integration of process modeling functionality and GIS aim at the integration of a specific model into the software packages of choice (cf. section 3.2).

Extending GIS with process modeling functionality that covers the specifics of the large set of existing models is very unlikely to happen. Moreover, integration approaches focusing on a specific model have a limited effect on improving the overall process modeling functionality of GIS. GIS need to be complemented with a generic functionality to represent processes in order to move towards process-enriched GIS. Crow (2000) came to the same conclusion in a review of the Virtual GIS project. She names criteria that have been identified in this project for the development of spatial modeling systems. These criteria include a graphical user interface, a component for the interactive development of scenarios, functionality for spatial analysis and visualization, and "a generic system that operates as a toolbox independent of a specific domain" (Crow, 2000, p.3). The idea of extending GIS with general modeling functionality was already discussed by Hornsby (1996); she started to investigate conceptualizations of spatial spread and had the extension of current GIS with basic abilities to represent dynamic processes in mind.

Previous contributions to process modeling in GIS like PCRaster or the Vector Map Algebra as discussed in section 3.3 are in general directed towards experienced modelers; the tools do provide the required constructs for building a model. A user is, however, not supported at the task of modeling. These contributions assume that their users know the model describing their process of interest. When integrating generic modeling functionality in GIS, non-expert modelers could be users of the modeling functionality as well.

Two specific requirements on the way to GIS with process modeling capabilities are addressed in this thesis: A first step requires an abstraction from details of quantitative models and an identification of prototypical behaviors of geographic physical processes. A second requirement is the development of a general method to describe geographic physical processes and to compose process components to models. This method should be usable for non-expert modelers as well. A *process description language* for geographic physical processes on a qualitative level is the tool I propose to meet these requirements.

5.2 Design of the Process Description Language

According to one of the first linguists, Ferdinand de Saussure, "...all languages have as their basic elements arbitrary signs. They then have various processes for combining these signs, but that does not alter the essential nature of language and its elementary constituents" (Culler, 1976, p.20). By combining the elements of a language - words - complex structures with a certain meaning are created. The same words of a language can be reused in different contexts, which influence their semantics.

The complex structures created with languages follow Frege's Principle of Compositionality: "the Principle of Compositionality is the principle that the meaning of a complex expression is determined by the meanings of its constituent expressions and the rules used to combine them"[1].

This general view on languages names the required components of our process description language: it needs a vocabulary and rules for composing the elements of the vocabulary. The process description language is intended to serve as a computer tool for modeling geographic physical processes. Therefore, an additional component is required for making the language tool accessible: a user interface.

The basis for the development of the process description language is provided by principles of mathematical modeling of physical processes as introduced in chapter 4. As said before, geographic physical processes are a subset of physical processes, which suggests the reusability of knowledge on modeling physical processes. The equations used in a mathematical model are a *language*. They fulfill both requirements of a language: the elements of the equations are the vocabulary and the mathematical constructs used for formulating an equation provide the rules for composing the vocabulary.

The mathematical model resulting from the application of the process description language is a *qualitative sketch model*. The sketch model can be handed on to a process simulation tool contributing quantitative analyses. The identification of elementary process modeling functionality is in the foreground of the development of the process description language. The testing and evaluation of specific models are not discussed in detail in this thesis; these steps have, however, to be performed in practical process modeling.

[1] Wikipedia, Principle of compositionality, 2009

5.2.1 A Conceptualization of Geographic Physical Processes

The development of a process model follows a general modeling procedure introduced in section 4.1. This procedure guides the modeler from the definition of a problem to a mathematical model that comprises the specification of the system of interest, the equations describing the behavior of a process, and the required conditions and parameter values. The modeling procedure related to deterministic models incorporates a conceptualization of processes with stock and flow elements and storage equations.

Partial differential equations and difference equations can both be used for the formulation of storage equations (cf. section 4.2). The process description language can use both representations. Partial differential equations are used for the formal specification of the vocabulary of the language (section 5.2.2). Difference equations are linked to blocks models, because both are discrete representations of a process (cf. section 4.2.2 and 4.2.4). Block models can be used for a representation of flows and components in a system; these models, therefore, support the visualization and development of a process model. Conceptualizing a process with block models can help at establishing the required model. The definition of a model can be done either with difference equations or with partial differential equations, because these formulations are exchangeable.

A geographic physical process occurs in space and we can cut out a small piece of space, a cell or block, and describe the change in the relevant parameters describing the process (Thomas and Huggett, 1980). In a block model the spatial domain is defined as a set of blocks. Blocks can be combined in various ways: they can be aligned next to each other, on top of each other, or on top and besides each other, just as required to represent a process in 1D, 2D, or 3D in the model. For studying, e.g., water flow in a river, blocks may be arranged in a line; for investigating the spread of a pollutant in a lake blocks can be arranged side by side; for modeling the spread of exhaust fumes in the atmosphere blocks can be arranged as a cuboid (Figure 5.1).

Figure 5.1: A sequential alignment of blocks for studying, e.g., water flow in a river.

Part of the conceptualization of the process in a model is the choice of the spatial dimensions of the domain of interest. Geographic physical processes happen in three-dimensional space; reducing the spatial dimensions of a process can, however, facilitate its description in a model. Van Deursen (1995, p.28) discusses possible reductions from 3D to 2D or to 1D: "2D Flow models can be used to describe processes where the third dimension (usually height) is less important, where the magnitude of transport in this third dimension is much smaller than in the other dimensions. This may be the case with groundwater and diffusion processes. 1D Transport descriptions can be used if one direction is dominant, such as the case of infiltration, or if the driving force has a predefined direction, as with overland flow in rugged areas or streamflow in a channel".

An example for the conceptualization of a geographic physical process is given for the process of water storage in a channel. The storage element of this process is the water storage and we are interested in its change over time. In a simplified model the change of the water storage is caused by flow of water down the river and runoff from grid cell (Huggett, 1993). The runoff from grid cell is a source of water in the model that is caused by rain and snow. The water added by rain and the water coming from upriver are the two kinds of flows that have to be considered in the storage equations; Figure 5.2 shows the flows affecting the water storage in a block. The spatial domain of the model can be conceptualized as follows: The model of water storage can be built as 2-dimensional model; the channel is a rectangular object and the blocks at the border of this rectangle have as additional inflow the runoff from gridcells. The process description language will supply the vocabulary for specifying the storage equations in mathematical terms and a user interface for entering the model.

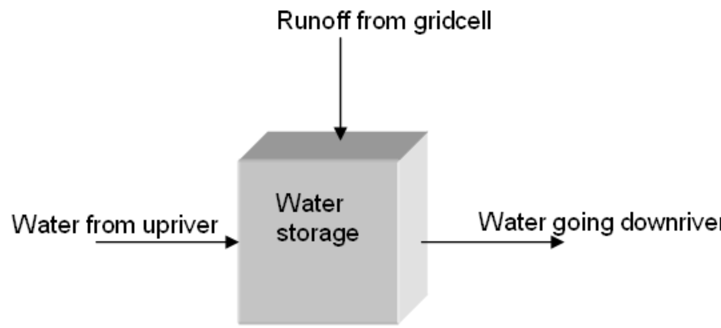


Figure 5.2: Water storage is affected by channel flow and runoff from gridcells.

5.2.2 Approach to a Vocabulary

The vocabulary of the process description language has to provide the means to specify equations and related model components that create a mathematical model of the process at hand. Physical principles, especially conservation laws, provide the basis for deriving the vocabulary of the process description language.

A systematic analysis of the mass conservation law leads to a set of well-known, basic PDEs and provides a physical interpretation of these mathematical formulations. With well-known, basic PDEs I refer to linear PDEs of at most second order. I argue that the equations derived from this conservation law, model prototypical behaviors of geographic physical processes; these equations are considered a starting point for the establishment of a process description language. The same approach can be applied to other conservation laws and combinations of conservation laws like the combination of mass and momentum conservation; the inclusion of these laws leads to an extension of the vocabulary for non-linear PDEs. This extension of the vocabulary is left for future work.

Partial differential equations have long been used for modeling, analyzing, and simulating continuous physical phenomena as well as geographic phenomena (Thomas and Huggett, 1980; Tobler, 1981; Mitasova and Mitas, 2002; Giudici, 2002). The Vector Map Algebra (VMA) introduced by Wang and Pullar (2005) focused on PDEs as well for modeling processes of interest. These previous contributions support the hypothesis that PDEs are a suitable formal tool for modeling geographic physical processes.

The terms of the vocabulary required for specifying the equations describing a process are the main part of the process description language. The language is complemented with components for specifying input data, parameters, and boundary conditions. The equations together with these components provide a sketch model of a process.

Partial differential equations consist of specific terms that are combined by addition. Founding the vocabulary of the process description language on mathematical equations supplies the rules related to the composition of terms of the vocabulary. Composition of terms is fundamental for developing powerful languages. A basic description of a process can be extended by adding additional terms to the original description; this means that single components of processes can be composed to more complex descriptions of processes.

5.2.3 Approach to a User Interface

Which terms of the vocabulary of the process description language have to be combined to describe the behavior of a certain geographic physical process? The assignment of an equation to a process requires guiding the user through the general modeling procedure introduced in section 4.1. This procedure builds on the conceptualization of processes with stock and flow elements and is represented in the user interface of the process description language. The modeling procedure indicates the components required for specifying a model that have to be included in the user interface:

- system of interest,
- equation specification,
- boundary conditions,
- initial conditions,
- parameter values.

The design of the user interface prototype of the process description language is based upon findings by Vass et al. (2006) and is spreadsheet-based. Vass et al. (2006) developed the JigCell Model Builder for modeling biochemical processes. In the course of the development of this model builder they analyzed four options for user interfaces used in modeling software: a graphical diagram for depicting the components of a system and their relationships graphically; a *wizard* consisting of a series of screens for defining the process equations; a script-based interface for the direct input of equations in a text editor; and spreadsheets defining the equation and related laws in a rows of the spreadsheet (Vass et al., 2006). They chose the spreadsheet approach as user interface for their model builder based on the results of usability studies. The conclusions drawn from Vass et al. (2006) study for this thesis are:

- the user interface should provide an overview over the process model during its specification;
- predefined lists of choices should be provided where applicable to reduce errors during data input;
- text-based description should be complemented with graphical depictions of relationships of model components.

A spreadsheet-based interface has the disadvantage that every row appears under the same column title even when the row type does not exactly correspond to these headings (Vass et al., 2006). An advantage of the design approach is the ease of extending the model at hand by adding an additional row specifying an equation term.

5.3 Summary and Expected Contribution

The process description language is a tool for establishing deterministic models of geographic physical processes based on a conceptualization of processes with stock and flow elements. It consists of three main components: a vocabulary derived from conservation laws underlying physical processes, rules for composing the elements of the vocabulary given by mathematical rules, and a user interface for leading the user through the modeling procedure.

The main task of the proposed process description language is the assignment of a mathematical model to a geographic physical phenomenon. The focus is on a qualitative description of phenomena with sketch models. The sketch models comprise the information required for a simulation of the processes with a process simulation tool. However, the sketch models do not compete with detailed and highly-specialized models of processes developed for quantitative analyses.

The process description language is intended to support non-expert modelers at the establishment of general models of a process. It can seen as layer on top of existing process modeling tools in GIS such as PCRaster and the Vector Map Algebra that assume that their users know the specifications of the models of interest (cf. section 3.3).

The development of the process description language is directed towards the identification of areas of improvement regarding process modeling in GIS. This motivation distinguishes the process description language from existing modeling tools such as the spatial modeling environment (SME) and the SIMILE process description language (cf. section 2.3.2). The process description language is intended to support non-expert modelers at the establishment of general models of a process.

6 A Vocabulary Based on Prototypical Process Equations

Models of physical processes require the definition of the following components, which strongly relate to the steps of deterministic model building discussed in section 4.1 (Hofierka et al., 2002):

- configuration space: The configuration space for a model states the choice of a modeling approach together with the specification of state variables, physical parameters and conditions, including initial and boundary conditions.

- interactions between elements of the configuration space: The elements of a process model - fields and/or particles in the work of Hofierka et al. (2002) - interact with each other. Those interactions have to be modeled that “control the modeled process at the given scale” Hofierka et al. (2002, p.2).

- governing equations: The governing equations of physical models are based on natural laws, “which describe the behavior of the system in space, and time” (Hofierka et al., 2002, p.2). These equations were previously referred to as storage equations.

- constituent or state equations: Constituent or state equations are required to fully describe the model of the process; they correspond to the previously mentioned flow elements. “These equations are often based on a combination of physical and empirical approaches and may include a high level of uncertainty” (Hofierka et al., 2002, p.2).

The vocabulary of the process description language needs to provide the terms for specifying the model components stated above. A systematic analysis of conservation laws leads to a set of prototypical partial differential equations that constitute the language’s vocabulary. This chapter builds upon the basics of physical process modeling introduced in chapter 4; section 6.1 provides details on physical process models that are used for the derivation of the language’s vocabulary in section 6.2.

6.1 Components of Physical Process Models

Physical principles underlie the equations of mathematical models as introduced in chapter 4. A fundamental principle is conservation laws that lead to continuity equations; continuity equations correspond to storage equations mentioned in the context of stock and flow elements of models. Continuity equations are completed with constitutive relations that specify specific kinds of flow taking place in a physical system. The provision of a continuity equation with constitutive relations and information on sources or sinks and initial and boundary conditions provides a mathematical description of a process. This section discusses continuity equations (section 6.1.1), constitutive relations (section 6.1.2), and additional model components (section 6.1.3).

6.1.1 Conservation Laws and Continuity Equations

A conservation law for closed physical systems states that the amounts of a quantity going in, going out, being created or destroyed in a control volume have to correspond to the amount of change in the control volume (Logan, 2004). This general conservation principle can be formulated in continuity equations that apply to mass, energy, momentum and other quantities. I focus on the continuity equation for mass.

I use difference equations and the conceptualization of the conservation principle for a block for deriving the continuity equation. The block of interest is referred to as *control volume* in the following derivation (Figure 6.1). The following derivation of the continuity or transport equation is based on Holzbecher (2007).

The change of mass in a control volume given by$\Delta x \Delta y \Delta z$ is expressed by the difference in mass concentration at the beginning and the end of a time interval Δt. The concentration of mass is denoted by $c(x, y, z, t)$ with the units of mass per volume [M/V]; the concentration is the state variable of interest. The term describing the change in mass concentration over time with the units [M/T] is:

$$\frac{c(x, y, z, t + \Delta t) - c(x, y, z, t)}{\Delta t} \cdot \Delta x \Delta y \Delta z \ .$$

The change in the concentration of mass in the control volume is caused by flows of mass across the opposite faces of the block. Flows can occur in all three spatial dimensions. Considering the flow in x-direction, there is the flow across the left face $\underline{\phi_{x-}(x, t)}$ and across the right face $\phi_{x+}(x, t)$ of the block. The area of the face across which a flow takes place is denoted by $\Delta y \Delta z$ for the flows in x-direction. The difference of the flow terms gives the balance between the flows:

$$(\phi_{x-}(x,t) - \phi_{x+}(x,t)) \cdot \Delta y \Delta z \,.$$

The units of mass flow are mass per area times time [M/(L^2*T)]; the multiplication of mass flow by the area of a face gives the flow term the units [M/T]. Flow is positive if mass is added to the control volume and negative if the flows transport mass out of the control volume.

