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Large-scale water resources management within the framework of GLOWA-Danube. Part A: The groundwater model

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Abstract

The research project GLOWA-Danube, financed by the German Federal Government, is investigating long-term changes in the water cycle of the upper Danube river basin (77,000 km^2) in light of global climatic change. Its aim is to build a fully integrated decision-support tool "DANUBIA" that combines the competence of 11 different research institutes in domains covering all major aspects governing the water cycle—from the formation of clouds, to groundwater flow patterns, to the behaviour of the water consumer. Both the influence of natural changes in the ecosystem, such as climate change, and changes in human behaviour, such as changes in land use or water consumption, are considered. DANUBIA is comprised of 15 individual disciplinary models that are connected via customized interfaces that facilitate network-based parallel calculations. The strictly object-oriented DANUBIA architecture was developed using the graphical notation tool UML (Unified Modeling Language) and has been implemented in Java code. All models use the same spatial discretisation for the exchange of data (1×1 km grid cells) but are using different time steps. The representation of a vast number of relevant physical and social processes that occur at different spatial and temporal scales is a very demanding task. Newly developed up- and downscaling procedures [Rojanschi, V., 2001. Effects of upscaling for a finite-difference flow model. Master's Thesis, Institut für Wasserbau, Universität Stuttgart, Stuttgart, Germany] and a sophisticated time controller developed by the computer sciences group [Hennicker, R., Barth, M., Kraus, A., Ludwig, M., 2002. DANUBIA: A Web-based modelling and decision support system for integrative global change research in the upper Danube basin. In: GSF (Ed.), GLOWA, German Program on Global Change in the Hydrological Cycle Status Report 2002. GSF, Munich, pp. 35–38; Kraus, A., Ludwig, M., 2003. GLOWA-Danube Papers Technical Release No. 002 (Danubia Framework), Software-Release No.: 0.9.2, Documentation Version: 0.10, Release Date: 27 March 2003] are required to solve the emerging problems. After a first successful public demonstration of the DANUBIA package (nine models) in May 2002 [Mauser, W., Stolz, R., Colgan, A., 2002. GLOWA-Danube: integrative techniques, scenarios and strategies regarding global change of the water cycle. In: GSF (Ed.), GLOWA, German Program on Global Change in the Hydrological Cycle (Phase I, 2000–2003) Status Report 2002. GSF, Munich, pp. 31–34], the research consortium is now preparing a first validation run of DANUBIA for the period 1995–1999 with all 15 models. After successful completion of the validation, a scenario run based on IPCC climate scenarios [IPCC, 2001. Climate Change 2001: Synthesis Report. In: Watson, R.T., Core Writing Team (Eds.), A Contribution of Working Groups I, II, and III to the Third Assessment Report of the Intergovernmental Panel on Climate Change. Cambridge University Press, Cambridge, UK and New York, NY, USA, 398pp] for a five year period between 2025 and 2040 will follow at the end of 2003.

The research group "Groundwater and Water Resources Management" at the Institute of Hydraulic Engineering, Universität Stuttgart, is contributing both a three-dimensional groundwater flow model of the catchment and an agent-based model for simulating water supply and distribution. This paper gives a general overview of the GLOWA-Danube project and describes the groundwater modeling segment. Nickel et al. deal with the water supply model in a second contribution to this special issue.

A three-dimensional numerical groundwater flow model consisting of four main layers has been developed and is in a continual state of refinement (MODFLOW, [McDonald, M.G., Harbaugh, A.W., 1988. A modular three-dimensional finite-difference ground-water flow model: US Geological Survey Techniques of Water-Resources Investigations, Washington, USA (book 6, Chapter A1)]). One main research focus has been on the investigation of upscaling techniques to meet the requirement of a fixed 1×1 km

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cell size. This cell size is compulsory for all models in DANUBIA in order to facilitate a one to one parameter exchange. In a second stage, a transport model (nitrogen) will be added (MT3D: [Zheng, C., Hathaway, D.-L., 1991. MT3D: a new modular three-dimensional transport model and its application in predicting the persistence and transport of dissolved compounds from a gasoline spill, with implications for remediation. Association of Ground Water Scientists and Engineers Annual Meeting on Innovative Ground Water Technologies for the '90s, National Ground Water Association, Westerville, Ohio, USA. Ground Water 29 (5)].

Keywords: Danube; Groundwater model; MODFLOW; Hydrogeology; Decision-support system; Integrated modelling

1. The GLOWA-Danube project

1.1. The upper Danube basin

The total area of the upper Danube catchment up to the gauging station Passau is approximately 77,000 km^2, which is about 10% of the whole Danube catchment. The catchment basin, which is spread over five European countries, has a population of about 10 million people (Fig. 1).

The climatic, geomorphologic and geological conditions as well as land use show a wide range over the model domain. Figs. 2 and 3 show the distributions of average annual precipitation and surface geology as examples of this diversity. The elevation difference between the highest peaks of the Alps to the lowest flatlands in the Danube valley is more than 3000 m.

1.2. Starting point and aims of GLOWA-Danube

The investigation and prediction of long-term water cycles with a view to sustainable water use in large catchment areas such as the upper Danube basin requires an interdisciplinary approach. While physical processes control the natural water cycle, water demand and quality are widely determined by human behaviour. GLOWA-Danube, therefore, pursues an entirely integrated strategy. The areas of expertise of the GLOWA-Danube members cover the following disciplines: meteorology, hydrology, soil sciences, plant ecology, remote sensing, groundwater, water-resources management, glaciology, economy, agricultural economy, tourism, environmental psychology, and computer science.

