A groundwater flow and particle tracking model for the Iraí-basin, Paraná, Brazil

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Summary

The explosive expansion of the population of the Metropolitan Region of Curitiba raised a high increase in the demand for water resources and the uncontrolled settlement poses a large problem for the environment. The greatest menace to the water supply sources of this region is the urban occupation (invasion) into the areas that contain these resources. This occupation continues with its slow, silent, although progressive march, threatening precious and irreplaceable resources. From this background an area in the direct vicinity north-east of Curitiba has been studied. In this area a drinking water reservoir was constructed in the time that the study took place in the Iraí-basin. The Iraí-reservoir even though an area around the lake will be protected may be polluted by two tributaries which flow through more or less densely populated areas. In the study area on the same time wells have been constructed.

To estimate what the impact may be from the possibly polluted reservoir on the aquifer a groundwater flow model has been constructed. On the same time to estimate the water balance and the spatial distribution of pollution vulnerability the hydrological model MODBIL has been used. Also other methods have been used to estimate the pollution vulnerability to make a comparison and because none of the methods takes every aspect into account.

With the calibrated groundwater flow model for the situation before the construction of the Iraí-reservoir and after its construction, simple particle tracking transport models are constructed as scenarios how the water of the aquifer may be influenced.

Kurzfassung

Die Bevölkerungsexplosion in der Region von Curitiba während der letzten Jahre verursachte eine große Zunahme des Wasserbedarfs; die zunehmend unkontrollierte Besiedlung stellt dabei ein großes Problem für die Umwelt dar. Die größte Bedrohung für die Wasserversorgung dieser Region ist die urbane Invasion in Gebiete, wo die Herkunft der Wasserressourcen liegen. Diese Invasion geht langsam aber stetig voran und bedroht kostbare und nicht ersetzbare Ressourcen. Vor diesem Hintergrund wurde ein Gebiet in der direkten Nähe der Großstadt Curitiba als Studienobjekt ausgewählt. In diesem Gebiet, dem Iraí-Becken, wurde während der Untersuchungszeit ein Trinkwasserspeicher geplant und gebaut.

Es besteht die große Gefahr, dass das Iraí-Reservoir kontaminiert wird, obwohl das engere Gebiet rundum den See geschützt werden soll. Die Verschmutzungsgefahr geht hauptsächlich von zwei Nebenflüssen aus, die durch mehr oder weniger besiedeltes Gebiet strömen.

Im Arbeitsgebiet befinden sich Brunnen, die der Trinkwasserversorgung dienen. Um die negativen Folgen einer möglichen Verschmutzung des Reservoirs abschätzen zu können, wurde ein Grundwasserfließmodell erstellt. Die erforderliche Wasserbilanz und die räumliche Verteilung der Verschmutzungsempfindlichkeit wurde mit dem hydrologischen Modell „MODBIL“ abgeschätzt. Weitere Methoden zur Abschätzung der Verschmutzungsempfindlichkeit wurden angewandt, um die differierenden Ergebnisse der angewendeten unterschiedlichen Methoden mit einander vergleichen und bewerten zu können.

Mit dem kalibrierten Grundwasserfließmodell ist mit der gegebenen hydraulischen Situation vor und nach der Konstruktion des Reservoirs, ein einfaches Particle Tracking Transport Modell eingesetzt worden, um mit unterschiedlichen Szenarien die Beeinflussung vom Reservoirwasser auf das Grundwasser zu simulieren.

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List of symbols

DURCH1	real border permeability	[mm/day]
E	evaporation	[mm]
f	a function	
f´	derivative of a function	
F14(i)	relative humidity at 2 p.m.	
GD	border permeability	[m/s]
h	hydraulic head	[m]
H	thickness of the aquifer	[m]
h_0	initial hydraulic head or for pumping tests static head	[m]
h´	the recovered head	[m]
HP	saturation state	[%]
I	Infiltration	[mm/day]
I_n	precipitation	[mm]
K	hydraulic conductivity	[m/s]
KF	hydraulic conductivity at saturation	[m/s]
KFBOD1	ground permeability	[m/s]
KFBOD2	permeability of subsoil	[m/s]
KPSI	the percolation velocity	[m/s]
LKFN	logarithm of unsaturated hydraulic conductivity	
MAB	thickness of the soil layer	[m]
n	groundwater flow direction normal to boundary (normal component)	[m]
n_e	effective porosity	
NFAKT	height correction factor for precipitation	
nFK	effective field capacity	[mm]
N(i)	precipitation	[mm]
NRD	reduction	
NZ	slope	[°]
P	precipitation	[mm]
P_e	effective precipitation	[mm]
PS	water content	
q	flow	[m^3/s]