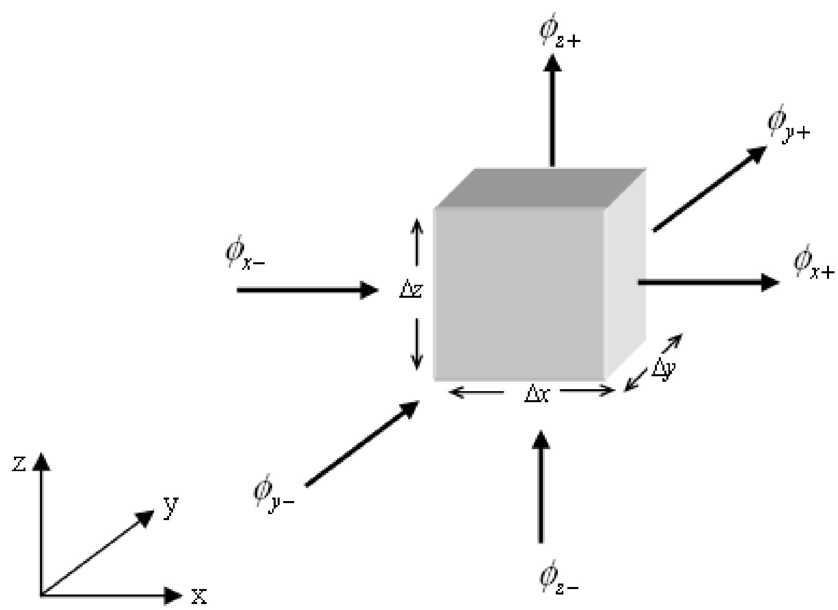


Figure 6.1: Control volume and flows in and out of this control volume.

The continuity equation may contain a source or sink term. Holzbecher (2007) refers to this term as source or sink rate $q(x,y,z)$ with the unity [M/(L^3*T)]; the term is positive when it represents a source and negative when it represents a sink. This term has to be added to the equation as integral term; because of the integral over the volume the units are [M/T]:

$$\int_{\Delta x} \int_{\Delta y} \int_{\Delta z} q(x,y,z) dx dy dz \,.$$

Following the conservation law the change in mass concentration over time has to be equal to the flows of mass taking place and source or sinks in the system. In this derivation only the flows in x-direction are considered:

$$\begin{aligned}\frac{c(x,y,z,t+\Delta t)-c(x,y,z,t)}{\Delta t}\cdot\Delta x\Delta y\Delta z &= (\phi_{x-}(x,t)-\phi_{x+}(x,t))\cdot\Delta y\Delta z \\ &\quad+\int_{\Delta x}\int_{\Delta y}\int_{\Delta z} q(x,y,z)dxdydz\,.\end{aligned}$$

Dividing by the volume $\Delta x\Delta y\Delta z$ gives:

$$\begin{aligned}\frac{c(x,y,z,t+\Delta t)-c(x,y,z,t)}{\Delta t} &= \frac{(\phi_{x-}(x,t)-\phi_{x+}(x,t))}{\Delta x} \\ &\quad+\frac{1}{\Delta x\Delta y\Delta z}\int_{\Delta x}\int_{\Delta y}\int_{\Delta z} q(x,y,z)dxdydz\,.\end{aligned}$$

For making the definition of a gradient applicable (cf. section 4.2.4) the order of the flow terms is turned by extracting *(-1)* from the sum of flow terms leading to the following equation:

$$\begin{aligned}\frac{c(x,y,z,t+\Delta t)-c(x,y,z,t)}{\Delta t} &= \frac{-(\phi_{x+}(x,t)-\phi_{x-}(x,t))}{\Delta x} \\ &\quad+\frac{1}{\Delta x\Delta y\Delta z}\int_{\Delta x}\int_{\Delta y}\int_{\Delta z} q(x,y,z)dxdydz\,.\end{aligned}$$

Taking the limit of Δx and Δt, which corresponds to reducing these terms to infinitesimal expressions, leads to the formulation of the continuity equation as partial differential equation. Taking the limit of the integral source term leaves the source rate $q(x,y,z)$[1]:

$$\frac{\partial c(x,y,z,t)}{\partial t}=-\frac{\partial}{\partial x}\phi_x(x,t)+q(x,y,z)\,. \tag{6.1}$$

The equation resulting from the derivation (Equation 6.2) is called continuity or transport equation in one dimension. Taking into consideration flows across faces in y and z direction of the control volume leads to an extension of the equation in 2D and 3D. The three dimensional version of the continuity equation is:

[1]The explanation of this step for one dimension is: $\int_{\Delta x} q(x)dx=\int_x^{x+\Delta x} q(x)dx = Q(x+\Delta x)-Q(x)$ and $Q'=q(x)$ with Q' denoting the derivative. Now we multiply both sides with $\frac{1}{\Delta x}$ and take the limit: $\frac{1}{\Delta x}\int_{\Delta x} q(x)dx = \frac{Q(x+\Delta x)-Q(x)}{\Delta x}$; $lim_{(\Delta x\to 0)}\frac{1}{\Delta x}\int_{\Delta x} q(x)dx = lim_{(\Delta x\to 0)}\frac{Q(x+\Delta x)-Q(x)}{\Delta x} = q(x)$. This results in $q(x)$ because of the relation $Q'=q(x)$.

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}\phi_x - \frac{\partial}{\partial y}\phi_y - \frac{\partial}{\partial z}\phi_z + q(x, y, z)\,. \tag{6.2}$$

A more compact way to write Equation 6.2 is by using the Nabla operator ∇:

$$\frac{\partial c}{\partial t} = -\nabla \boldsymbol{\phi} + q(x, y, z)\,. \tag{6.3}$$

where $\boldsymbol{\phi}$ is the flow vector:

$$\boldsymbol{\phi} = (\phi_x, \phi_y, \phi_z)^T \ .$$

The specification of the three components of the transport equation, change over time, flow terms and source term, is sufficient for describing the general behavior of a physical phenomenon (Logan, 2004).

6.1.2 Constitutive Relations

The terms $c(x, y, z, t)$ or simply c and $\boldsymbol{\phi}$ in the equation are unknowns, when assuming that sources and sinks are given (Logan, 2004). For describing the unknowns, an additional equation is required: a constitutive relation or state equation (Logan, 2004). These constitutive relations generally define the flow terms of the conservation equation. They give a rule to link flow $\boldsymbol{\phi}$ and concentration $c(x, y, z, t)$ of a substance (Holzbecher, 2007). The definition of the constitutive relations is based on physical characteristics of the system and founded on empirical evidence. Two commonly differentiated kinds of flow are advective flow and diffusive flow.

Advection is transport by flow; the word comes from the Latin word *vehere* that means to carry or to bring. This kind of flow refers to the transfer of a quantity with a certain velocity; the distribution of the quantity thereby remains unchanged. Flow due to advection is described by the product of concentration c and flow velocity v, which can be specific for each spatial dimension (Holzbecher, 2007):

$$\phi_x = v_x c,\ \phi_y = v_y c,\ \phi_z = v_z c\,.$$

Advective flow in different spatial dimensions $\boldsymbol{\phi_a}$ can be written in a more compact form with vector notation; the vector $\mathbf{v}$ contains the velocities in three dimensions ($\mathbf{v} = (v_x, v_y, v_z)^T$)

$$\boldsymbol{\phi_a} = \mathbf{v} \cdot c = c{\cdot}\mathbf{v}\,.$$

Diffusion is the random spread of a quantity due to concentration differences, which implies that the transfer of the quantity is proportional to the concentration of the quantity. This kind of flow is described by the flow of a quantity *down the concentration gradient*; the minus sign in front of the diffusion term assures that the flow goes from higher to lower concentrations of a quantity (per definition the gradient points into the direction of greatest increase, cf. section 4.2.4). The parameter D is the diffusion coefficient describing the diffusivity property of the matrix in the control volume.

$$\phi_x = -D_x \frac{\partial c}{\partial x},\ \phi_y = -D_y \frac{\partial c}{\partial y},\ \phi_z = -D_z \frac{\partial c}{\partial z}\,.$$

The constitutive relation describing diffusive flow $\boldsymbol{\phi_d}$ in vector notation with $\mathbf{D} = (D_x, D_y, D_z)^T$ and the Nabla operator ∇:

$$\boldsymbol{\phi_d} = -\mathbf{D} \cdot \nabla c\,.$$

The flow term $\boldsymbol{\phi}$ in the continuity equation is composed of the advective component $\boldsymbol{\phi_a}$ and the diffusive component $\boldsymbol{\phi_d}$. Depending on the process both advective and diffusive components of flow can be present or either of them can be zero.

$$\boldsymbol{\phi} = \boldsymbol{\phi_a} + \boldsymbol{\phi_{d.}} = \mathbf{v} \cdot c - \mathbf{D} \cdot \nabla c\,. \tag{6.4}$$

6.1.3 Additional Model Components

Initial and boundary conditions are required for making a PDE model consisting of governing equations and constitutive relations well-posed (cf. section 4.2.2). For initial boundary value problems both kinds of conditions need to be specified: initial and boundary conditions. Boundary value problems require only boundary conditions.

Initial conditions specify the concentration of the state variable at time zero. For example, the initial concentration of the state variable can be specified by a function f: $c(x, y, z, 0) = f(x, y, z)$. Boundary conditions specify a condition of the unknown dependent variable at the boundary of the model region. They can be of three different kinds (Holzbecher, 2007):

- Dirichlet boundary condition: provision of a fixed value for a boundary; $c = c_1$ specified.

- Neumann boundary condition: specification of the flux across a boundary by a spatial gradient; e.g., $\frac{\partial c}{\partial x}$ specified.
- Cauchy boundary condition: mixed condition, which means the provision of a value and a flux for a boundary with $\alpha_0$and α_1 being given coefficients; $\alpha_0 c + \alpha_1 \frac{\partial c}{\partial x} = j$.

The specification of initial and boundary conditions together with parameter values depends on the specific process at hand. The choice of the conditions and parameters values is critical for the applicability of a model. Tools like MATLAB support modelers at the identification of appropriate conditions and parameter values that lead to stable solutions of the PDE problems. The focus of this thesis is on modeling the qualitative behavior of a process; the quantification of the models is, therefore, in a mostly abstracted form.

The term $q(x, y, z)$ in the continuity equation (Equation6.2) refers to sources and sinks in the system. In case amounts of the quantity are added to the system, the term is considered as a source; if amounts of the quantity are removed from the system the term is considered as a sink. The source term can additionally depend on time; the term would then be referred to as $q(x, y, z, t)$.

The source or sink term can in more general terms be understood as a function that describes *reactions* in the system. Reactions frequently occur in the contexts of chemistry and biochemistry; they describe the interaction of elements involved in a process model. In the consideration of process models from the viewpoint of geography we refer to source and sink terms rather than reaction terms in the investigated models.

Sources in PDE models can have different characteristics. A source can by a non-point source which means that there is no specific source location but amounts of the quantity of interest are added throughout the considered system. An example for a non-point source would be precipitation adding water throughout the system. A source can also be at a specific location. When thinking of a problem domain being divided into blocks, the source can be thought of being located in a specific block or in a series of specified blocks. Sources may depend on time and add different amounts of a quantity over time or they may be independent of time and, therefore, be constant. The discussion of different characteristics of source terms similarly applies to sink terms.

The single components referring to inputs, outputs, sources or sinks in the system, can require the specification of separate equations. A process description can, therefore, lead to a system of modeling equations. The process' description is not restricted to a single equation that has to capture all influences. In the particular example of water storage in a channel, Huggett (1993) draws up an additional equation for the runoff from grid cell (cf. section 5.2.1). This runoff from grid cell is the sum of runoff from rain and runoff from snow.

6.2 A Vocabulary Consisting of Prototypical Process Equations

Inserting the constitutive relations in the continuity equation and going through possible combinations of terms in the equation leads to a series of partial differential equations. The PDEs that are derived in that way are basic, linear PDEs of at most second order that I consider prototypical process equations. One equation that complements this set of prototypical PDEs, but is not directly established by the combination of terms in the continuity equation, is the wave equation.

The components of the continuity equation (Equation 6.2) as considered in the subsequent analysis are the term referring to time dependent change of the state variable T, the flow term J consisting of the sum of advective flow Ja and diffusive flow Jd, and the source or sink term Q:

$$\frac{\partial c(x,y,z,t)}{\partial t} + \nabla \boldsymbol{\phi} = q(x,y,z)\ .$$

$$T + (Ja + Jd) = Q\ .$$

These terms can be combined in various ways; the different cases resulting from the combination of terms are shown in Table 6.1. The equation names displayed in bold in Table 6.1 are the partial differential equations derived from the analysis of the continuity equation (cf. Table 6.2). Case 3 and the first two combinations shown in case 2 and case 6 are special cases that describe ordinary differential equations (ODEs) when they depend on one independent variable. Case 3, for example, is an ODE that describes growth or decay. The combination of advective flow and a source in the second combination of case 2, can be an ODE modeling advection and growth or decay. These equations are discussed as special cases of transport involving decay in Holzbecher (2007); they have no correspondence in a partial differential

Cases	Setting of Terms	Variation	Equation names
Case 1	$T \neq 0; J \neq 0; Q \neq 0$	T + (Ja + Jd) = Q	**Advection-diffusion equation with source term**
		T+ (Ja + 0) = Q	**Advection equation with source term**
		T + (0 + Jd) = Q	**Diffusion equation with source term**
Case 2	$T = 0; J \neq 0; Q \neq 0$	Ja + Jd = Q	
		Ja + 0 = Q	
		0 + Jd = Q	**Poisson Equation**
Case 3	$J = 0; T \neq 0; Q \neq 0$	T = Q	
Case 4	$Q = 0; J \neq 0; T \neq 0$	T + (Ja + Jd) = 0	**Advection-diffusion equation**
		T + (Ja + 0) = 0	**Advection equation**
		T + (0 + Jd) = 0	**Diffusion equation**
Case 5	$Q = 0; J = 0; T \neq 0$	T = 0	
Case 6	$T = 0; Q = 0; J \neq 0$	Ja + Jd = 0	
		Ja + 0 = 0	
		0 + Jd = 0	**Laplace Equation**
Case 7	$T = 0; J = 0; Q \neq 0$	Q = 0	
Case 8	$T = 0; J = 0; Q = 0$	0 = 0	

Table 6.1: Variations of the continuity equation.

equation and are, therefore, not further considered. Cases 5, 7, and 8 have reasonable interpretation.