GLOWA-Danube was started in 2001 with the aim to develop integrative techniques, scenarios, and strategies

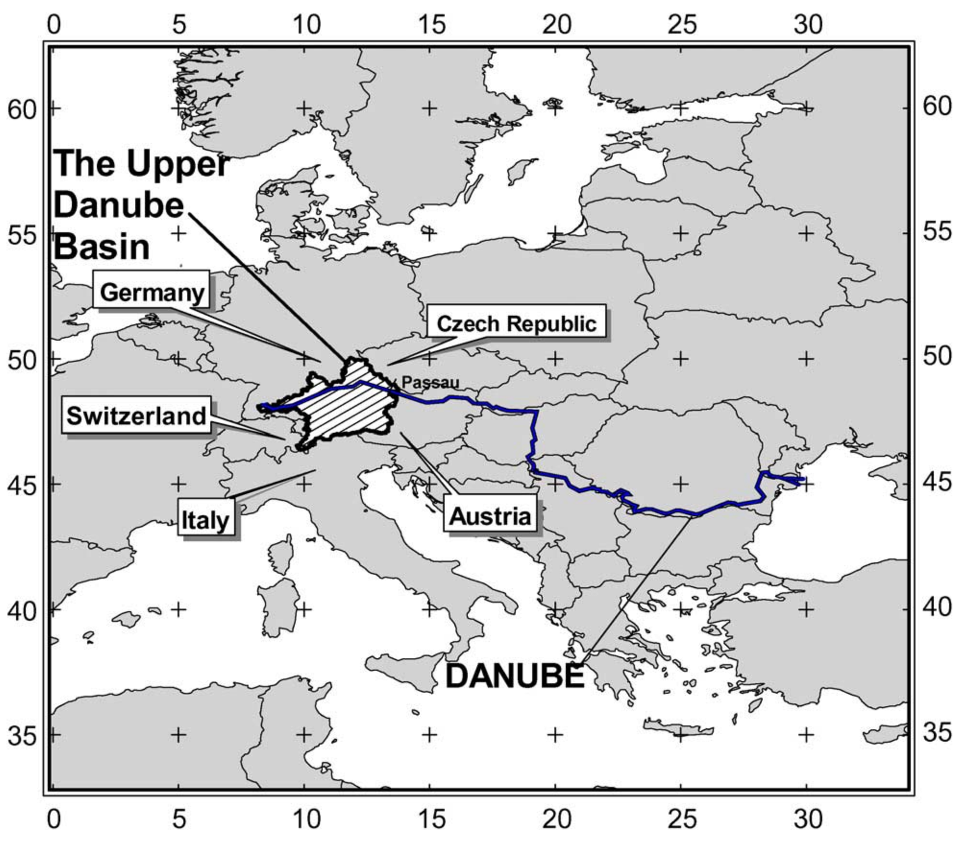
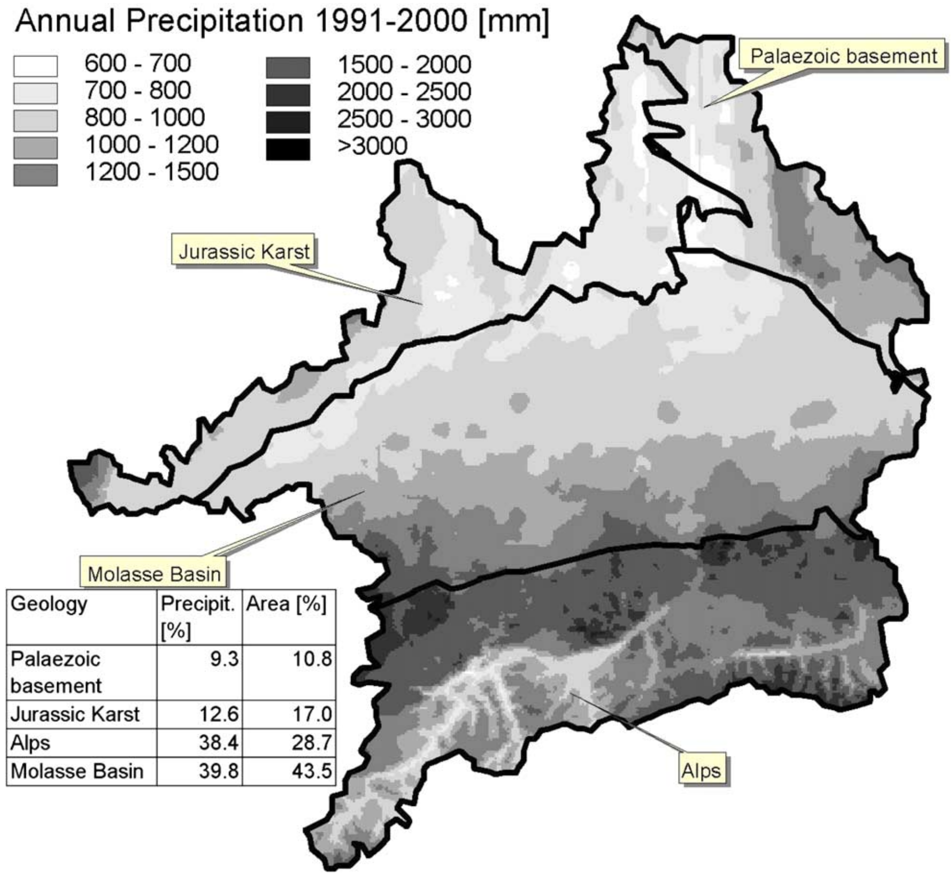


Fig. 1. The location of the upper Danube Basin in the Centre of Europe.