Q	pumping rate	[m^3/s]
Q_{INT}	maximum infiltration rate	[mm/day]
Q_{LECK}	leakage	[mm/day]
Q_{Ob}	surface runoff	[mm/year]
Q_p	pumping withdrawal	[m^3/day]
Q_{Quelle}	spring flow (Maillait)	[mm/dag]
r	distance to the well	[m]
$R_{interfl}$	interflow	[mm/year]
R_o	surface runoff	[m^3/day]
R_r	groundwater recharge	[m^3/day]
s	drawdown	[m]
S	storativity	
s´	residual drawdown	[m]
S_s	specific storativity	[1/m]
T	transmisivity	[m^2/s]
t´	time since pumping stopped	[s]
T14(i)	temperature at 2 p.m.	[°C]
THETAHAFK	water content at field capacity	
THETAMAX	water content at saturation	
T_m(i)	the mean daily temperature	[°C]
v	linear velocity of groundwater	[m/s]
VPOT	potential evatransporation	[mm/year]
VAKT	actual evatransporation	[mm/year]

Preface

The explosive expansion of the population of the Metropolitan Region of Curitiba raised a high increase in the demand for water resources and the uncontrolled settlement poses a large problem for the environment. The greatest menace to the water supply sources of this region is the urban occupation (invasion) into the areas that contain these resources. This occupation continues with its slow, silent, although progressive march, threatening precious and irreplaceable resources. From this background an area in the direct vicinity Northeast of Curitiba has been studied. In this area a drinking water reservoir was constructed in the time that the study took place in the Iraí-basin. The Iraí-reservoir even though an area around the lake will be protected may be polluted by two tributaries which flow through more or less densely populated areas. In the study area on the same time wells have been constructed.

To estimate what the impact may be from the possibly polluted reservoir on the aquifer a groundwater flow model has been constructed.

On the one hand this study is written for the people who work and know the situation in the area and on the other hand for general scientific purpose. For this reason the description of the situation in the survey area may be a little to extensive for some people, but the modelling study is build on the information and data which are applied to the problems which are discussed in this description. The modelling study was carried out with the software available at that time in the Geological Institute in Würzburg. It is clear that software packages used will not be used eternally, but their discussion helps to understand the methodology for building the model. It is actually the methodology of modelling that is the focus of this study.

How to construct a model from scratch ?

Is a modelling study the goal or just an instrument for understanding the system and for planning ?

In this study the model is extracted from various type of data from an area in the Municipal Region of Curitiba applied on problems specific for areas in the direct vicinity of rapidly expanding urban areas.

The result of this modelling is a hydraulic model and based on that a particle tracking model.

This is done to make scenarios of how the impact on the aquifer that is subject of this study may be when the water of the Iraí-reservoir is polluted.

1 Introduction

From the background from uncontrolled settlement which poses a large problem for the environment and with it for the fresh water resources an area in the direct vicinity Northeast of Curitiba has been studied. In Brazil mainly surface water is used but in the area the groundwater is exploited as well. In the near future more surface water will be exploited in the study area. Only because of the possible urban development the water quality may be at risk and possible polluted surface water may also have its influence on the groundwater. To estimate possible impacts on the groundwater quality the goal of this study was to study the groundwater hydraulics –and transport in the Iraí-basin.

In this study the approach to achieve a groundwater model from available data is described. In this case a hydraulic and a particle tracking model for the study area is constructed.

The Iraí is a tributary of the Iguaçu river basin that lies in the Curitiba-basin. The modelled area is Northeast of Curitiba the capital city of the state Paraná with about 5.2 million inhabitants in the city and its direct region. The modelled area is actually in the direct vicinity of the urban region around Curitiba (Metropolitan Region of Curitiba). The Iraí-reservoir is constructed in this catchment area, which will most probably be polluted by its tributaries and which water quality is additionally endangered by the founding of illegal settlements in its direct vicinity in the near future.
With the modelling study scenarios are constructed to see what are the probable impacts on an aquifer if the pollution of the water of the Iraí-reservoir is severe enough.

To make a clear illustration how this model was achieved the description of this approach is subdivided in chapters, that describe and clarify each step. Chapter 2 makes an extensive description of the survey area and also presents the data used for the modelling study. In this chapter the possible influences of the several described factors on the groundwater are considered as well. Natural factors influencing the groundwater e.g. geology, soils, and climate. Quantitative and qualitative factors of the surface waters. The development of the Municipal Region of Curitiba, its tremendous growth in the last decades, the problems of the water supply of Curitiba, the stresses posed on the surface waters, the uncontrolled settlement and littering are shortly touched on.
The questions to be solved which make a modelling approach necessary are posed in this chapter.