Table 6.2 summarizes the PDEs following from the analysis of the continuity equation that I refer to as prototypical process equations. I assume that the identified equations model types of general process behaviors. The equations of Table 6.2 constitute the core of the vocabulary of the process description language. The equations are displayed for one or two spatial dimensions and in vector notation. The diffusion, advection, and advection-diffusion equations are represented without source terms; they can of course have a source term as well.

The equations from Table 6.2 can be grouped into transport processes, steady-state processes, and wave-like processes. Transport processes comprise the diffusion (Equation 1), advection (Equation 2), and advection-diffusion equation (Equation3). These processes appear frequently in applications of geography; this is indicated, for example, in Holzbecher's (2007) book on environmental modeling that discusses

Formulation of 1D or 2D Equations	**Formulation with Vector Notation**	**Equation Name and Number**
$\frac{\partial c(x,,t)}{\partial t} - D * \frac{\partial^2 c(x,t)}{\partial x^2} = 0$	$\frac{\partial c(x,y,z,t)}{\partial t} - \nabla(\mathbf{D} \cdot \nabla c(x,y,z,t)) = 0$	diffusion equation without source term (Equation 1)
$\frac{\partial c(x,t)}{\partial t} + \frac{\partial (v * c(x,t))}{\partial x} = 0$	$\frac{\partial c(x,y,z,t)}{\partial t} + \nabla \mathbf{v} \cdot c(x,y,z,t) = 0$	advection equation without source term (Equation 2)
$\frac{\partial c(x,t)}{\partial t} + \frac{\partial (v * c(x,t))}{\partial x} - D * \frac{\partial^2 c(x,t)}{\partial x^2} = 0$	$\frac{\partial c(x,y,z,t)}{\partial t} + \nabla \mathbf{v} \cdot c(x,y,z,t) - \nabla(\mathbf{D} \cdot \nabla c(x,y,z,t)) = 0$	advection-diffusion equation without source term (Equation 3)
$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = 0$	$\nabla(\mathbf{D} \cdot \nabla c(x,y,z)) = 0$	Laplace equation (Equation 4)
$\frac{\partial^2 c(x,y)}{\partial x^2} + \frac{\partial^2 c(x,y)}{\partial y^2} = q(x,y)$	$\nabla(\mathbf{D} \cdot \nabla c(x,y,z)) = q(x,y,z)$	Poisson equation (Equation 5)
$\frac{\partial^2 c(x,t)}{\partial t^2} - v^2 \frac{\partial^2 c(x,t)}{\partial x^2} = 0$	$\frac{\partial^2 c(x,y,z,t)}{\partial t^2} - v^2 \triangle c(x,y,z,t) = 0$	wave equation, v...wave speed, $\triangle$... Laplace operator (Equation 6)

Table 6.2: Prototypical PDEs derived from the continuity equation.

transport processes but does not contain an account of the wave equation. Steady-state processes are modeled with the Laplace equation (Equation 4) and Poisson equation (Equation 5); the wave equation (Equation 6) models wave-like processes. The discussion of the prototypical process equations in the following subsections is based on Logan (2004) and Holzbecher (2007).

6.2.1 Advection Equation

The advection equation describes the bulk movement or transport by flow of a substance in a transporting matrix. Water or wind are flow fields in which advection takes place among others. Examples for advection processes are the transport of contaminants by the currents of a river and a dust particle or pollen carried by wind (Figure 6.2). The flow direction and velocity v of the transporting matrix determine in which direction and how fast the quantity is transported; the transporting medium constitutes a flow field. The spatial density profile of a quantity being transported shows that the original distribution of a quantity remains and is transported as it is through the flow fields (Figure 6.3).

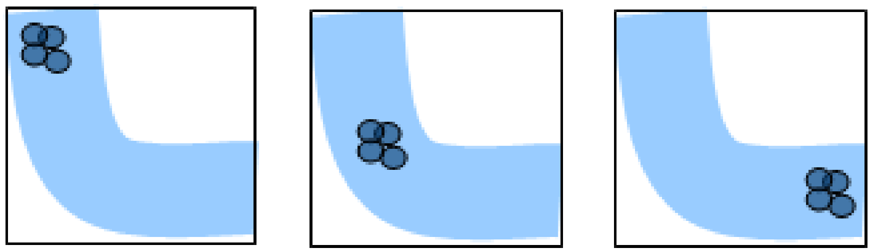


Figure 6.2: Advective transport of contaminants in a river.

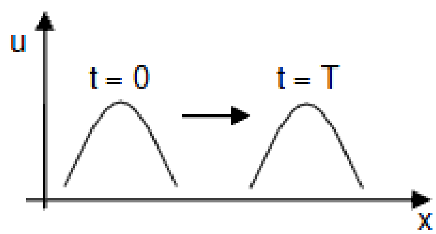


Figure 6.3: Spatial density profile of a transported quantity (Logan, 2004).

The advection equation was Equation 2 in Table 6.2; it is shown again in Equation 6.7:

$$\frac{\partial c(x,y,z,t)}{\partial t} + \nabla \mathbf{v} \cdot c(x,y,z,t) = 0\,. \tag{6.5}$$

The terms included in this equation are:

- The first term specifies the change of the state variable over time.
- Flow term: Advective flow is specified by the multiplication of a flow velocity v with the state variable of interest (cf. Equation 6.5); the v in the equation specifying advective flow has to have the units of length per time, e.g., $[\frac{m}{s}]$. The velocity is depending on the transporting medium and can be constant or varying across space and time. In case the flow velocity is different in the

spatial direction, a vector of the flow velocity is used $\mathbf{v} = (vx, vy, vz)$ as shown in Equation 6.7.

- Sources or sinks: When the advection equation contains a source or sink term, variants of the equation like the advection-decay equation or the advection-growth equation are established.

The advection equation is a time-dependent equation and, therefore, requires initial and boundary conditions to be specified. The parameter value that is required is the flow velocity, which is part of the flow field constituted by the transporting matrix.

6.2.2 Diffusion Equation

The diffusion equation describes a process where a substance spreads from areas of higher concentrations of the substance or areas of higher pressure to areas with lower concentrations or pressure. Diffusive flow is flow down the concentration gradient in a matrix; the rate of flow is proportional to concentration differences. Natural systems have a tendency to balance differences in concentrations, which is the expressed is this process (Holzbecher, 2007). The motion of the particles itself is random. Examples for diffusion processes are the spread of a chemical in standing waters, heat flow in a soil profile, and the flow of water in a porous medium (Thomas and Huggett, 1980). Figure 6.4 gives an impression of diffusing particles. The spatial density profile of a diffusion process is shown in Figure 6.5. It shows that diffusion processes tend to smear out the initial configuration of a quantity.

The diffusion equation was Equation 1 in Table 6.2. It is represented again below in Equation 6.6:

$$\frac{\partial c(x,y,z,t)}{\partial t} - \nabla(\mathbf{D} \cdot \nabla c(x,y,z,t)) = 0\,. \tag{6.6}$$

The terms of the diffusion equation are:

- The first term specifies the change of the state variable over time.

- Flow term: Diffusion is specified by flow down the concentration gradient. Per definition the gradient points into the direction of greatest increase; flow down the concentration gradient is therefore assured by the minus sign in the flow term. The flow term includes the diffusion constant D, which describes the diffusivity characteristics of the matrix in which the diffusion process takes place; it has the dimension of length square per time, e.g., $\frac{m^2}{s}$. D can be a vector of several components accounting for various characteristics of the medium; for more details consult (Holzbecher, 2007, p.49ff). The constitutive relation describing diffusive flow appears with different names in different contexts: Darcy's law models the "flow rate of water in a porous medium" by evaluating the hydraulic head (Thomas and Huggett, 1980, p.99); Fourier's law is used in the context of heat conduction; Fick's first law of diffusion specifies the rate of diffusion of a solute.

- Sources or sinks: The diffusion equation may include a source, respectively, sink term. In the case of a system without sources, the process leads to a balanced distribution of particles in the system. A source or sink term in the diffusion equation leads to the description of diffusion together with growth or decay.

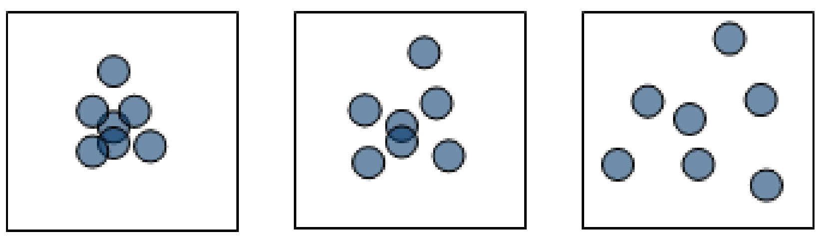


Figure 6.4: Diffusion of particles.

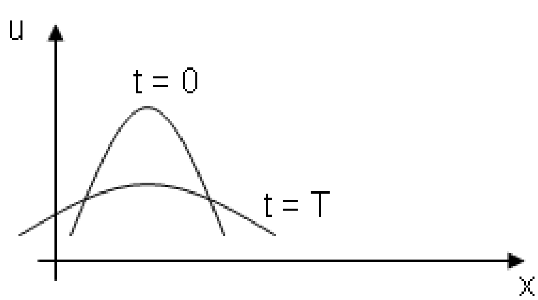


Figure 6.5: Spatial density profile representing a diffusion process after Logan (2004).

The diffusion equation is an evolution equation requiring initial and boundary conditions to be specified. The parameter value needed is the diffusion constant D.

6.2.3 Advection-Diffusion Equation

The total amount of flow in a system consists of the sum of advective and diffusive components of flow (cf. Equation 6.4). Inserting both kinds of flow terms in the continuity equation leads to the advection-diffusion equation. This equation is applied for modeling processes where a substance is spreading randomly down the concentration gradient and at the same time transported by a flow field. Examples for such processes are the spread of exhaust fumes of a factory in the air, the spread of a contaminant in a river, and salt movement in an enclosed sea (Thomas and Huggett, 1980). Figure 6.6 shows particles in a river being affected by the processes of advection and diffusion; this figure constitutes an extension of the example given for advection in section 6.2.1.

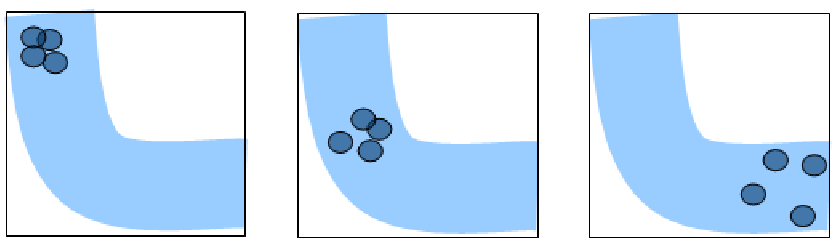


Figure 6.6: Contaminants in a river being affected by advection and diffusion.

The advection-diffusion equation was Equation 3 in Table 6.2. It is shown again in Equation 6.7 for the subsequent discussion of its terms.

$$\frac{\partial c(x,y,z,t)}{\partial t} + \nabla \mathbf{v} \cdot c(x,y,z,t) - \nabla(\mathbf{D} \cdot \nabla c(x,y,z,t)) = 0\,. \tag{6.7}$$

The components of the advection-diffusion equation are:

- The first term specifies the change of the state variable over time.
- The flow term is the sum of the advection and diffusion terms, which were discussed in the previous subsections.

- Source or sink term: the equation may have a source respectively sink term specified, which leads to the advection-diffusion equation with growth or decay.

The advection-diffusion equation is an evolution equation, which requires the specification of initial and boundary conditions. The parameters required are the velocity of the flow field v and the diffusion coefficient D.

6.2.4 Steady-state Equations

A steady-state equation models changes in the amount of a quantity occupying a position in space in a system; it describes steady-state flow in fields. The available amount of a quantity remains unchanged over time. The term including time is zero ($\frac{\partial c(x,y)}{\partial t} = 0$) and the source is a function of space only *q(x,y,z)* (Holzbecher, 2007). "In real systems steady state is achieved when the relevant time-scale for the problem is too long compared to the internal time-scale" (Holzbecher, 2007, p.165). An example for a steady-state process is the flow of groundwater in a certain region with fixed boundary conditions (Kemp, 1992). In the case of groundwater flow the change in amount of groundwater over time can be neglected, because it is a much slower process in comparison to the flow of the available groundwater.

Two representatives of equations modeling this kind of processes are the Laplace equation (Equation 4 in Table 6.2) and the Poisson equation (Equation 5 in Table 6.2). In contrast to the Laplace equation, the Poisson equation contains a source or sink term. The following equation shows the Poisson equation (Equation 6.8):

$$\nabla(\mathbf{D} \cdot \nabla c(x,y,z)) = q(x,y,z)\,. \tag{6.8}$$

Explanation of the terms of the Poisson equation:

- The flow term of the Poisson equation and also of the Laplace equation is the diffusive flow term. These equations are the time-independent versions of the diffusion equation as the analysis of the continuity equation showed (cf. Table 6.1).

- Source or sink term: the source term is only depending on spatial variables and not on time.

This kind of equations is known as equilibrium equation and differs from evolution equations because of their independence of time; a model based on equilibrium equations requires only boundary conditions to be specified.

6.2.5 Wave Equation

A wave-like phenomenon shows an alternation between two opposed states in the system as, for example, states of higher kinetic or potential energy. The wave equation describes the propagation of sound waves or water waves among others.

The wave equation differs from the previously discusses equations, because it does not only depend on the continuity of mass, but also on the conservation of momentum (Logan, 2004). This equation is an evolution equation with the wave speed being the required parameter. The wave equation is (as already shown in Table 6.2 as Equation 6):

$$\frac{\partial^2 c(x,t)}{\partial t^2} - v^2 \frac{\partial^2 c(x,t)}{\partial x^2} = 0\,. \tag{6.9}$$

The two terms in the wave equation are (Equation 6.9):

- Time dependent term: the first term is a second-order derivative in time. In the derivation of the wave equation an advection equation is differentiated in time, which leads to this term. The term corresponds to acceleration, which is the second-order derivative of path in time.
- Flow term: The derivation of the equation starts with an advection term, which is differentiated in space and leads to the second derivative of space in the equation. The term contains the parameter v which is the wave speed.

6.3 Summary

The behavior of physical processes is modeled with mathematical languages. One representative of such a language is partial differential equations. I derived a set of prototypical process equations through a systematic analysis of the continuity equation of mass. The prototypical process equations describe three groups of processes: transport processes, wave-like processes, and steady-state phenomena. The derived equations are assumed to capture the general behavior of prototypical geographic physical processes. The process equations together with additional model components (initial and boundary conditions, parameter values) constitute the vocabulary of the process description language. The equations imply rules for composing the elements of the vocabulary. The vocabulary of the process description language is, therefore, formally grounded on mathematical models used for modeling physical phenomena.