Geology	Precipit. [%]	Area [%]
Palaezoic basement	9.3	10.8
Jurassic Karst	12.6	17.0
Alps	38.4	28.7
Molasse Basin	39.8	43.5

Fig. 2. Distribution of the average annual precipitation in the upper Danube basin. The higher values of slightly more than 3000 mm/a in the south are caused by the Alpine mountain chain. The table shows the precipitation in specific zones of the groundwater model.

to cope with regional effects of global change on the water cycle in the upper Danube basin with respect to human activities (water and land use). Climate change, vulnerability of mountain environments, water-use conflicts, water-management technologies, and transboundary water management, are global-change issues that are treated in the project. The heterogeneity of the mountain catchment requires an explicit representation of all processes considered within GLOWA-Danube. The main integrative challenge of the first project phase of GLOWA-Danube (2001–2003) is to develop and apply the Web-based global-change decision-support system "DANUBIA" (Mauser and Ludwig, 2002). DANUBIA will, in a consistent and transferable manner, combine the expertise of all disciplines involved. In its final state, DANUBIA will be used to monitor, analyse, and model the impacts of global change on nature and society by combining a multitude of water-related environmental, social and economic aspects formulated by the stakeholders. In the second phase of the project (2004–2006), DANUBIA will be used to formulate and test complex future scenarios and by measuring the degree of sustainability of different scenarios. DANUBIA will thereby enable the identification of the most appropriate alternatives in watershed management.

1.3. The decision-support system DANUBIA

The concept of DANUBIA is based on the parallel execution of independent disciplinary models. The main characteristic of DANUBIA is its strictly modular, object-orientated concept. At each time step, the required parameters are exchanged. For example, the groundwater model, which will be dealt with in more detail later in this paper, has on the "physical side" interfaces to soil water and surface water models respectively ("*Soil*" and "*RiverNetwork*" see Figs. 4 and 5) which provide important parameters that are used as model boundary conditions (Fig. 5).

On the "socio-economic side", the groundwater model exchanges data with the so-called "Actors" component, a group of models concerned with the human impact on the water cycle. The amount of groundwater extracted for drinking water and other purposes is a boundary condition of the groundwater model calculated by the Actors models. The feedback between demand and supply creates a need for complex optimi-

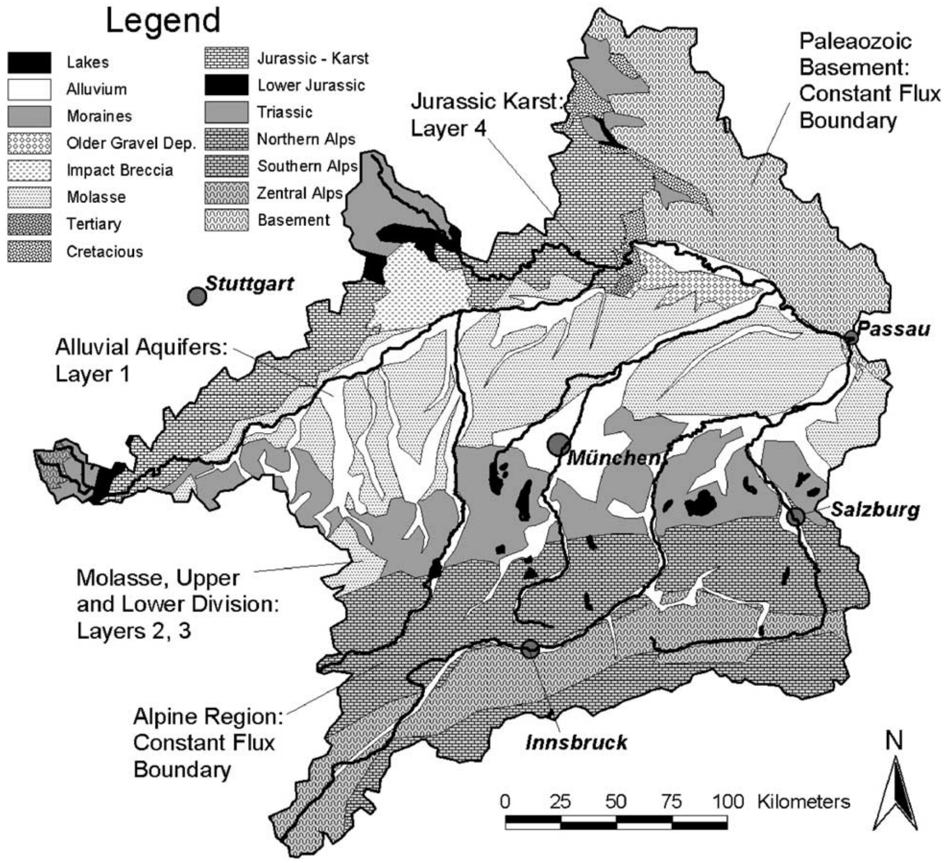


Fig. 3. Schematic geological map of the upper Danube basin.

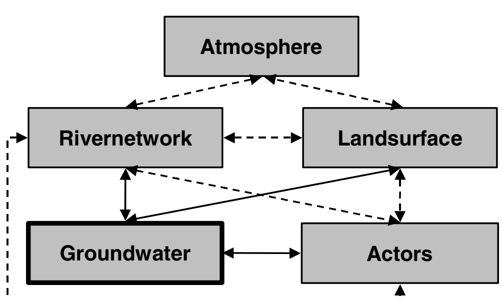


Fig. 4. Connections and dependencies between the main model components. Each main component can contain several individual models (e.g. Atmosphere: 3, Landsurface: 5). Solid lines symbolize the dependencies of the Groundwater Model.

sation algorithms to calculate the maximum possible extraction rates.