In chapter 3 the methodology of making a hydraulic model and a conjunctive particle tracking model is discussed.
How is it designed and what kind of software is applied ?
What kind of algorithms were used, and what choices could be made as solution methods to solve them and because why a specific solution method was chosen.
Further something is written about some of the criteria used trying to construct a conceptual model that does corresponds with the natural situation and about the further calibration and finally the further use of the calibrated groundwater flow model.

Chapter 4 describes the water balance modelling with the MODBIL Water Balance model to compare the results of the hydrological balance described in chapter 2 with emphasis on recharge. MODBIL works on the basis of meteorological data, soil physical data, topography and land use. In this chapter the several types and principles of hydrological modelling are discussed. The way MODBIL functions and the results are discussed.
In chapter 5 the build-up of the hydraulic model is described. What is the concept of the hydraulic model and how is it build-up. What are the boundary conditions ? What are the results of the modelling study ? In this chapter the models of the hydraulic regime before and after the construction of the Iraí-dam will be described.

The pollution vulnerability assessment for the Iraí-basin is described for the Iraí-basin in chapter 6. For several methods of generalised aquifer pollution vulnerability systems a comparison is made. A new method considers the accumulation of debris and contaminant matter by overland flow in depressions of the land surface. This assessment was done originally for a symposium of the “Deutsche Geologische Gesellschaft” in cooperation with my college Günter Kus. Here the results of the pollution vulnerability assessment is presented to give an idea where the highest pollution potential for the groundwater is for the study area and as a help for the transport model.

In chapter 7 the results of a simple particle tracking transport model are presented. This is actually a scenario of what may be the influence on the groundwater water quality of the water of the Iraí-reservoir.
Chapter 8 summarises the findings and is at the same time the conclusion of this thesis.

2 Description of the survey area

The locality of the study area is about 15 km Northeast of the city of Curitiba in the state of Paraná, around the exposition park ‘Castelo Branco’, in the municipality Pinhais-PR in Brazil. The study area is part of the Iraí- river basin which has a total area of 163 km^2. Near the park a well field (Iapar) has been developed. Other nearby wells have been drilled at Fazenda Canguiri, in the ‘Parque Castelo Branco’ and Colonia Penal (the state prison dominion).
In this chapter the geology, the geomorphology, the soils, climate and meteorological data, the possible stresses on the water resources together with the hydrologic data, water quality of the surface waters and the groundwater system with its water chemistry will be discussed.

The geology has been divided in a paragraph about the geological history of the region, the geological structure of the region and the lithology within the study area. To win an insight into the formation of rocks in the region and on the other side to describe the geological materials in the study area. These geological materials also determine very much of the geomorphology in the study area. The geomorphology determines the course of streams, the distribution of wet areas, distribution of soils, the suitability even for well construction. The properties of the soils have been described to get insight on possible influences on the groundwater chemistry. The climate is responsible for the quantity of water that is contained in the water balance of the study area and the temperatures that may be reached. The factors water and temperature play a very important role in weathering and soil formation. The meteorological data are some of the raw data that will be used for the water balance. Possible stresses on the water resources will be discussed, using quality data of surface waters, the development of the Municipal Region of Curitiba (MRC), the planning of the water supply of the MRC, and the circumstances prevailing in Brazil. For the planning of the water supply several benefits and disadvantages of the water supply from surface water and groundwater should be mentioned.
For the groundwater system the hydraulical and hydrochemical properties of the aquifer will be discussed and how these data were achieved. These data were gathered mainly by a desk study (well construction reports, dam construction study, geological literature, etc.) and for some part in the field by assisting and joining the staff of the Hydrogeology Department of the UFPR and Sanepar (well construction, geoelectrical pseudo-sections, sampling and measuring). This approach for the discussion of the survey area has been chosen to present the data that will be used for the modelling study and to make the necessary considerations about the area that is modelled.

2.1 Geology

2.1.1 Geological history of the region

The South American platform is a large geotectonic entity that was consolidated between the end of the Precambrian and the Cambrian. It comprises the entire extra-Andean area of the continent North of the Colorado river in Argentina (de Almeida, 1972).

The area around Curitiba is part of the Mantiquera structural province from which the lithological and structural features were chiefly imposed during the Brasiliano orogenetic cycle (450 - 700 m.y), with evidence of a Proterozoic geosynclinal evolution.

The Mantiqueira structural province is situated along the Atlantic coast South of latitude 15° S, extending to the frontier with Uruguay, with structural trends parallel to the Atlantic coast.. It is bordered by the coastal basins and continental margin and at the other side by the São Francisco, Tocatins and Paraná Provinces (de Almeida et al, 1981).

This is also called the Ribeira Fold Belt by several authors (Cordani, 1973; Ulbrich and Comes, 1981).

The Mantiqueira province presents an almost entirely mountainous region, with altitudes higher than 1500 m in the coastal mountain range.