The approach regarding the analysis of conservation laws can be extended to other conservation laws and combinations of laws such as the combination of mass conservation and momentum conservation, which was indicated in the context of the wave equation. Such an extension would lead to the identification of additional PDEs, which could be integrated in the vocabulary of the process description language. Work on the extension of the vocabulary is left for future work; the PDEs that have been identified in this chapter provide the starting point for the specification of the process description language.

7 Using the Process Description Language

The process description language is accessible via a user interface, which is introduced in section 7.1. The application of the process description language is demonstrated by means of two application examples (section 7.2). The presentation of the examples shows how a sketch model of a process is established and how components of models of processes can be composed by using the process description language. The focus of the process description language is on the specification of this sketch model of a process; the testing and evaluation of a specific model are not in the foreground of the discussion.

The process description language is based upon the modeling procedure related to deterministic modeling (cf. chapter 4). This procedure requires to state a problem and to define the system of interest, the state variables and the flows. The starting point for the application of the process description language is, therefore, the knowledge of the physical components of a geographic physical process and an idea of the prevailing kinds of flow. The user can think of a cell or a block and then write down what the quantities of interest are, and what is going in, going out, created or destroyed in a block. This conceptualization captures the conservation principle that underlies a physical phenomenon (cf. section 5.2.1).

The main components of a process model are: state variables, flow laws, sources or sinks. A component referring to the matrix in which a process takes place can help at identifying involved flow laws. In order to specify these components in more detail a user can pose a series of questions:

- State variables: the state variables refer to the quantities changing in the process model. Is there one or several state variables involved in the process? Is the change of the quantities depending on time?

- Matrix: the matrix is the medium in which a process takes place. Is the matrix moving or static? Is it a porous medium? Specifying the matrix gives hints on the existing kinds of flow in a system. For example, if the matrix is a porous medium like soil and the quantity of interest is water, diffusive flow will take place. If the matrix is moving and thus providing a flow field, advective flow can be expected.

- Flow laws: the process description language differentiates between advective and diffusive flow. Advection requires a flow field; diffusion is caused by differences in the concentration of a state variable between neighboring blocks. The third possible flow law is describing wave motion.

- Sources or sinks: Sources or sinks increase or reduce the available amount of a quantity. Is a source constantly adding a quantity to the system or is the source time dependent? Is a source or sink existing at a certain point in space or does add a quantity throughout the study area (like, e.g., rain)?

The description of these model components is completed with a description of the system of interest. The system of interest is specified by choosing the spatial dimension for modeling a process, by determining the geometry of the study area, and by information regarding parameter values, initial and boundary conditions.

The user interface of the process description language is not yet fully implemented and not linked to GIS and process simulation tools. An implementation of a process description tool can be based upon the outline of the system components given in the following subsections; the contribution of this research is, therefore, the identification of the required components for a process description tool.

7.1 User Interface Components

The process description language has to allow also non-expert modelers to derive general descriptions of their processes of interest. The user interface of the process description language is, therefore, intended to guide a user from a (textual) description to a sketch model of a process. The interface consists of five panels for specifying the information required for a sketch model; these panels of the user interface are (cf. section 5.2.3):

- system of interest,

- equation specification,

- boundary conditions,
- initial conditions,
- parameter values.

The screenshots in the subsequent discussion of the components show presentation sketches of the envisioned interface. A future implementation of the user interface has to consider the linkage of the tool to GIS in the long run. Currently the description of a process with the presented user interface is geared to the simulation of the process with the PDE-solver software FlexPDE. FlexPDE is a mathematical tool that solves PDEs on geometrical shapes like cylinders, rectangles, cuboids, etc. In the long run the user interface should use data from GIS as input for the specification of the geometry of the problem domain, sources, parameter values, etc. Real data change the requirements regarding the specification of boundary conditions, because the geometry of the domain of interest would no longer be regular. One could think of a diagram representing the problem domain as blocks and functionality allowing the user to select blocks and specify boundary conditions, source locations etc. The extension of the textual description of a model with a graphical tool was proposed by Vass et al. (2006).

System of interest

The system of interest panel requires the user to specify the name of the model, the system dimensions (1D, 2D, or 3D), the geometry of the problem domain and the dimensions of the chosen geometrical shape (Figure 7.1). Given that the geometry of the problem domain is a cylinder, for example, the dimensions of the geometry could be a radius of 3 meters and a height of 10 meters. Depending on the selected geometry the fields in the boundary conditions panel are updated; the automatic update of related panels is supposed to reduce possible error sources (Vass et al., 2006). As said in the introduction to this section, the specification of the problem domains as geometrical shapes is a simplification that has to be overcome by the integration of GIS data as input for the specification of the system of interest.

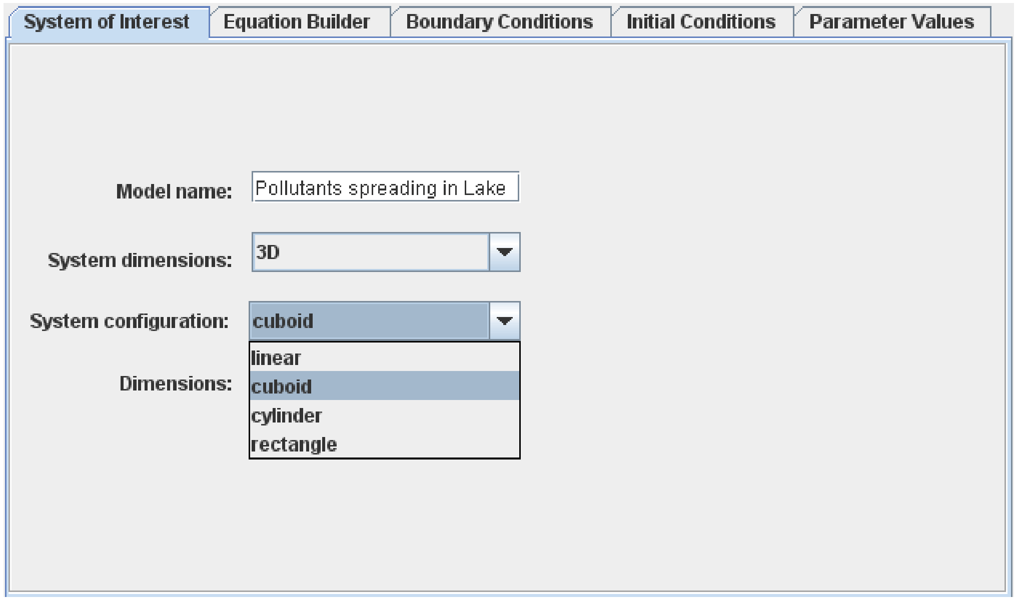


Figure 7.1: Interface panel: *system of interest*.

Equation Builder

The panel for the specification of the model equation is the main part of the interface of the process description language (Figure 7.2). A spreadsheet is used for entering the terms of the model equations (cf. Vass et al., 2006). The main components of a process equation are the terms for the state variable, flow terms and sources and sinks. The state variable thereby corresponds to the name of a layer in the GIS. The state variable is generally time dependent; in case of a steady-state description of a process the state variable is, however, independent of time. The dependence of the state variable on time is accounted for by the introduction of a *time dependent term* that can be included in a model or not. The choice of the flow terms and source and sink terms depends on the process at hand; the number of flow terms and the appearance of source and sink terms, therefore, varies for different models. In the *term* column of the equation spreadsheet, a combo box element provides the following choices of equation terms:

- state variable,
- time dependent term,
- flow law,

- source,
- sink.

The *description* column asks the user to specify the description of the variable in the respective term. The *expression* column contains the mathematical expression in the notation of partial differential equations referring to the selected type of variable term; this expression can automatically be inserted for the terms after giving a name for the state variable. If a term requires additional input by the user, as in the case of a particular source or sink in the system, the expression column can be edited. In the *parameters* column the parameters of an equation term are identified and automatically transferred to the parameter value panel where the detailed specification of the parameters takes place.

A model equation describes the change of a state variable; process models can, however, contain several state variables. Therefore, the equation spreadsheet has to provide the possibility to specify equations for more than one state variable. This could be solved by specifying collections of rows that indicate which terms belong to a specific equation.

The user is given freedom in adding rows referring to the terms included in an equation to build the description of a specific process. There has to be some mechanism to check the combination of terms chosen by the user. This mechanism could be based on an internal comparison of the specified terms with the prototypical PDEs identified as the core of the vocabulary of the process description language (section 6.2). A required extension of the current version of the spreadsheet-based equation builder is the possibility to add new kinds of equation terms as required; these terms may, for example, describe the specifics of source terms in the model of interest.

The model equation describing a process is established by *adding up* the terms specified in the expression column referring to a specific state variable; all terms are added up except the term specifying the name of the state variable. (Referring to the example given in Figure 7.2, the expression C in the first row of the spreadsheet would not be part of the equation.) Addition is the composition rule related to the vocabulary of the process description language. The ability to sum up the expressions defined in the equation spreadsheet indicates how models of processes can be composed by using the process description language.

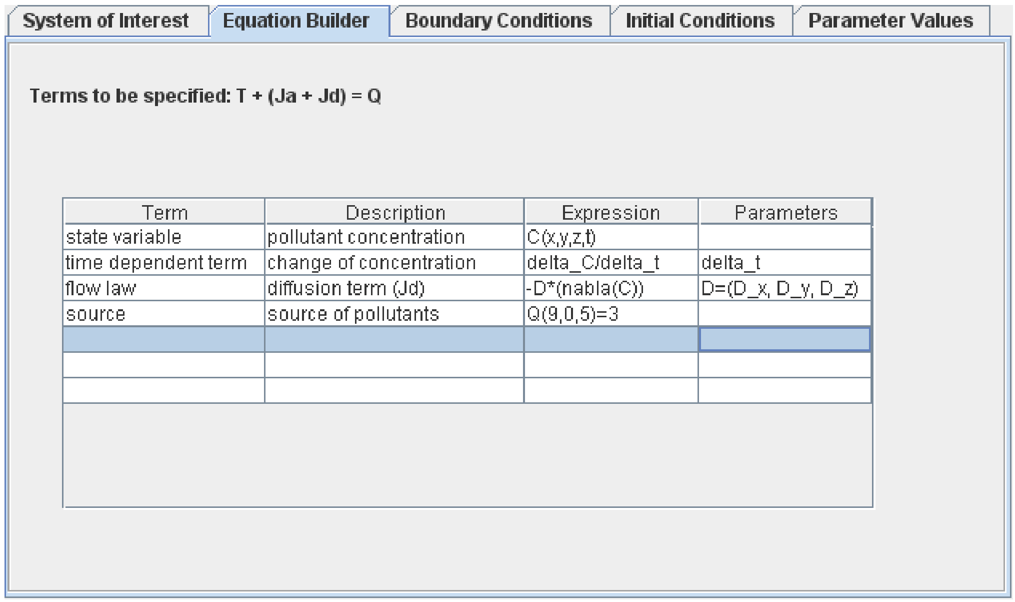


Figure 7.2: Interface panel: *equation specification.*

Boundary Conditions

The boundary conditions panel asks the user to specify the boundary conditions for the given geometry of the system. In the case of, for example, a cylinder the user gives conditions for the bottom, top and cylinder jacket (Figure 7.3). The following options for the specification of boundary conditions are provided:

- no boundary condition: this boundary condition is used in case no diffusion takes place along the boundary (Holzbecher, 2007).
- value: the value boundary condition is a Dirichlet condition that requires the user to set a specific value at the boundary.
- natural: the natural boundary condition describes flow at the outward normal component of the system. If the natural condition is set to zero, *natural = 0*, it represents a reflective boundary condition.
- combined boundary conditions allow to describe specific kinds of flows that take place along a boundary.

The selection of a kind of boundary condition as shown in Figure 7.3 is not sufficient for the complete specification of the conditions. As said above, the value and natural boundary conditions, for example, may require specifying certain values.

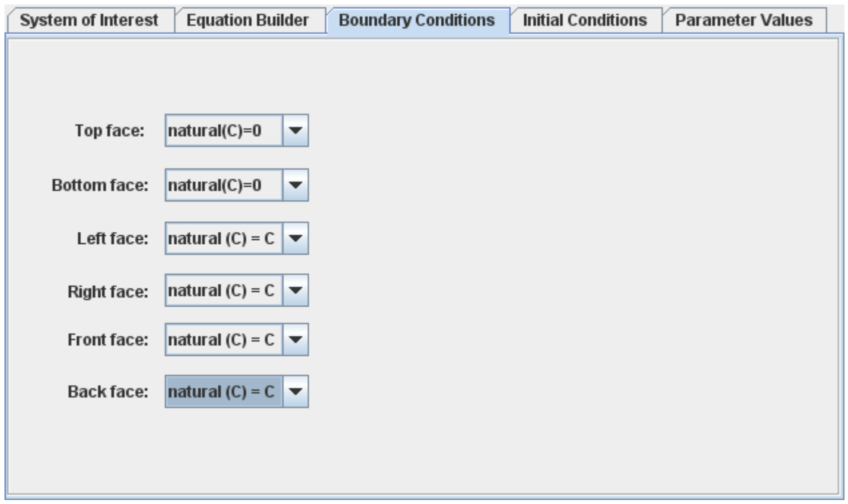


Figure 7.3: Interface panel: *boundary conditions.*

Initial Conditions

The initial conditions need to be specified for the selected state variables; they give the initial distribution of values in the system. The initial conditions may in the long run be given by GIS data. For the simplified example given in Figure 7.4, the specification of initial conditions states that the initial concentration of the quantity is *zero* everywhere except at a specific point in the problem domain; at that specific point the initial concentration of the quantity amounts to 15 units. The specific point can be seen as acting like a source adding a certain amount of the quantity once.

Parameter Values

The parameter names are defined in the equation builder panel and automatically inserted in the table of parameter values (Figure 7.5). The user completes the specification of the parameter values with a description and a value. In the long run, parameter values should be estimated from GIS data.