The strong coupling of models that run in parallel both in model time and in real time (meaning that the output of one model is the input of another at run-time) requires that the area of competence of each of the 15 models be clearly defined. No redundancies may occur in the numerical computation of the physical processes. This means that no physical variable may be computed by more than one model. Despite the apparent simplicity of this statement, one has to remember that models treating different parts of the water cycle usually overlap. When modelling saturated groundwater flow, for example, it is common to use simplified estimates of groundwater recharge and evapotranspiration rates, although these processes occur in the unsaturated zone. This overlapping is done at the expense of an accurate description of the physical and chemical processes. This inherent problem of disciplinary models is solved by the integrated approach of DANUBIA. Each model computes only those processes that belong to its core area of competence. The input and output data are clearly defined by the interfaces that connect the models (see Figs. 4 and 5). UML was used for that purpose by all groups to describe all processes within models, model interfaces, exchange parameters and more. UML (Unified Modelling Language, Booch et al., 1999) is a scripting language that uses a diagrammatically defined syntax to describe static and dynamic relationships and processes.

The following steps were taken to develop the DANUBIA prototype (Mauser et al., 2002):

1. Inventory of available disciplinary modelling approaches and definition of a common model architecture and interfaces between disciplines. The grid-based object-oriented "proxel" concept was invented

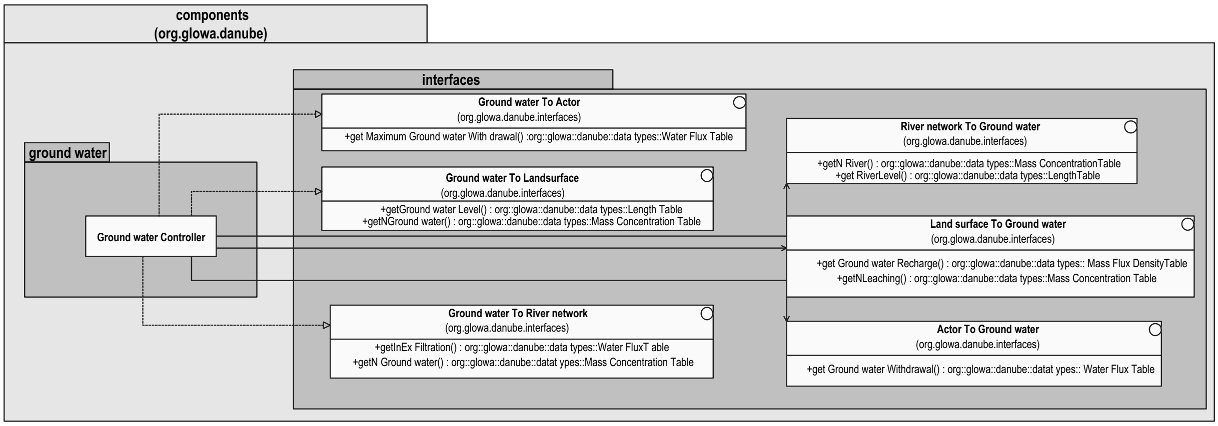


Fig. 5. Class diagram of the groundwater component in UML graphical notation. Only external interfaces to other model components (as listed in Fig. 4 and Table 1) are shown.

to allow common spatially explicit modelling in each disciplinary field (see below).
2. Definition of a common description of space on the basis of a 1×1 km grid (→ Proxels).
3. Utilisation of a common description language to diagrammatically describe the architecture of DANUBIA and the interfaces between the disciplines. UML was used for this purpose (Fig. 5).
4. Selection of a suitable common programming language to implement the disciplinary model and interfaces on the web in accordance with the formalised UML description. Java is used for this purpose because of its cross-platform capabilities. Java "wrappers" are used to integrate models written in different programming languages into the DANUBIA system (e.g. the groundwater flow model MODFLOW written in FORTRAN).
5. Careful analysis of timing and development of execution sequences for the different models by means of a simulation manager and a time controller created by the computer science group.

The utilisation of UML as mentioned in steps 3 and 4 proved to be very helpful and important in the process of conceptualizing the modelling system DANUBIA. Fig. 5 shows only one out of many options to model processes in UML, namely the static "class diagram" view. Dynamic aspects are not represented in Fig. 5.

To explain Fig. 5: The object "Groundwater" is one of the components of DANUBIA, represented by a class named "groundwater". The communication between the core groundwater module (which is basically MODFLOW; McDonald and Harbaugh, 1988), is carried out through a class "GroundwaterController" which has external interfaces with the other main model component as shown in Figs. 4 and 5 and internal interfaces to the core module not represented in Fig. 5. Interfaces are defined by their "from model...to...model" relation, e.g. "GroundwaterToRiverNetwork" and the "get"-methods in these interfaces, e.g. "getNGroundwater" (= method used to import Nitrogen concentrations from the Groundwater model to the RiverNetwork model). In the GroundwaterToRiverNetwork interface we find, among others, the method "getInExFiltration". This get method allows the RiverNetwork model to import "get" infiltration or exfiltration (from groundwater to surface waters or vice versa depending on the sign) calculated by the groundwater model in the previous time step. The physical meaning of the parameter "InExfiltration" will be explained later on. The return type "WaterFluxTable" specifies the imported value as L^3/T as specified in the package [org::glowa::danube::datatypes].