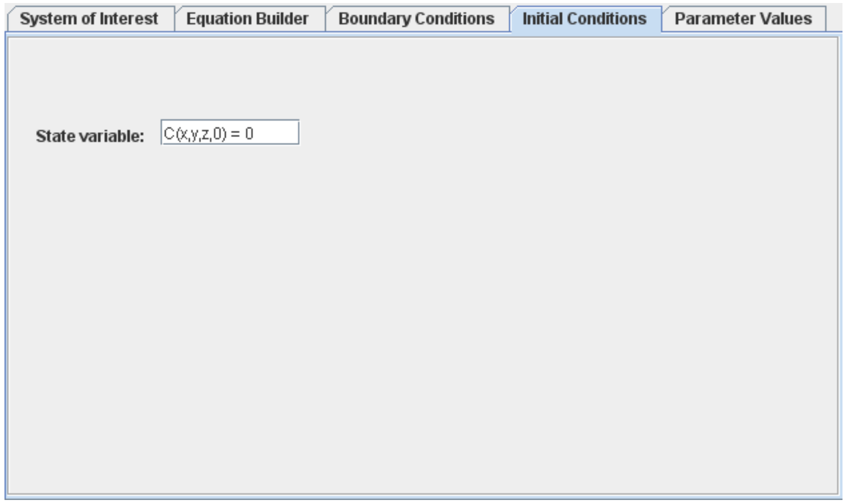
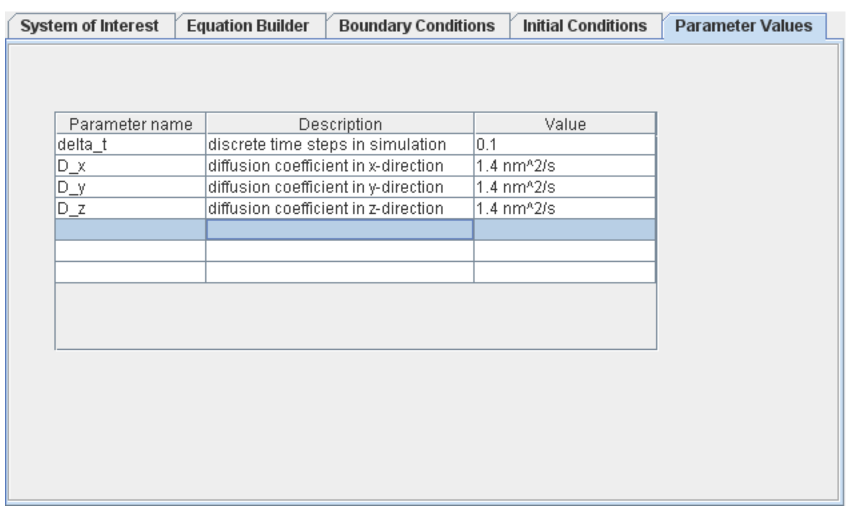


Figure 7.4: Interface panel: *initial conditions*.

The specification of the information in the five panels is sufficient for establishing a sketch model that allows the simulation of a process in a tool like FlexPDE (cf. chapter 8). Two application examples for the usage of the process description language are given in the following section.



Parameter name	Description	Value
delta_t	discrete time steps in simulation	0.1
D_x	diffusion coefficient in x-direction	1.4 nm^2/s
D_y	diffusion coefficient in y-direction	1.4 nm^2/s
D_z	diffusion coefficient in z-direction	1.4 nm^2/s

Figure 7.5: Interface panel: *parameter values*.

7.2 Application Examples

Two application examples are presented that differ in complexity. The first example models how a pollutant spreads in a lake; the second example describes the dispersion of exhaust fumes. The description of the examples starts with the conceptualization of the processes of interest and continues with the specification of the information that needs to be provided for the five panels of the user interface. All parameter values chosen in the following model descriptions are estimated values.

7.2.1 Example 1: Pollutant Spreading in a Lake

The first example investigates how a pollutant spreads in the standing water of a lake; the pollutant is constantly added to the lake by a pipe. The goal of modeling and simulating this process is to answer questions like how the pollutant spreads, how long it takes until a certain amount of a pollutant is diluted in the water, and what pollutant concentrations can be found. A reverse view on the process is possible as well, where one starts from a certain concentration of a pollutant to determine the initial amount of the pollutant that was added to the lake.

For the conceptualization of the process at hand I look at a representative block in the lake (cf. Figure 7.6). The representative block is filled with water and the variable of interest is the concentration of a pollutant in that block. The concentration is changed by amounts of the pollutant coming in and going out of the block across any of the six faces of the block. The movement of the pollutant is caused by differences in pollutant concentrations between neighboring blocks; the center of the distribution of the pollutant is thereby the point where the pollutant is added to the water. The components of the process model are:

- State variable: pollutant concentration is the state variable whose change is investigated over time; the chemical is added to the water as a liquid.
- Matrix: water; in this simple example the water is standing.
- Flow law: differences in pollutant concentration between neighboring blocks leads to a diffusion process. Because the water in the lake is standing it does not provide a flow field; therefore, diffusive flow is the only kind of flow occurring.
- Sources or sinks: the pollutant is added through a pipe into the lake; the source of pollutants is assumed to be constant.

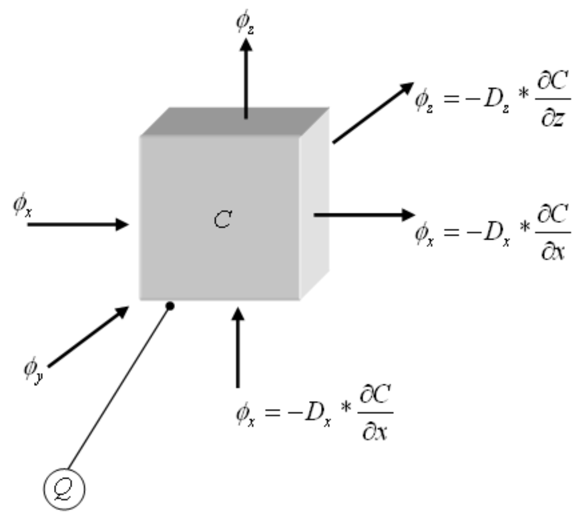


Figure 7.6: Representative block in the problem domain affected by flows.

This qualitative conceptualization of the process provides the basis for the application of the process description language. The information entered into the five panels of the user interface of the process description language is given below.

System of interest

The process takes place in a lake with a complex shape. For simplifying the model I reduce the problem domain to a cuboid that represents the area around the source of pollutants. The problem domain is three dimensional, the sides of the cuboid are 10 meters long and its height is 4 meters. Summarizing the description of the system of interest gives the following entries in the user interface:

- model name: Pollutant spreading in a lake,
- problem dimension: 3D,
- geometry: cuboid,
- geometry dimension: side length 20 meters, height 4 meters.

Equation Builder

The equation builder specifies the model equation. The state variable of interest is the pollutant concentration C; the change of the state variable is time dependent as specified in the second row of the equation builder in Table 7.1. In this example the flow law affecting the change of the state variable is the diffusive flow law that has a diffusion coefficient $\mathbf{D}$ as parameter; the parameter can have different values in the three spatial dimensions. The source Q is located at a certain position and has a constant value of 3 units of the pollutant being added. The source represents a pipe through which the pollutants flow into the lake; this is described by a cuboid with side length 2 around the point with the coordinates *(9,0,5)* in *x, y,* and *z-direction*; it is located above the surface of the lake. The equation builder yet has to be extended with an option for specifying the shape of the source in detail.

Term	Description	Expression	Parameters
state variable	pollutant concentration	*C(x,y,z,t)*	
time dependent term	change of concentration	$\frac{\partial C}{\partial t}$	∂t
flow law	diffusion term (Jd)	$-\mathbf{D} * \nabla C$	$\mathbf{D} = (D_x, D_y, D_z)$
source	source of pollutants	*Q(9,0,5)=3*	

Table 7.1: Pieces of information specified in the equation builder.

Boundary conditions

Boundary conditions have to be given for the cuboid representing the lake and for the cuboid referring to the source. Water can flow across the faces of the cuboid in *x* and *y-direction*; no water can flow across the top and bottom faces of the cuboid. The type of boundary conditions applied is Neumann conditions that refer to the flow across the boundary; these conditons are referred to as natural boundary conditions in the terminology used in the FlexPDE software (cf. section 6.1.3). Setting the natural condition to *0* means that there is no flow taking place. Setting the natural condition to the value of the state variable means that there is flow depending on the present concentration of the state variable C.

- Bottom and top faces: natural(C) = 0,
- Left, right, front, and back faces: natural(C)=C.

The cuboid representing the source can have flow only through its bottom face; all other faces do not show a flow of pollutants:

- Bottom face: natural(C)=C,
- Top, left, right, front, and back faces: natural(C)=0.

Initial conditions

The initial conditions specify the values of the state variable in the problem domain at the start of the simulation. The concentration of the state variable C is set to *0* in this model.

C(x,y,z,0) = 0.

Parameter values

The parameter values come from the expressions stated in the equation builder. In this model we have the change of the state variable over time; the time steps of the simulation are set to *0.1*. The diffusion coefficient is a vector consisting of three components, one component for each spatial dimension. In this model the three coefficients all have the same values. The values themselves represent the estimated diffusion coefficient of the pollutants in water. The parameter values are summarized in Table 7.2.

Parameter name	Description	Value
∂t	discrete time steps in simulation	0.1
D_x	diffusion coefficient in x-direction	1.4 nm^2/s
D_y	diffusion coefficient in y-direction	1.4 nm^2/s
D_z	diffusion coefficient in z-direction	1.4 nm^2/s

Table 7.2: Specification of parameter values for the model.

Resulting Model Equation

The model equation is derived by adding up the entries of the expression column of the equation builder as described in section 7.1. The equation set up by using the process description language is the following diffusion equation:

$$\frac{\partial C(x,y,z,t)}{\partial t} = \nabla(\mathbf{D} \cdot \nabla C(x,y,z,t)) + Q\,. \tag{7.1}$$

Equation 7.1 describes how pollutants that are added by a source diffuse in the problem domain. (The equation corresponds to the diffusion equation specified in section 6.2.2; the flow term has here been moved to the right side of the equation.) This description of the process is very general. One aspect that is neglected, for example, is the reaction of pollutants with bacteria in the water. This reaction destroys some of the pollutants, which means that it acts like a sink of pollutants. The model can easily be extended for this additional model component. Adding a sink to the model requires the insertion of an additional row in the table describing the model equation. The updated equation builder now contains the following rows (Table 7.3.):

Term	Description	Expression	Parameters
state variable	pollutant concentration	*C(x,y,z,t)*	
time dependent term	change of concentration	$\frac{\partial C}{\partial t}$	∂t
flow law	diffusion term (Jd)	$-\mathbf{D} * \nabla C$	$\mathbf{D} = (D_x, D_y, D_z)$
source	source of pollutants	*Q(9,0,5)=3*	
sink	reaction between pollutants and bacteria	*Q2 = - C*0.001*	

Table 7.3: Updated equation builder including a sink term.

The sink is referred to as *Q2*; it occurs throughout the problem domain and depends on the concentration of pollutants. The minus sign shows that it represents a sink in the model; the value of the sink is again estimated. The equation resulting from the extension of the model for a sink is:

$$\frac{\partial C(x,y,z,t)}{\partial t} = \nabla(\mathbf{D} \cdot \nabla C(x,y,z,t)) + Q + Q2\,. \tag{7.2}$$

Looking at Equations 7.1 and 7.2 shows the idea of composability; the model of the process was extended for an additional model component by adding the respective term to the model equation.

7.2.2 Example 2: Exhaust Fumes of a Factory

The second example process is the dispersion of exhaust fumes of a factory. A previous discussion of this example was given in Hofer and Frank (2009). The question of interest in relation to the dispersion of exhaust fumes is where the areas are that are most affected by the fumes (Thomas and Huggett, 1980). In order to answer this question, the spreading of the exhaust fumes in the atmosphere has to be modeled. From the moment the exhaust fumes are released to the air from the smoke stack, they spread continuously and are moved by air currents. The exhaust fumes affect the air quality in a region surrounding the factory. Figure 7.7 gives a picture of the situation sketched above.

Figure 7.7: A smoke stack releasing exhaust fumes to the atmosphere.

The foundation of the model is the assumption that exhaust fumes are subject to mass conservation; the process is investigated in three spatial dimensions. For the conceptualization of the process the change in fume concentration in a representative block of the atmosphere is described. In this block fumes are homogeneously distributed with a certain density that indicates the ratio between fumes and air. The change in fume concentration depends on inputs, outputs, sources and sinks of fumes. The source of fumes is the smoke stack; possible sinks are ignored in this simple model. The inputs and outputs of fumes require the identification of ongoing flows. Fumes spread from areas of higher concentrations to areas of lower concentrations of fumes. Therefore, the amount of flow between two blocks depends on the difference in fume concentration between the two blocks. This characterization corresponds to the behavior of a diffusion process. In addition to diffusive flow, the fumes are transported by air currents. The air currents are modeled as a flow field with a certain velocity and direction of flow. The impact of air currents leads to advective flow. The flow in z-direction also depends on the influence of gravity ρ; this influence is not considered at the moment. The flows acting on a block in this model are shown in Figure 7.8. The components of the process model are:

- state variable: concentration of exhaust fumes.
- matrix: air moved by air currents with a certain velocity and direction.
- flow law: the first flow law involved is diffusive flow caused by differences in fume concentration between neighboring blocks. The second flow law is advective flow, which captures the influence of air currents on the fume distribution.
- sources or sinks: the smoke stack is a constant source of exhaust fumes at a certain location. In the particular model of the dispersion of exhaust fumes, we do not consider possible sinks.

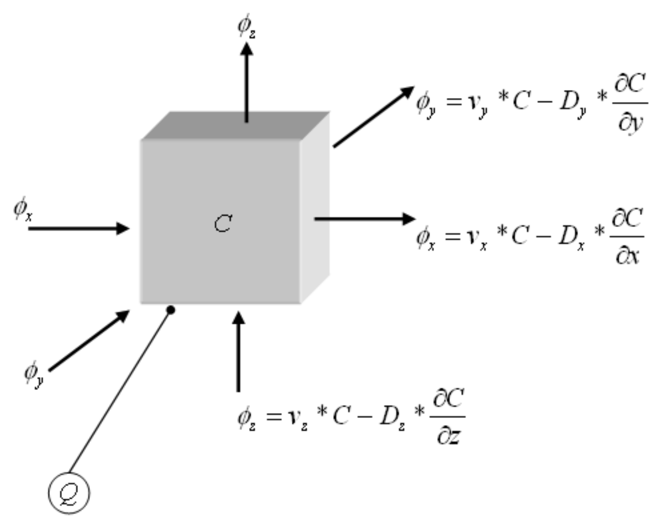


Figure 7.8: Total flow in the model of the dispersion of exhaust fumes.

The conceptualization of the process of the spread of exhaust fumes given above is the basis for the application of the process description language. The pieces of information specified in the five panels of the user interface of the process description language are discussed below.

System of interest

The problem domain is represented by a cuboid around the smoke stack. The problem domain is three dimensional and the sides of the cuboid have a length of 100 meters; the height of the cuboid is set to 50 meters. The system of interest panel of the user interface contains the following pieces of information:

- model name: exhaust fumes from a factory,
- problem dimension: 3D,
- geometry: cuboid,
- geometry dimension: side length: 100 meters; height: 50 meters.

Equation Builder

The equation modeling this process consists of a term describing the change of the fume concentration over time, two flow terms, and a source term. These terms are specified as rows in the equation builder given in Table 7.4. The diffusive flow law includes the diffusion coefficient $\mathbf{D}$, which can have different values in the three spatial dimensions. The advective flow law includes the paramter $\mathbf{v}$, which is a vector giving the flow velocity of the air currents in the three spatial dimensions. The source in this model is the smoke stack that constantly releases exhaust fumes to the air at a rate of 15 units of exhaust fumes. The source is located at a corner point of the problem domain; it is represented by a cuboid with a side length of 2 meters and a height of 50 meters (the equation builder yet has to be extended with an option for the detailed specification of the shape of the source).

Boundary conditions

The boundary conditions have to be set for the cuboid representing the problem domain and the cuboid that acts as a smoke stack. The fumes can flow through

Term	Description	Expression	Parameters
state variable	fume concentration	*C(x,y,z,t)*	
time dependent term	change of concentration	$\frac{\partial C}{\partial t}$	∂t
flow law	diffusion term (Jd)	$-\mathbf{D} * \nabla C$	$\mathbf{D} = (D_x, D_y, D_z)$
flow law	advection term (Ja)	$\mathbf{v} * C$	$\mathbf{v} = (v_x, v_y, v_z)$
source	release of fumes	$Q(0, 0) = 15$	

Table 7.4: The equation builder for the model of exhaust fumes.

all faces of the cuboid of the problem domain except the bottom face if this face is connected to the surface of the earth; no flow is indicated by setting the boundary condition to *0*. As briefly discussed in the boundary conditions section of the previous example, the kind of boundary conditions applied are Neumann conditions. These conditions are termed *natural* boundary conditions in the context of the simulation software FlexPDE.

- Bottom face: natural(C) = 0
- Top, left, right, front, and back faces: natural(C) = C.

The source is a cuboid that adds fumes to the problem domain. The conceptualization of this cuboid in this model is such, that fumes are added along all faces of the cuboid. The boundary conditions for this cuboid express that flow can take place across all faces of the cuboid:

- Left, right, front, and back faces: natural(C) = C,
- The boundary conditions for the top and bottom faces are provided by the boundary conditions of the problem domain.

Initial conditions

The initial concentration of fumes in the air is set to *0*.

C(x,y,z,0) = 0.

Parameter values

The parameter values of model describing the spread of exhaust fumes are summarized in Table 7.5. These parameter values contain estimated values of the diffusion coefficients of exhaust fumes in the air and the flow velocity of air currents in the three spatial dimensions. The air currents show a higher velocity or speed in *x-direction*. In addition, the discrete time steps for the simulation of the model are provided.

Parameter name	Description	Value
∂t	discrete time steps of simulation	0.1
D_x	diffusion coefficient in x-direction	1.7
D_y	diffusion coefficient in y-direction	1.7
D_z	diffusion coefficient in z-direction	1.7
v_x	wind speed in x-direction	5.5 m/s
v_y	wind speed in y-direction	2.5 m/s
v_z	wind speed in z-direction	2.5 m/s

Table 7.5: Parameter values for the model of exhaust fumes.

Resulting Model Equation

The following model equation is established by combining the terms specified in the equation builder (Table 7.4). The general structure of the resulting equation was discussed in section 6.2; the flow terms are here move to the right side of the equation:

$$\frac{\partial C(x,y,z,t)}{\partial t} = \nabla(\mathbf{D} \cdot \nabla C(x,y,z,t)) - \nabla \mathbf{v} \cdot C(x,y,z,t) + Q\,. \tag{7.3}$$

Equation 7.3 is an advection-diffusion equation that models how exhaust fumes spread in the air; the movement of exhaust fumes is caused by diffusion and advection in this model. The resulting equation shows the idea of compositionality again, because the two kinds of flows taking place in the model can simply be added to give the total amount of flow in the system. The extension of the model for additional components is possible by adding other process components of interest.

7.3 Summary

Using the process description language is a procedure comprising several steps. Starting point is a conceptualization of the process of interest. The conceptualization aims at clarifying the general principles that shape the behavior of a process and allow the mapping between the process' behavior and a prototypical process equation. The process description language is accessible via a user interface that consists of the following five panels for describing the behavior of a process: system of interest, equation builder, boundary condition, initial condition, and parameter values. The application of the process description language results in sketch models of processes that contain the required information for a subsequent simulation of the process (cf. chapter 8).

A strength of the process description language is the ability to compose process models by adding a line in the equation builder. This means that additional process components are included in the model by adding a term in the model equation. Thereby, complex application processes can be composed from prototypical process equations. The idea of the composability of model parts was indicated in the first application example, where the model was extended for a sink that accounts for ongoing reactions in the system of interest.

8 Process Modeling in GIS - An Outlook

The process description language provides a versatile vocabulary of limited breadth for modeling geographic physical processes that can be integrated in GIS. The language aims at a qualitative description of the behavior of geographic physical processes with prototypical process equations. The process description language does not aim at competing with existing modeling tools as it is the task of special purpose modeling tools to reach perfection in the creation and analysis of realistic and complex models. The objective behind establishing the process description language is to learn more about the connection between process modeling and GIS. The presented language has two major strengths:

- The elements of the language's vocabulary are composable and allow the stepwise extension of process models. Complex models of application processes can be composed from descriptions of process components.
- The language can be accessed via a user interface that guides through the modeling procedure and supports its users at the derivation of a mathematical model of a process.

The question addressed in this chapter is what the presented language contributes to process modeling in GIS in the long term. The output of the application of the process description language are mathematical models of geographic physical processes; these models can serve as input for process simulation tools. Section 8.1 discusses the simulation of sketch models as a proof of concept regarding the applicability of the derived sketch models for process simulations.

The components of a user interface required for specifying a model in a process description tool were discussed in the previous chapter (chapter 7). Establishing a user interface of a such a tool is not sufficient; a process description tool needs to combine GIS and process simulation tools for deriving input data and generating simulation results. Considerations of a possible framework for the combination of process modeling functionality and GIS are discussed in section 8.2.

8.1 Simulation of Sketch Models with FlexPDE

Sketch models of geographic physical processes resulting from the application of the process description language are a step towards the numerical analysis and simulation of processes. This section shows a simulation of the two example processes discussed in the previous chapter with the PDE solver tool FlexPDE. The quantitative analysis of the models remains simple and is not compared to real world data. The successful simulation of the example processes shows, however, that the information contained in the sketch models is sufficient for a simulation of the process at hand.

8.1.1 FlexPDE Models

FlexPDE[1] is a finite element solution environment for numerically solving partial differential equations. This tool has been successfully applied to simulating processes involving electricity, chemical reactions, fluids, heatflow, magnetism, etc. The problems simulated with FlexPDE can have one, two or three spatial dimensions; the equations involved in a simulation can be linear or non-linear. A screenshot of the FlexPDE software tool is shown in Figure 8.1.

FlexPDE was chosen in this research, because the specification of a model in this tool is strongly related to the components provided by the sketch models generated with the process description language. Other tools to solve PDEs like MATLAB could have been used as well.

The description of a PDE model in FlexPDE is done in a text file having a structure defined by sections; the screenshot in Figure 8.1 shows a part of such a model formulation. The sections that can be specified in the text file are:

- TITLE: indicate the model name.
- COORDINATES: select the coordinate system appropriate for the process model.
- VARIABLES: in the variable section the state variables of interest are defined.
- SELECT: an optional section for specifying details regarding solution methods if a user wants to change the default settings of FlexPDE.

[1] http://www.pdesolutions.com

- DEFINITIONS: parameter values and functions are defined in this section; parameters can represent sources.
- INTIAL VALUES: in case of an initial value problem the initial values for the state variables have to be provided.
- EQUATIONS: section specifying one PDE for each state variable.
- CONSTRAINTS: an optional section which may be used in steady state problems to specify values of integrals.
- BOUNDARIES: In the boundaries section the dimensions of the problem domain and the boundary conditions are set.
- TIME: for a time dependent problem a run time has to be given.
- MONITORS, PLOTS: graphical outputs of the simulation.
- END: this keyword indicates end of script.

For the definition of a model in FlexPDE one has to consider some specifics of this software. FlexPDE does not know any units of quantities; the user has to make sure that the ranges of parameters chosen in the model formulation fit together.

The specification of the problem domain is done in the *boundaries* section of the model description. The keyword *start* specifies a starting point and the boundary conditions are set along a line to the next point in the problem domain; this means that the boundary of a problem domain is set by walking along the periphery of the domain. It is possible with this approach to specify different regions in a problem domain in two dimensions and also in three dimensions. (Regions may be differentiated, for example, by the material they consist of.) In case of three dimensional problems the problem domain is first defined in 2D and then extruded to three dimensions; this is done in the *extrusion* section, which is only part of models defined in three dimensions. Layers of the problem domain can be defined in the extrusion section; the layers themselves may contain different regions. This procedure of defining the boundaries of a problem domain allows the specification of various geometric objects with different characteristics.

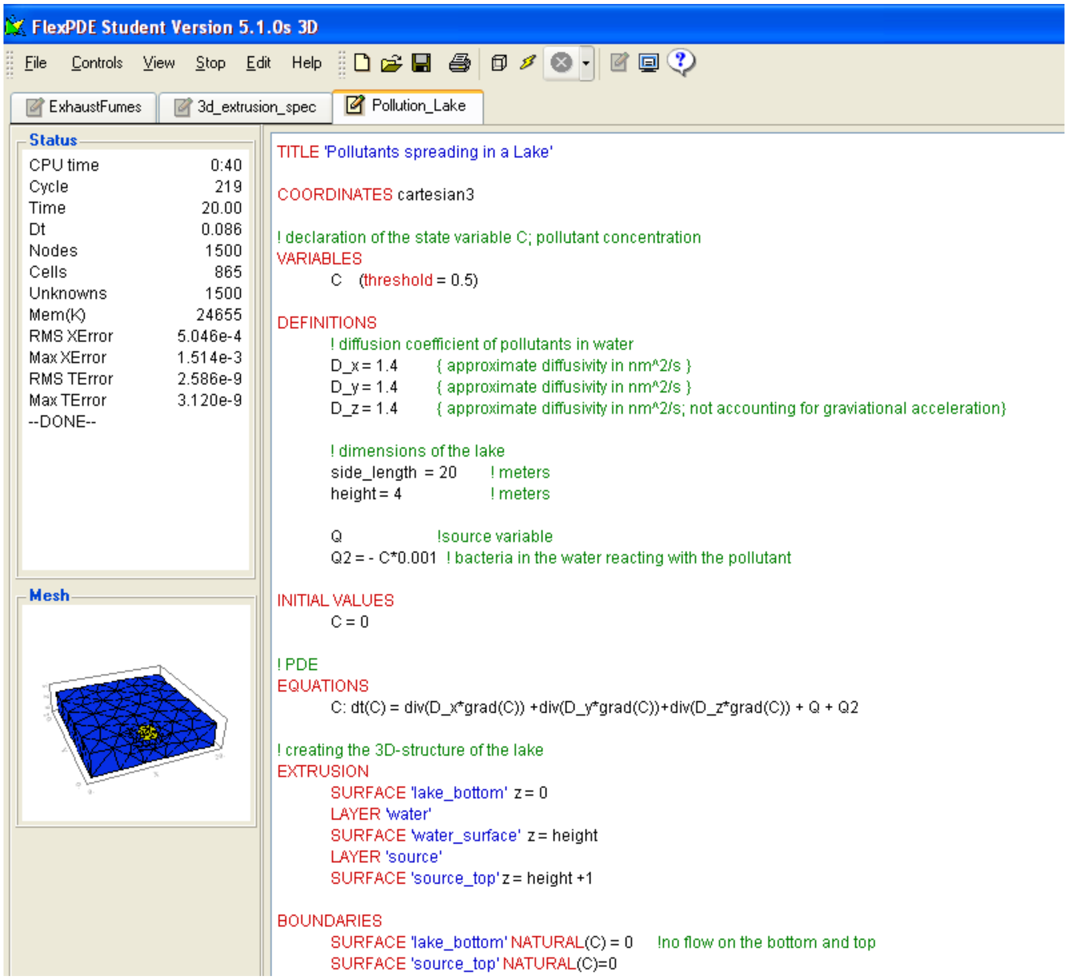


Figure 8.1: Screenshot of the FlexPDE software tool.

There is no specific section in FlexPDE for defining a source. A source is defined in the *definitions* section of the model description by defining a parameter that represents the source. The value or function representing the parameter can be set directly in the respective section or defined in the *boundaries* section. In case the parameter is specified in the *boundaries* section, different parameter values can be set for regions of the problem domain. This idea will be used to describe a region in the problem domain acting as a source in the subsequent simulations of the application examples.

8.1.2 Simulation of Example 1: Pollutant Spreading in a Lake

The description of the spread of a pollutant in a lake with the process description language led to a diffusion equation with a source and a sink (cf. section 7.2.1). For the simulation of this process the sketch model is transferred to a formulation of the model in FlexPDE. The resulting model description in the format of FlexPDE is shown below.

```
TITLE 'Pollutants spreading in a Lake'
COORDINATES cartesian3
!declaration of the state variable C; pollutant concentration
VARIABLES

     C (threshold = 0.5)

DEFINITIONS

     !diffusion coefficient of pollutants in water
     D_x = 1.4
     D_y = 1.4
     D_z = 1.4
     side_length = 20  !dimensions of the lake
     height = 4
     Q             !Q.. source; Q2.. sink
     Q2 = - C*0.001

INITIAL VALUES

     C = 0

EQUATIONS

     C: dt(C) = div(D_x*grad(C)) +div(D_y*grad(C))+div(D_z*grad(C))+
                + Q + Q2

!creating the 3D-structure of the lake
EXTRUSION

     SURFACE 'lake_bottom'  z = 0
     LAYER 'water'
     SURFACE 'water_surface'  z = height
     LAYER 'source'
     SURFACE 'source_top' z = height+1

BOUNDARIES

     SURFACE 'lake_bottom' NATURAL(C) = 0
     SURFACE 'source_top' NATURAL(C)=0
     LIMITED REGION 'water' Q=0
```

```
            LAYER 'water'
            START(0,0) NATURAL(C)=C
            LINE TO (side_length, 0)
            TO (side_length, side_length)
            TO (0, side_length)
            TO CLOSE
        LIMITED REGION 'source_box'
            SURFACE 'water_surface' NATURAL (C)=C
            LAYER 'source' Q=3
            START(8,0) NATURAL(C)=0
            LINE TO (10, 0)
            TO (10,2)
            TO (8, 2)
            TO CLOSE
    TIME 0 TO 20 BY 0.1
    PLOTS
        FOR t = 0 BY 0.1 TO endtime
            CONTOUR(C) on y = 0
            SURFACE (C) on z = 0
            VECTOR (C) on y = 0
    END
```

The formulation of the model in FlexPDE follows the structure of FlexPDE models outlined in section 8.1.1. The specification of the parameters, the state variable C, the initial values, and the equation was directly taken from the information provided on the model in section 7.2.1. The extrusion of the 3D problem domain, the specific setting of the boundary conditions, the statement concerning the time, and the visualization of the simulation are adapted to the requirements of FlexPDE. In the extrusion section the problem domain is divided into a layer *water* and a layer *source*. In the boundary section the boundary conditions for these layers and the respective surfaces are set. The specification of the boundary conditions thereby includes the definition of the problem domain, which is shown in Figure 8.2. The source is modeled by setting the parameter value of Q to the source value in the specified source layer, respectively, source box. The simulation is run for 20 time steps and during this simulation plots are shown.