Currently, 12 of the 15 model components are running in parallel on a LINUX cluster. From May 2003 on, all 15 models will be implemented. After a validation phase of 3 months, run a first scenario simulation based on a Global Climate Change scenario from IPCC IPCC (2001). In the final stage, each model will run on a different computer in a different location using internet connections for the data exchange.

1.4. Description of space and time in DANUBIA

The direct coupling of different models requires the unique description of the model time and space. A *time* controller, which will not be dealt with in this paper, secures the synchronisation of different model time steps and the explicit parallel operation of the individual models. It should be mentioned that the harmonisation of the time factor was and is a particular challenge, as the time steps used by the different models during their parallel runs vary from minutes to months. Details are provided in Hennicker et al. (2002).

To allow an explicit description of the model *space*, the proxel concept was developed. A proxel (*PRO*cess-pi*XEL*) is, at first view, a rectangular, 1×1 km grid cell. Firstly, unlike the classical pixel that just stores co-ordinate and attribute information, proxels use the inheritance concept of the object-oriented approach. A general proxel class that describes basic proxel properties and functionality can be further expanded and specialised to comprise various subclasses according to the needs of the individual disciplines. Secondly, a proxel as an "object" may not only contain simple values but may also have "methods" for performing different actions, e.g. executing a calculation. Despite all capabilities that a specialised proxel subclass might have, data exchange between models is always done via "proxel tables" that contain a single value for each proxel (one variable = one proxel table). The identifier of a proxel is globally valid for the upper Danube basin and for all sub-areas for which simulations can be performed. For detailed information on the proxel concept and on the functionality of the Java proxel class, see Hennicker et al. (2002) and Kraus and Ludwig (2003).

The 1×1 km grid that forms the geometric basis of the proxel concept was agreed upon after a careful analysis of the significant scales of each physical process to be modelled. The computer power currently available was also considered in several cases. This common 1×1 km grid, based on which the data exchange can take place, is of great significance for many aspects of the GLOWA-Danube project. For most of the involved disciplines, the 1×1 km grid requires either up- or downscaling of model input and/or output data. For a groundwater model, for example, this is a very coarse grid, the use of which results in serious problems that will be dealt with later in this paper.

1.5. Contributions of the research group "Groundwater and Water Resources Management" to Danubia

The research group "Groundwater and Water Management", within the framework of GLOWA-Danube, is developing a model of the three-dimensional groundwater flow for the upper Danube catchment area, and a model for the simulation of water supply and water consumption in the domestic and industrial sectors. The groundwater and the water-resources models are linked to each other and to the models of the other contributing institutes following the aforementioned DANUBIA scheme.

2. The groundwater component

2.1. Overview

The main aim of the groundwater model is to assess and forecast the quantity and quality of the groundwater resources together with the other physically based models under conditions of global change. Upon completion, the groundwater flow and transport model currently being developed will be the largest multi-purpose numerical groundwater model ever created in Germany with respect to area and complexity. The construction of a conceptual hydrogeological model for such an enormous area is a demanding task which requires not only the collection of extremely large quantities of data but also the use of advanced data managing and evaluation tools. Additionally, interpolation methods capable of considering the different degrees of confidence of the values and the existence of discontinuities such as geological boundaries are utilised.

The groundwater flow and transport (Nitrogen) model developed by the research group uses a finite-difference approach (MODFLOW; McDonald and Harbaugh, 1988). A three-dimensional conceptual hydrogeological model consisting of four layers was developed. Only aquifers with basin-wide occurrence are considered. Aquifers on the local scale cannot be included in the model due to insufficient data availability, the model grid resolution (1 km^2) used, and various limitations arising from the MODFLOW-approach. The cell size of 1 km^2 is compulsory for all models in DANUBIA in order to facilitate parameter exchange (see above). Local refinements are planned for the next project phase. The (flow) model receives data that is used to parameterise the boundary conditions from the following:

- The Landsurface component: groundwater recharge.
- The RiverNetwork model: in- and exfiltration from and to the rivers.
- The Actors component: groundwater extraction.

The connection between "Groundwater" and "Landsurface" is defined by the computation of recharge rates into the saturated zone and of evapotranspiration rates occurring through capillary rise from the saturated groundwater. The exchange between "Groundwater" and "Rivernetwork" is defined by means of infiltration and exfiltration rates between the aquifer and the surface water body. The hydraulic connection is a function of the water level of the surface water body (averaged over one cell), the piezometric head in the hydraulically connected layer in the groundwater model and a parameter signifying the hydraulic conductivity of the aquitard separating the two water bodies. Groundwater extraction (to parameterise the well boundary condition) is calculated from the water demands of the Actors. The actual groundwater extraction at a certain location is limited by a maximum extraction rate which is calculated based on the hydraulic conditions at that location. If the water demand sent to a certain well exceeds this maximum value, supply will be less than demand.

MODFLOW was chosen in accordance with the size of the model area and the constraints imposed by the DANUBIA Proxel concept. The finite-difference approach fulfils the requirements in a nearly ideal way.

Furthermore, MODFLOW was chosen because of its robustness, which has been proven over many years, and its modular, adaptable concept. In a second stage, a transport model simulating nitrogen transport (MT3D; Zheng and Hathaway, 1991) will be added.