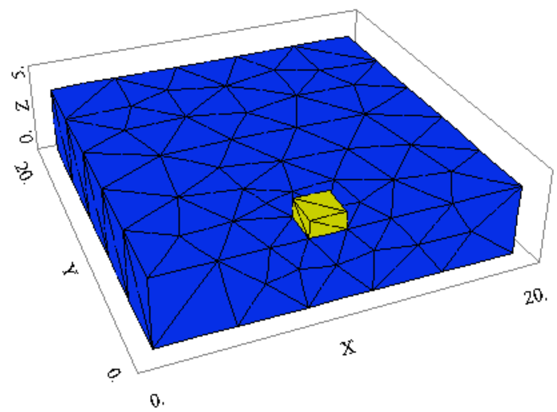


Figure 8.2: Geometry of the problem domain of Example 1.

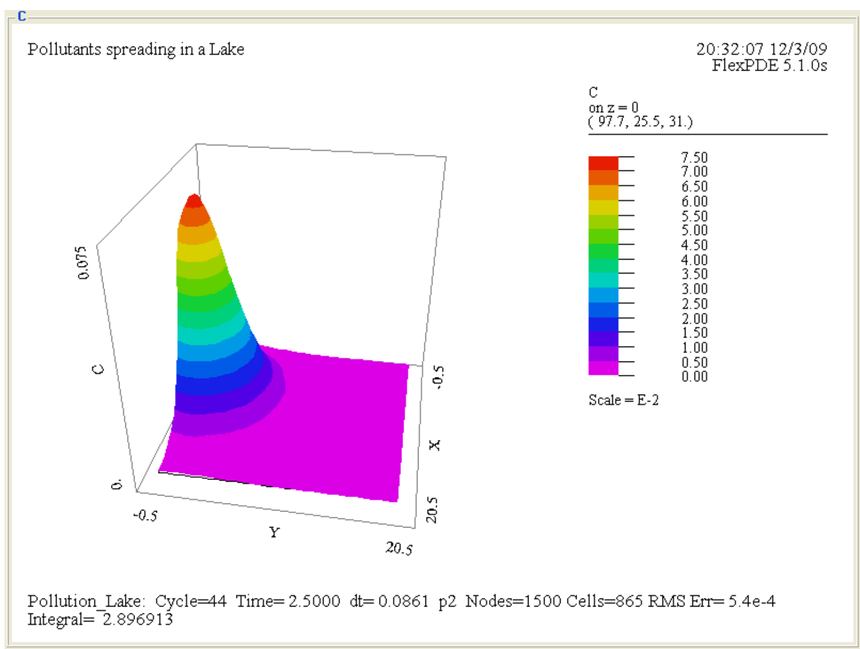


Figure 8.3: Distribution of the pollutant shortly after the start of the simulation.

Figure 8.3 and 8.4 show two snapshots of the simulation of the spread of a pollutant in a lake. The snapshots show a graph of a surface representing the concentration of the state variable, a legend for interpreting the values, and information on how long the simulation is running, how many nodes and cells are used in the calculation, and an estimation of errors.

Since the initial concentration of pollutants is zero, a large section of the problem domain is not yet affected by pollutants in the beginning of the simulation (c.f. Figure 8.3). The highest concentration of pollutants is, of course, at the source location and gradually dropping from there. In Figure 8.4 more time of the simulation has elapsed and the pollutant has spread through the problem domain. The values displayed indicate that the differences in the concentration have been evened out. The distribution of pollutants represented in Figure 8.4 does not change significantly when letting the simulation run longer. The represented behavior of the process is typical for diffusion processes, which reduces differences in concentrations over time.

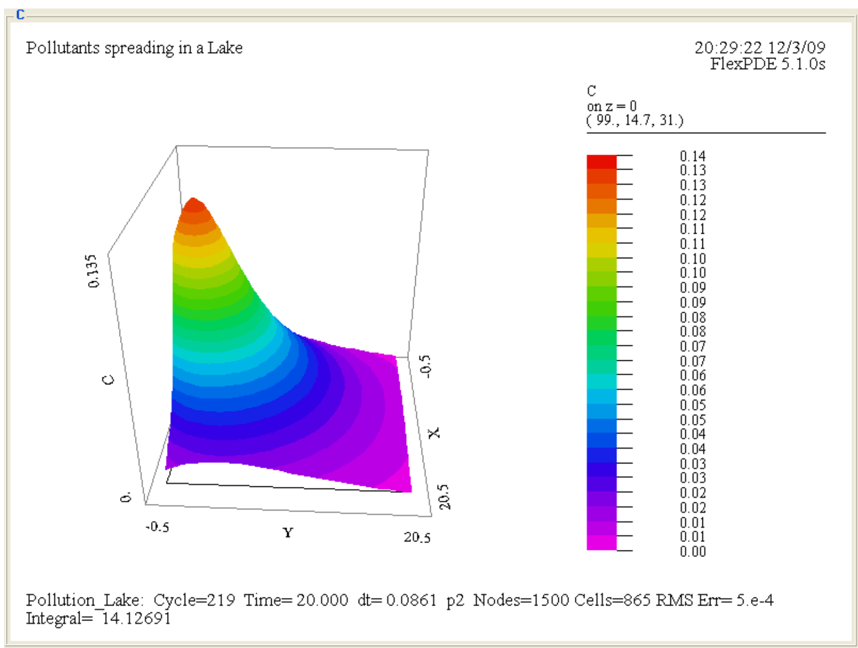


Figure 8.4: Distribution of the pollutant in the lake after 20 time steps.

The simulation shows the qualitative behavior of the process. Since the parameters used in the model simulation are estimated, the quantitative results would have to be compared with observations to check their reliability. In the context of this thesis the important contribution of the simulation is to show that the models established with the process description language contain all pieces of information required for the model simulation.

8.1.3 Simulation of Example 2: Exhaust Fumes of a Factory

The process of exhaust fumes spreading from a smoke stack is modeled with an advection-diffusion equation with a source at a specific location (cf. section 7.2.2). As with the previous example, the sketch model is transferred to a model formulated in FlexPDE. The FlexPDE model description is shown below.

```
TITLE 'Exhaust fumes from a factory'
COORDINATES cartesian3
!declaration of the state variable C; exhaust fume concentration
VARIABLES

     C (threshold 0.5)

DEFINITIONS

     !diffusion coefficient for air
     D_x = 1.7
     D_y = 1.7
     D_z = 1.7
     ! wind speed; stronger wind in x-direction
     v_x = 5.5
     v_y = 2.5
     v_z = 2.5
     side_length = 30 ! side length of the cube
     Q                !source

INITIAL VALUES

     C = 0

EQUATIONS


     C: dt(C) = div(D_x*grad(C)) +div(D_y*grad(C))+div(D_z*grad(C)) -
                - dx(v_x*C) - dy(v_y*C) - dz(v_z*C) + Q

EXTRUSION

     SURFACE 'cube_bottom' z = 0
     LAYER 'air'
     SURFACE 'cube_top' z = side_length/2

BOUNDARIES

     SURFACE 'cube_bottom' NATURAL(C) = 0
     SURFACE 'cube_top' NATURAL(C) = C
     REGION 'air' Q = 0
```

```
        START (0,0) NATURAL(C) = C
        LINE TO (side_length, 0)
        TO (side_length, side_length)
        TO (0, side_length)
        TO CLOSE

     REGION 'smoke_stack' Q = 15

        START (0,0) Natural(C) =C
        LINE TO (2, 0)
        TO (2, 2)
        TO (0, 2)
        TO CLOSE

TIME 0 TO 15 BY 0.1
PLOTS
FOR t = 0 BY 0.1 TO endtime

     CONTOUR(C) on x = 0
     SURFACE(C) on z = 0
     SURFACE(C) on x = 0
     VECTOR (C) on z = 0

END
```

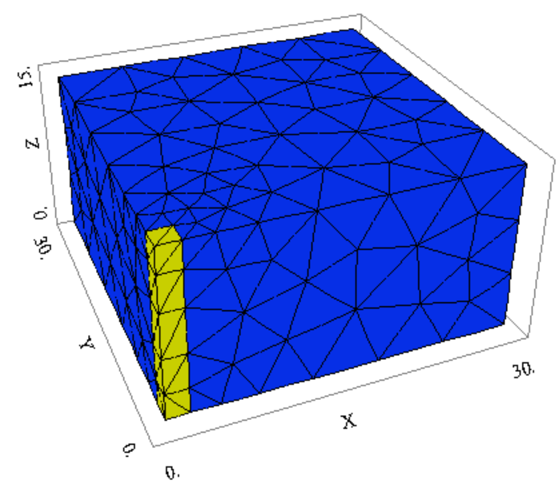


Figure 8.5: Geometry of problem domain of Example 2.

The model formulation in FlexPDE contains the pieces of information specified in the sketch model of the process. The problem domain is a cube with a layer *air* (Figure 8.5). In the boundary section two regions of this layer are defined; one represents the atmosphere and one represents the source. The difference between these regions is that the source parameter is set to the source value in the cuboid modeling the source and set to zero outside this region.

Two snapshots of the simulation are shown in Figure 8.6 and 8.7. Figure 8.8 shows the same snapshot of the simulation as Figure 8.7 as a vector field. In Figure 8.8 the source location is at the corner in the front whereas in the other two figures the source location is at the back of the problem domain, which allows to view the distribution in the problem domain.

Figure 8.6 is a snapshot showing an early time step in the simulation. The concentration of exhaust fumes is highest at the source location and gradually distributes through the problem domain. The surface already shows some indication that the fumes spread more quickly along the x-axis, because the wind speed is higher in this direction. The snapshots in Figure 8.7 and 8.8 are taken at a later point of the simulation and show a distribution that does not change considerably in subsequent time steps. These snapshots show the strong effect of wind on the concentration of exhaust fumes. The higher wind speed in x-direction has the effect that the concentration of exhaust fumes does not spread evenly in all directions as in the previous example; some parts of the problem domain are, therefore, much less affected by the exhaust fumes than others.

As for the previous example the idea behind the simulation was to assess if the sketch model provided the information required for a simulation. The parameter values are estimated and the quantitative results not reliable without comparison to real world observations. The qualitative behavior of the spread of exhaust fumes could be simulated successfully.

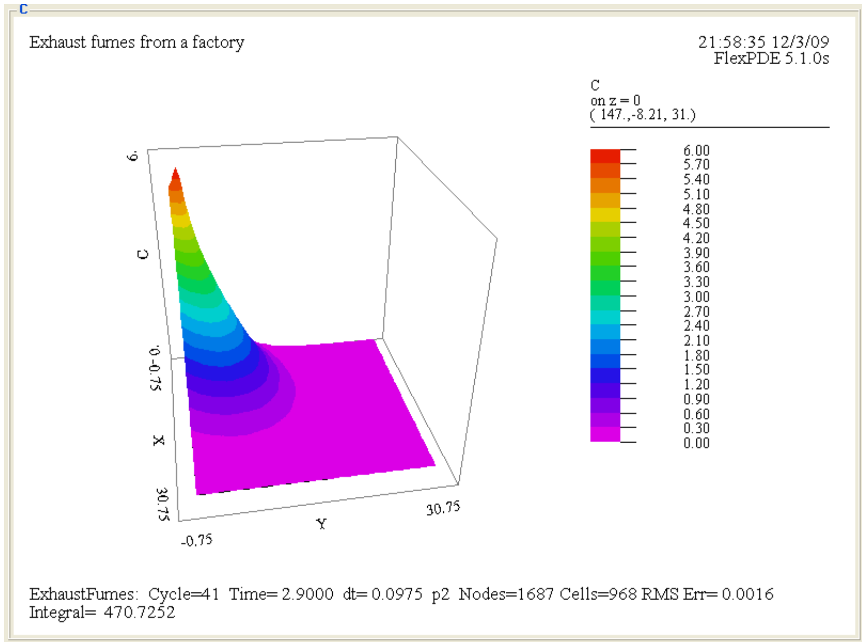


Figure 8.6: Distribution of exhaust fumes shortly after the start of the simulation.

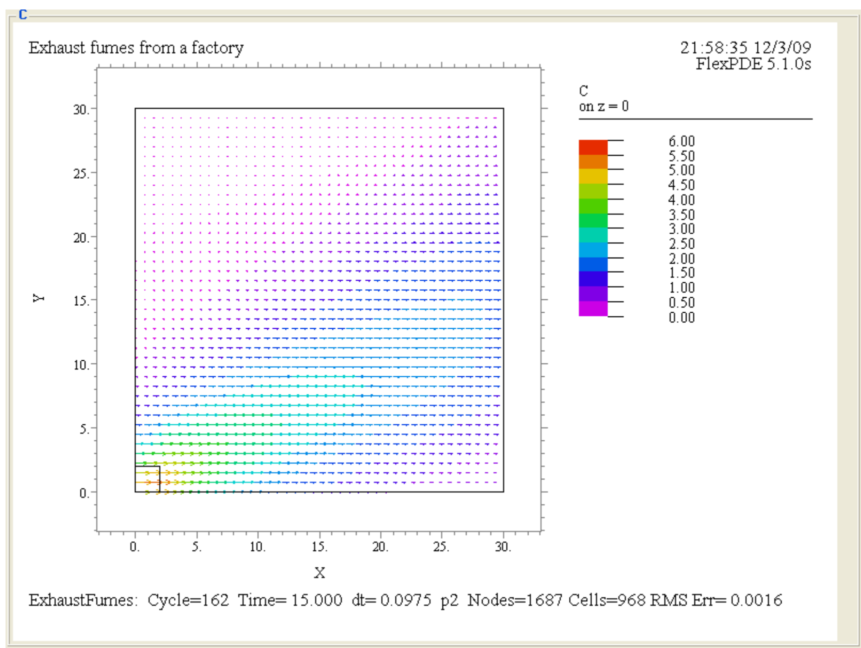


Figure 8.8: Distribution at the end of the simulation represented as vector field.

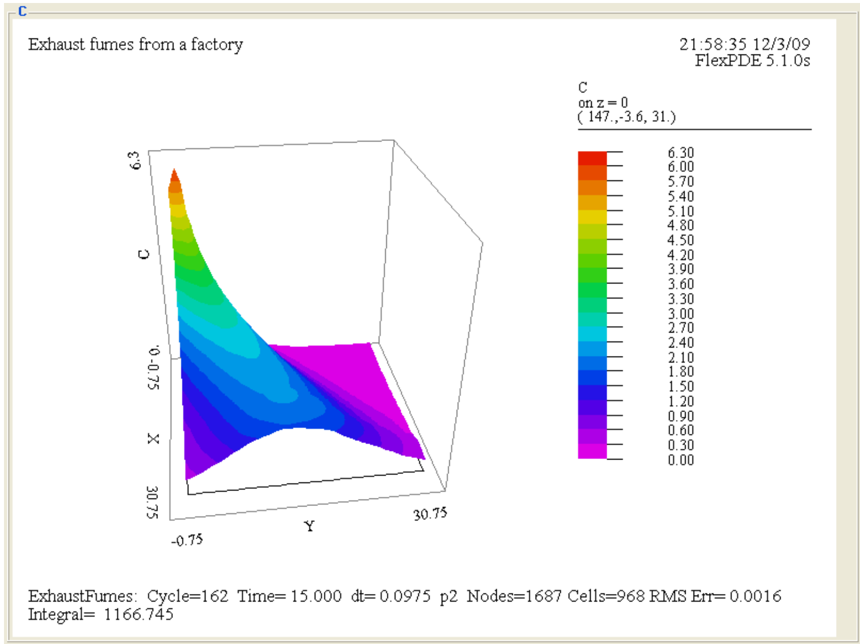


Figure 8.7: Distribution at the end of the simulation.