The main focus of research in the first two years of the project has been on the development of the conceptual hydrogeological model of the catchment. The gathering and processing of data for a drainage area of this magnitude has been, and remains, one of the major tasks. For areas that are not yet or only poorly investigated, geostatistical methods are utilised, and, if necessary, enhanced to describe the sub-surface. A particular challenge lies in the modelling of groundwater flow and substance transport for a very coarse grid fixed to 1×1 km and in the constant exchange of input and output data with the other research groups (parallel calculations). The proxel architecture of DANUBIA, necessary to ensure communication between the different models, requires the development of new upscaling methods to reproduce soil heterogeneity and geo-hydraulic boundary conditions in order to simulate groundwater flow and substance transport without an adaptation of the grid.

2.2. The conceptual hydrogeological model

Over the course of the first project year, it became apparent that the data situation in the basin is highly variable. Many important raw data such as borehole logs are not directly accessible to the authors (the number of boreholes existing in the study area can only be estimated to be several 10,000, however only a small fraction is hydrogeologically evaluated and digitally available). Instead of using raw borehole data directly to interpolate layer tops and bottoms, the model geometry relies mainly on contour maps created in previous studies. Such contour maps do not exist throughout the area; they were calculated for different layers and have different resolutions and accuracies. Time series of weekly data on groundwater levels or piezometric heads for the calibration period 1990–2000 exist for about 1800 observation wells. However most of the observation wells are located in the alluvial aquifers close to rivers and in many cases it is not obvious which aquifer is actually filtered.

Geological data of satisfactory coverage and quality, which are required for the geometrical description of the aquifers, is available for most areas of the catchment. However, only small parts of this data are available in digital format. Data in printed format had first to be compiled from various sources and subsequently digitised and processed. In contrast, data on the hydraulic properties of the sub-surface is infrequent or inaccessible. Other important data, e.g. the hydraulic properties of the riverbeds, do not exist at all. The hydraulic properties of the riverbeds are needed to calculate the amount of leakage per river cell. River levels are an exchange parameter calculated by the RiverNetwork Model (Fig. 5, Table 1). The hydraulic conductivity of the river bed (conductance) can only be estimated by calibration.

For the hydraulic conductivity, data are scarce. This important parameter should normally be based on as many field observations as possible. Estimation by use of calibration leaves too many uncertainties and leads to unreasonable model results. To increase the number of sample values for the hydraulic conductivity (or transmissivity), co-kriging will be applied in order to correlate hydraulic head measurements and hydraulic conductivities that are mathematically connected in the general groundwater flow equation.

Regardless of the evident importance of a correct representation of the hydraulic parameters in a groundwa-

Table 1
Principle exchange parameters of the groundwater component within the DANUBIA system (please compare with Fig. 5)

Exchange parameter	Model...to...groundwater	
	Main component	Model
GroundwaterWithdrawal	Actor	WaterSupply
RiverLevel	RiverNetwork	SurfaceWaterFlow
NRiver (N = Nitrogen)	RiverNetwork	SurfaceWaterQuality
GroundwaterRecharge	Landsurface	Soil
NLeaching (N = Nitrogen)	Landsurface	Soil
Parameter	Groundwater...to...model	
	Main component	Model
GroundwaterLevel	Landsurface	Soil
NGroundwater	Landsurface	Soil
	Rivernetwork	SurfaceWaterQuality
	Actors	WaterSupply
InExfiltration	Rivernetwork	SurfaceWaterFlow
MaximumGroundwater		
Withdrawal	Actors	WaterSupply

ter model, the appropriate definition of the model geometry (layer top and bottom) has proven to be the critical and dominating factor for the model behaviour (see below). It shows that the calibration of hydraulic conductivities can be considered to be "fine-tuning" if one deals with such large and coarse models.

Based on the data currently available for the catchment area, a first conceptual hydrogeological model has been conceived as a prerequisite for the development of the numerical model (Figs. 6 and 7). The conceptual model consists of four layers, comprising the strata "Malm Karst", "upper Tertiary Molasse", "lower Tertiary Molasse" and "Quaternary". The units "upper" and "lower" Molasse are, for the most part, defined without regarding the actual complexity of the litho-stratigraphic units. The upper Tertiary unit is an approximately 50 m thick layer, within which the important local structures can be modelled independent of the properties of the subjacent Molasse. The Quaternary layer is mainly defined by small and thin local structures of high permeability (valley aquifers, alluvial gravel plains; Figs. 6–8). This uppermost layer is most important for short and medium term groundwater flow. Its importance in DANUBIA is obvious, because it represents the interface with the other models. Unfortunately, the complicated geometry of the Quaternary layer makes it the most difficult to model. The importance and complexity of the layer brought it into the centre of research activities.

The hydro-stratigraphical units subjacent to the Malm are not considered explicitly, as the groundwater exchange that takes place here is negligible for GLOWA. Therefore, the base of the "Jura" aquifer constitutes the base (lower boundary) of the model (Fig. 6).

In the Palaeozoic Basement in Northeast Bavaria, local hydraulically unconnected aquifers predominate. Since they are too small to be modelled on the predefined grid size, these areas are excluded from the groundwater model. Instead, a boundary allowing temporally variable inflows will be drawn along these sections. The task of quantifying such boundary inflows into the model area is still under investigation.

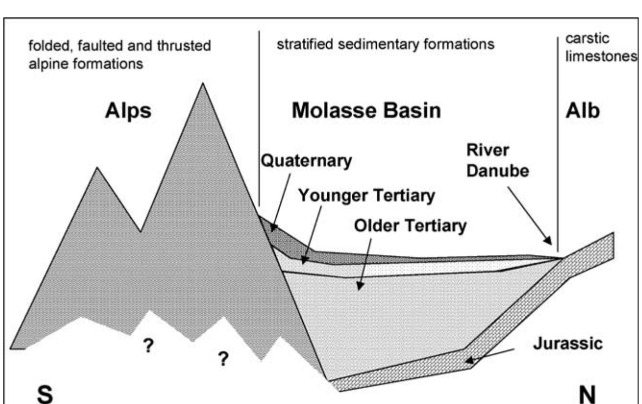


Fig. 6. Schematic geological cross section of the upper Danube basin showing the four model layers. See Fig. 7 for the horizontal distribution of the uppermost active model layers.