8.2 Consideration of a Framework for Process Modeling in GIS

Geographic information systems are no process modeling and simulation tools despite the importance of modeling spatial processes. Chapter 3 outlined limitations in the context of process modeling in GIS. Reasons for extending GIS with process modeling capabilities are the potentials of GIS for spatially explicit process modeling and for analyzing patterns in spatial data. In addition, the interoperation of GIS and existing process modeling tools can only be improved when the systems have a common understanding of the exchanged information. Process modelers currently employing GIS for process modeling could, therefore, benefit from GIS with process modeling functionality.

The idea for the development of the process description language originated from the variety of existing process models and process modeling approaches. A tool was considered necessary that allows the qualitative description of geographic physical processes with a manageable vocabulary. The presented process description language is formally grounded in principles of physical process modeling; its vocabulary consists of terms referring to six prototypical process equations. The expressiveness of the vocabulary is ensured by the property of compositionality of the elements of the language.

The process description language clarifies what pieces of information are required for the modeling of a process. It is a tool describing the data and mathematics of a process model at one place. Required data are geometry and dimensions of the problem, boundary conditions, initial conditions, and parameter values. These pieces of information are implicitly contained in the data collections stored in GIS and are ideally automatically derived from existing data sources. For example, the state variable referring to the concentration of exhaust fumes could be a layer in a GIS.

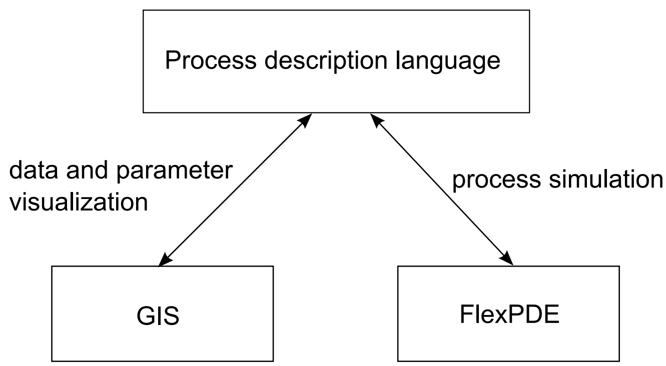


Figure 8.9: The process description language as a link between GIS and FlexPDE.

In a process description tool a request for required data could be sent to a GIS and the process calculations could be done in a mathematical process simulation tool like FlexPDE or MATLAB (cf. Figure 8.9). The results of the simulation should then be integrated and visualized in the GIS. GIS could thereby serve as process simulation tools.

Wang and Pullar (2005) showed by developing the vector map algebra that it is possible to connect models of processes based on PDEs and vector fields with GIS. The path towards an implementation is given by the closeness of raster or voxel representations and block models used in the conceptualization of a process (voxels are three dimensional volume elements used for the visualization of 3D data).

Extending GIS with process modeling functionality following the idea of monolithic GIS is outdated. We envision a framework for process modeling in GIS that follows a service-based approach. However, current attempts to describe processes such as web processing services of the Open Geospatial Consortium (OGC) mainly focus on procedures or schedules rather than the behavior of geographic physical processes. Bernard et al. (2002) worked on interoperable modeling software using standards of the OGC. A possible direction to go from our status quo is to look into integrating the process modeling tool with the layered modeling framework they propose.

8.3 Summary

The process description language leads to sketch models of geographic physical processes that can be simulated with PDE-solver software. The simulation of the two application examples in the software FlexPDE was shown in section 8.1.

The process description language describes the data and mathematics of a process model at one place. The data required in process models describing the problem domain, boundary and initial conditions, and parameter values are contained in GIS. One can think of a tool that sends a request for the required data to a GIS and uses a process simulation tool like FlexPDE for performing the simulation. Simulation results could then be displayed in GIS and make GIS serve as process simulation tools.

9 Results and Conclusions

The specific goal addressed in this research was the development of a method for establishing general models of geographic physical processes. Such a general method for process modeling needs to provide the following: a vocabulary for formulating the model, rules for composing the terms of the vocabulary, and a user interface for guiding through the modeling procedure. These components are provided by the *process description language* for the qualitative description of geographic physical processes. Characteristic for the process description language is that it focuses on process modeling from a GIS perspective and tries to make process modeling accessible for non-expert modelers by providing a user interface. A major strength of the proposed process description language is that it allows the description of process components and the composition of the components to application processes.

This chapter gives a summary (section 9.1) and critically reviews the research on the process description language by discussing the chosen approach (section 9.2) and results and contributions (section 9.3). Section 9.4 concludes this chapter and outlines future work leading further on the path to GIS with process modeling functionality.

9.1 Summary

The main outcome of this research is a *process description language* for the modeling of geographic physical processes. The focus of the process description language is hereby on the description of the general behavior of geographic physical processes. The motivation guiding this research was the identification of generic process modeling functionality that can provide a basis for the extension of GIS with process modeling functionality (chapter 5).

The approach to the specification of a vocabulary of the process description language focused on existing knowledge on modeling physical processes with deterministic models. Geographic physical processes are a subgroup of physical processes, which suggests the applicability of physical principles to the modeling of geographic physical processes. The physical principles referred to are conservation principles that specify the behavior of continuous physical processes. Conservation principles are formulated as continuity equation by using mathematical languages such as partial differential equations (PDEs) or difference equations (chapter 4). The continuity equation is composed by the following three components that describe the behavior of a process:

- specification of a state variable or state variables of interest,
- specification of the kinds of flow that are ongoing together with required parameters,
- specification of sources and sinks in the system.

Based on an analysis of the continuity equation of mass basic, linear PDEs were identified; the analysis considered alternative flow laws and alternative combinations of terms. These PDEs are considered as prototypical process equations and as a starting point for the specification of a vocabulary of a process description language. The terms included in these equations together with a specification of the problem domain, initial and boundary conditions, and parameter values constitute the vocabulary of the process description language (chapter 6).

The structure of the equations provides rules for composing the elements of the vocabulary of the process description language; the composition rule related to the vocabulary is addition. The ability to compose elements of the vocabulary assures that the model of a process can be composed from descriptions of components of a process.

Besides the provision of a vocabulary for modeling prototypical process behavior, a process description tool has to support its users at linking a specific process with the appropriate equation. A user interface was outlined for this purpose (chapter 7); the interface reproduces the general procedure of modeling physical processes introduced in chapter 4. A preparative step for the application of the user interface is a conceptualization of the process at hand according to conservation principles; this step is supported by block models (chapter 5).

The application of the process description language was tested for two geographic physical processes: the spread of a pollutant in a lake and the dispersion of exhaust fumes of a factory (chapter 7). The specification of the behavior of a process together with the indication of required parameters, initial and boundary conditions etc. are the output of the application of the process description language. The resulting models describe the general behavior of the processes and are considered as *sketch models*. The sketch models were transferred to a process simulation tool to test if the model descriptions suffice for a simulation, which was confirmed (chapter 8).

9.2 Discussion of the Approach

A particular modeling approach was chosen for establishing the process description language. This approach reverses the usual modeling procedure in which the tool is selected based on the process at hand (Lowry, 1965). An alternative approach towards developing a process modeling tool is the analysis of existing models and the derivation of required modeling functionality from these models. This approach was applied for developing the PCRaster software (cf. section 3.3). Predefining the modeling tool has the disadvantage that the processes that can be modeled have to fulfill requirements implied in the modeling approach. The advantages are that a formal basis for the specification of process modeling functionality is established and the completeness of the proposed vocabulary can be assured. In addition, the diversity of existing modeling approaches made it necessary to choose a particular approach for identifying generic process modeling functionality.

The choice of the particular approach is justified with the focus on geographic physical processes in this thesis. With geographic physical processes being a subset of physical processes, the reusability of existing deterministic modeling approaches can be assumed and has been successfully employed before (Thomas and Huggett, 1980; Wang and Pullar, 2005). The vocabulary of the process description language is appropriate for modeling the general behavior of geographic physical processes.

A process modeled with the proposed language has to comply with the conceptualization of continuous processes implied in the approach. Although the link to physical processes is strong, all processes - even social processes - that can be conceptualized based on state variables and flows laws, can be modeled with the process description language.

The restriction to geographic physical processes led to the successful establishment of a description language for geographic physical processes. This restriction constitutes a limitation, because a considerable group of spatial processes are initiated by social or political forces in contrast to physical forces. To what extend the currently available process description language is applicable to the modeling of geographic social processes has yet to be analyzed. Social and physical processes are ontologically different. The problem with the application of physical principles on social phenomena is twofold: people have their own will (cf. information causation); flights, telephone calls, long journeys with cars, etc. lead to unconnected, i.e., discontinuous, spaces. In some cases the general approach to model building focusing on changes in densities of quantities could be applied to social processes as well. A city, for example, can be seen as a system and the ongoing processes in the system can be understood as flows of people, ideas, goods, etc. Some social relations do strongly relate to physical principles: the amount of violence, for example, may depend on the gradient of economic power. In an area with a large discrepancy between economic power of people living close to each other, more violence is taking place when compared to the amount of violence in areas with a lower discrepancy in the economic power of people.

The derivation of the prototypical process equations is based on the continuity equation of mass. The identified partial differential equations are basic, linear second-order PDEs that are referred to as prototypical process equations. Because of the systematic analysis of the continuity equation, the derived equations are exactly those required for modeling processes grounded in the continuity equation of mass. The set of derived PDEs has a long history and wide applicability to processes in physics. The prototypical process equations are a first approach to a vocabulary of a process description language.

The analysis of linear, second-order PDEs excluded some PDEs and systems of PDEs that are used in environmental models like the Navier-Stokes equations, St. Venant equations, and Euler equations for the time being. For the derivation of the mentioned equations the continuity equations for mass and for momentum have to be combined (Sonar, 2009). The Navier-Stokes and St. Venant equations model processes of water flow such as Hortonian overland flow (Holzbecher, 2007). The analysis of conservation principles other than mass conservation and the combination of the resulting continuity equations opens a view on other PDEs and leads to extensions of the current vocabulary of the process description language. The present research does provide the methodology for extending the vocabulary by analyses of additional conservation laws.

The grounding of the process description language in mathematical models leads to the advantage that rules for composing the elements of the vocabulary are provided together with the terms of the mathematical models. The composition of terms applies to the establishment of the equations and likewise to the combination of simulation results. The process description language provides the means to add components that extend a model; these components can describe additional influences on a process like flow fields in the problem domain or additional sinks or sources. Based on the idea of composability, model equations of application processes can be extended step by step and eventually include various influences on the system of interest.

9.3 Results and Contributions

This research abstracted from details of quantitative process modeling in order to identify generic process modeling functionality that describes the behavior of processes on a qualitative level. The derived modeling functionality is encapsulated in a process description language that provides a vocabulary for assigning model equations to geographic physical processes. The presented process description language together with a user interface guiding the user through the modeling procedure are the major results of this thesis. The process description language allows to describe models of geographic physical processes; these models can be composed from descriptions of components of a process.

A language is powerful when its simple elements can be composed to complex expressions (cf. section 5.2). The process description language consists of the terms required to construct process equations; these terms are composed by addition. The composability of the elements of the language's vocabulary is the major strength of this language. The first application example of the process description language indicated how a process description can be extended by adding an additional component (cf. section 7.3.1). A simple description of the process of a pollutant spreading in a lake was extended for a sink of pollutants, because the modeler found out that pollutants are reduced by reacting with bacteria in the water. The change in the existing model was simple: it required the adding of a sink term in the model equation.

The process description language serves as sketching tool for processes. Non-expert modelers are given the possibility to specify the characteristics of a process on a qualitative level. In case the models are used for quantitative analyses, they can be linked to existing modeling tools providing the corresponding functionality. On the one hand, this quantitative analysis could be performed with mathematical tools like FlexPDE or MATLAB (cf. chapter 8). On the other hand, the process description tool could serve as layer on top of existing spatial process modeling tools such as PCRaster (Van Deursen, 1995) or the vector map algebra (Wang and Pullar, 2005); the purpose of linking the process description tool and these existing tools is, thereby, to support the users at specifying the model.

The simulation of the application examples in chapter 8 showed that the sketch model established with the process description language can be simulated. This research, therefore, identified what pieces of information have to be provided in a user interface of a process description tool. The implementation of such a tool can be based upon these findings.

9.4 Conclusions and Future Work

Three main issues need to be investigated further in the context of the process modeling language: the evaluation of resulting process models, the extension of the current vocabulary, and the implementation of a process description tool.

The establishment and simulation of models of two processes were discussed in chapter 7 and chapter 8. The next step in the process modeling procedure would be an evaluation of the models. The models created with the process description language are simple and largely ignore practical issues of process modeling regarding parameter determination, data provision, etc. These issues have to be considered in case the established models shall be used for prediction purposes.

The vocabulary of the process description language is restricted to prototypical partial differential equations derived from the continuity equation of mass. As discussed in section 9.2, other PDEs could be integrated in the vocabulary of the process description language. Extensions of the vocabulary to cover other kinds of process models might also lead to modeling functionality for social processes.

A topic that has not been covered is the combination of two models describing the change of two different state variables. Complex processes like the relocation of sand of the Sahara or the propagation of noise in a city include combinations of processes taking place on different scales. Composability provides a means to investigate the combinations of process models; this combination would allow to study interactions of processes.

The implementation of the process description language in order to approach process-enriched GIS is still an open issue. An obvious step is the implementation of the language's user interface. Implementing the process description tool requires, however, more than this step. The connection between process modeling and GIS has to be explored in more detail (cf. section 8.2). The language tool specifies the required data and mathematics for a process model at one place. GIS could be employed for data provision and parameter estimation. The required data are there, but (statistical) methods have to be discussed to extract and calibrate parameter values from data for the process models.

A direction to go from the process description language is to put the focus on the qualitative description of the processes and to link to research on qualitative models and simulations based on qualitative parameters (cf. Kuipers, 1994). In this case, the parameters to be provided by a GIS would have to be qualitative and tools would be required that can deal with qualitative models.

The lesson learned during the development of the process description language is that "[m]odelling is both an art and a science" (Huggett, 1993, p.51). Specifying the equations that describe the general behavior of a process is one part; providing the parameters, initial, and boundary conditions in such a manner that the simulation of a process is reasonable, is another part that requires further research.

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