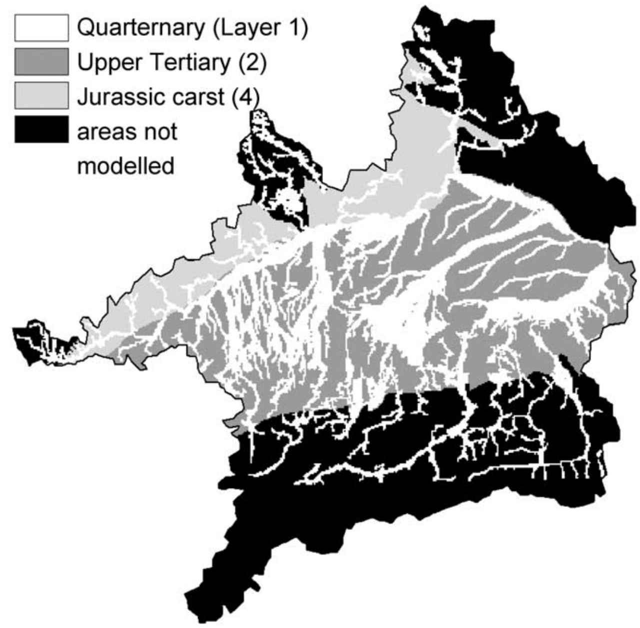


Fig. 7. Horizontal distribution of the uppermost active layer of the groundwater model. Please note the complex geometry of the Quaternary layer. Due to the general dip of the layers towards the Alps (south), layer 4 reaches the surface in the north of the model (compare Fig. 6).

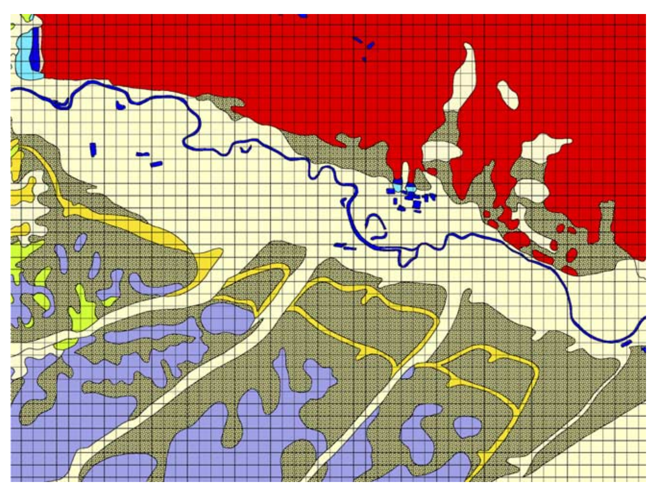


Fig. 8. Cut-out of the hydrogeological map of the upper Danube catchment (based on a very coarse map of the scale 1:500,000). The map was simplified by joining hydro-stratigraphic units with similar properties. The underlying GLOWA-Danube 1×1 km grid is also shown. White areas: high permeability alluvial aquifers (quaternary deposits) in river valleys (model layer 1). Please note the small horizontal dimensions and the diagonal orientation with respect to the model grid.

The alpine section of the model area is a subject of particular concern. On the one hand, the alpine regions, covering approximately 30% of the catchment area and contributing about 40% of the total precipitation (Fig. 2), evidently play a large role in the water cycle of the region. On the other hand, it is not possible to treat the extremely faulted, folded, and thrusted stratigraphic units of the Alps as ordinary quasi-horizontal layers as they are usually required in the MODFLOW concept. Karstification, which plays an important role in certain parts of the Northern Alps, adds to the difficulties in this area.

2.3. The numerical groundwater flow model

The task of developing a three-dimensional (3D) groundwater flow and transport model of this size has been divided into the following manageable sub-steps to allow for the simultaneous, painstaking process of data acquisition:

1. Creation of a two-dimensional steady-state model using the simplest assumptions concerning aquifer geometry, boundary conditions, and model parameters. Only the alluvial aquifers (Fig. 7) are modelled explicitly, whereas others are neglected or, where necessary, taken into account as boundary conditions. The Alps and the Palaeozoic Basement are excluded from the model area and are represented by constant flux boundary conditions (Fig. 7). The purpose of step one is mainly to set parameters and boundary conditions as a first approximation. It is based on the assumption that the alluvial aquifers are the most important for the processes that are recognised in the DANUBIA scale (space and time). The model calibration is primarily done by trying to achieve "reasonable" results, e.g. the minimisation of flooded areas.
2. Successive refinement and adjustment of the model from step one, replacement of estimated parameters by measured values where available, and the use of field observations for the model calibration. The model area is still reduced to the core part of the catchment, excluding the highlands and mountain areas.
3. Expansion of the two-dimensional model to 3D by adding the lower three layers.
4. Calibration and validation of the model for steady-state and transient conditions.
5. Detailed modelling of the mountainous areas using a conceptual hydrological approach.
6. Calibration and validation of the full 3D model for steady-state and transient conditions.

Currently (May 2003) the project group has completed steps 1–3 and is mainly concerned with step 4.

2.4. Integration of MODFLOW in Danubia—adaptation of the proxel concept

Parallel to the development of the flow and transport model, the integration of this model in the structure of DANUBIA is being pursued. The finite-difference models MODFLOW and MT3D, for flow and transport respectively, were chosen mainly because of the cell-based approach that matches the proxel concept of DANUBIA in a nearly ideal way. One to one data exchange with other models is possible without elaborate post-processing of the model output. Although the block-centred flow approach used by MODFLOW has numerous advantages (simplicity, robustness, perfect integration in DANUBIA), it also has clear disadvantages, particularly with regard to the implementation of boundary conditions and the representation of complex geometrical features.

The following input data are calculated by the models named in parenthesis: river level (River Network), nitrogen in surface water (River Network), groundwater recharge (Landsurface), nitrogen in percolating water (Landsurface), groundwater withdrawal (WaterSupplyActor). Likewise, the following output data are required by the models stated in parenthesis: groundwater level (Landsurface), nitrogen in groundwater (Landsurface, RiverNetwork, WaterSupply), infiltration and exfiltration between groundwater and surface water (RiverNetwork). The transfer parameters were implemented in UML-diagrams (Fig. 5), which in turn were used to create a Java code which can be integrated in the overall structure of DANUBIA.

3. Special issues of the large-scale groundwater model

Groundwater modelling on a very large scale brings about some problems that are not present or at least of less importance in small or medium scale models. Many of the features in nature that play an important role in the water cycle show heterogeneity on a scale much smaller than the 1 km grid. It seems important to point out again, that data exchange throughout DANUBIA is done on 1000×1000 m grid cells. Using a finer grid for the internal calculations and later recalculating the results for the 1000×1000 m grid would theoretically be an option, but it proves to be infeasible in practice because of performance aspects. The time frame for simulations with DANUBIA is 30 years at stress periods of one day.

Prime examples for this problem are the river valleys crossing the catchment from the bordering Alps with courses aligned from South to North or Southwest to Northeast (Figs. 7 and 8). While these alluvial river valleys have small cross sections (less than 500 m in many places), they are at the same time significant aquifers due to their deposit's coarse grain size, their thickness, and the valley's steep gradients. Their discretisation presents a particularly great challenge when such structures run at an angle to the grid. Rojanschi (2001) pursued these and other similar questions extensively and tested various methods for modelling the differences in hydraulic conductivity between a highly permeable Quaternary aquifer (Aitrachtal on the border between Bavaria and Baden-Wuerttemberg) and the surrounding Molasse based on the proxel size (1 km^2). His research showed that in many cases the upscaling methods currently in use yield unsatisfying results. Hence, the second major research emphasis of the research group "Groundwater" is in the development of new scaling procedures.

As shown in Rojanschi (2001), the difficulties are related mainly to the upscaling of layer parameters, such as hydraulic conductivity, and of point and linear boundary conditions, such as wells and rivers. The main aim of upscaling is to minimise the errors resulting from modelling on a coarse scale as compared to a theoretically correct but unmanageable fine grid model.

Scaling issues, however, affect not only the hydraulic parameters but also the model geometry itself. As previously mentioned, the correct and appropriate representation of the model geometry has a very high importance and influence on the conduct and performance of the model. The difficulties arise mainly from the fact that the uppermost, partly saturated (unconfined) quaternary layer is (a) of very complex geometry and (b) very thin (0–50 m, average 10 m) compared to the grid cell size. Moreover, the finite-difference method usually allows only one specific flow path through such structures (perpendicular to the cell faces). Therefore, the bottom and top of the cells upstream and downstream, and the possible positions of the hydraulic heads in such cells, must allow for a continuous flow through the structure. Otherwise, the smallest changes in recharge, extraction by wells, or any change in hydraulic head anywhere, can cause the most dramatic effects starting from the flooding of large areas to the drying up of cells. In this paper, we only want to point out that in large-scale models the aim should not be the most realistic representation of the aquifer geometry in nature, but a representation that respects the most realistic groundwater flow paths. This can be achieved manually, cell-by-cell, or by semi-automatic procedures currently under development in our working group.

It should be pointed out that grid refinements, which would seem to be a simple solution to that kind of problem, are generally not the answer. Firstly, even with a finer grid resolution, the question of how to parameterise the cells remains (data availability). Secondly, refinements require more computer power and calculating time. Finally, values calculated on the finer grid would have to be transferred to the 1 km grid again, since this is the compulsory grid cell size for the exchange with other models. The problem would only be shifted.

4. Conclusions

In the beginning of 2003, after 2 years of work, GLOWA-Danube has achieved a high degree of integration. A unique spatial model concept for 15 models with an efficient (and working) technical solution for the coupling of 15 independent models from different disciplines using UML, JAVA and Web techniques has been developed and successfully tested. The Groundwater component developed by the working group "Groundwater and Water Resources Management" has not reached a fully satisfactory state in all respects. However, it has already been possible to show that modelling groundwater flow on the very large scale under heterogeneous conditions is manageable if careful attention is paid to the model geometry. The "stumbling blocks" of large-scale modelling have been identified and addressed: regions within the model area where a layered model approach is not applicable (Alps), the coarse model grid and the involved upscaling questions. Finally, it should be pointed out that such a large model is not intended to, and never will, answer questions on a local scale. It is designed to forecast regional trends on a large time scale using boundary conditions provided by Global Climate Change models (GCMs). In turn, it can be used to generate boundary conditions for smaller scale local models. It can, therefore, be considered to be a link between the global and the local scale.

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