The fold belt was developed during the Brasiliano Cycle. The fold belt systems have been formed by geosynclinal sequences. These rocks have been metamorphosed into a greenschist and amphibolite facies under low P/T. In large areas they underwent migmatization processes. The folding was intense, polyphase and of linear type, with poorly evidence vergence. The pre-tectonic magmatism of maffic nature is poorly developed, contrary to the syntectonic magmatism of acid nature represented by numerous stocks and batholiths dated at about 650 m.y. There also exist post-tectonic intrusions, less frequently forming stocks and batholiths, dated about 540 m.y.

From the end of the Jurassic, the platform underwent a process of reactivation which affected its entire Eastern region, from North to South.

The relations between the activation and the evolution of the Atlantic continental margin seem evident.

Geothermal doming and crustal swelling above large-scale hot-spots rising from the underlying asthenosphere may have been instrumental in causing the splitting of Gondwanaland into its component crustal units, now separated by the Atlantic and Indian Oceans (Clapperton, 1993).

Sedimentological indications of source area renewal and more rapid supply in the Paraná basin are prove of uplift acceleration during the Triassic-Jurassic in the Paraná Basin’s Eastern margin. This uplift acceleration corresponds to the continental pre-rift, crustal uplift phase or pre-volcanic swelling (Soares and Landim, 1975). It is supposed that this uplift constituted a continental arch during the Triassic-Jurassic. During the Palaeozoic, the Ponta Grossa and Rio Grande arcs (fig. 1) were developed at the borders of the Paraná Basin, exercising their influence strongly on the modelling of the basin and the delimitation of the province (de Almeida et al, 1981).

At the end of the Jurassic to the beginning of the Cretaceous the uplift eased off and volcanism began.

Intensive magmatic activity occurred from the beginning of the tectonic activation (Campos, Ponte and Miura, 1974). During the Jurassic, and possibly persisting into the Albian, important fissure volcanism of tholeiitic nature occurred, which covered an area greater than 1,200,000 km^2 with lava of the Paraná synclise, representing a minimum volume of 650,000 km^3 (Almeida, 1972). At the same time, diabase dikes penetrated tension fractures and faults throughout the greater part of the areas consolidated at the end of the Precambrian. Especially notable is the

swarm of thousands of Northwest-oriented dikes which penetrated the then active Ponta Grossa arch.
Assuming the reality of continental drift, the Mesozoic activation of the South American platform represents a reflex of the tectonic and magmatic phenomena which accompanied the opening of the South Atlantic Ocean, beginning with the Upper Jurassic.

Basaltic volcanism reached its climax in the Lower Cretaceous. The flow of basaltic rocks, is grouped under the denomination of the Serra Geral Formation (Soares and Landim, 1975).
Southeast Brazil then suffered the greatest tectonic movements since the early Palaeozoic times: vertical faults with several dozen of km in length and up to 150 m of slip were originated; horsts, grabens and dome structures, with amplitude up to 200 m and 300 km^2 in area, were also formed. At the same time the Afro-Brazilian Arch collapsed, giving rise to the Afro-Brazilian Rift whereby the rupture and subsequent separation of South America from Africa began.
This set of events is denominated as the Wealdenian reactivation.

Tectonic rifting on a continental scale during the Mesozoic separated part of the Precambrian craton underlying Gondwanaland into half-domes now represented by the highlands of Eastern Brazil and equivalent highlands in Southwest and South Africa (Clapperton, 1993).
In Southeast Brazil, the modern expression of the former rift zone is the `Great Eastern Escarpment´ forming the Serra do Mar and Serra da Mantiqueira.

The epeirogenic uplift occasioned in the eastern region of the platform during the Tertiary was accompanied by the development of smaller sedimentary basins located next to ancient faults which were reactivated. Such as the São Paulo basin, the Itaboraí basin in the State of Rio de Janeiro, and some smaller basins like the Curitiba basin. Each contains exclusively continental sediments (Almeida, 1972). For the upper Tertiary - Quaternary period it is possible to make a correlation of the sediments in those basins that were formed by epeirogenetic tectonics with the climatic history that is known from e.g. Antarctic ice-cores and pollen data from Para State and the Colombian highlands.
Several authors proposed a model of landscape evolution that during glacial periods the climate became semi-arid over much of tropical and sub-tropical Brazil, causing a substantial change in the vegetation cover and in the main geomorphologic processes operating on the land (Clapperton, 1993). Figure 3 shows how the vegetation is thought to have been divided on the South-American continent during the Last Glacial Maximum, illustrating a likely situation for the Plio-Pleistocene period. In the upper Pliocene - lower Pleistocene it is thought that the climate in the area was resembling the semi-arid during the Last Glacial Maximum.

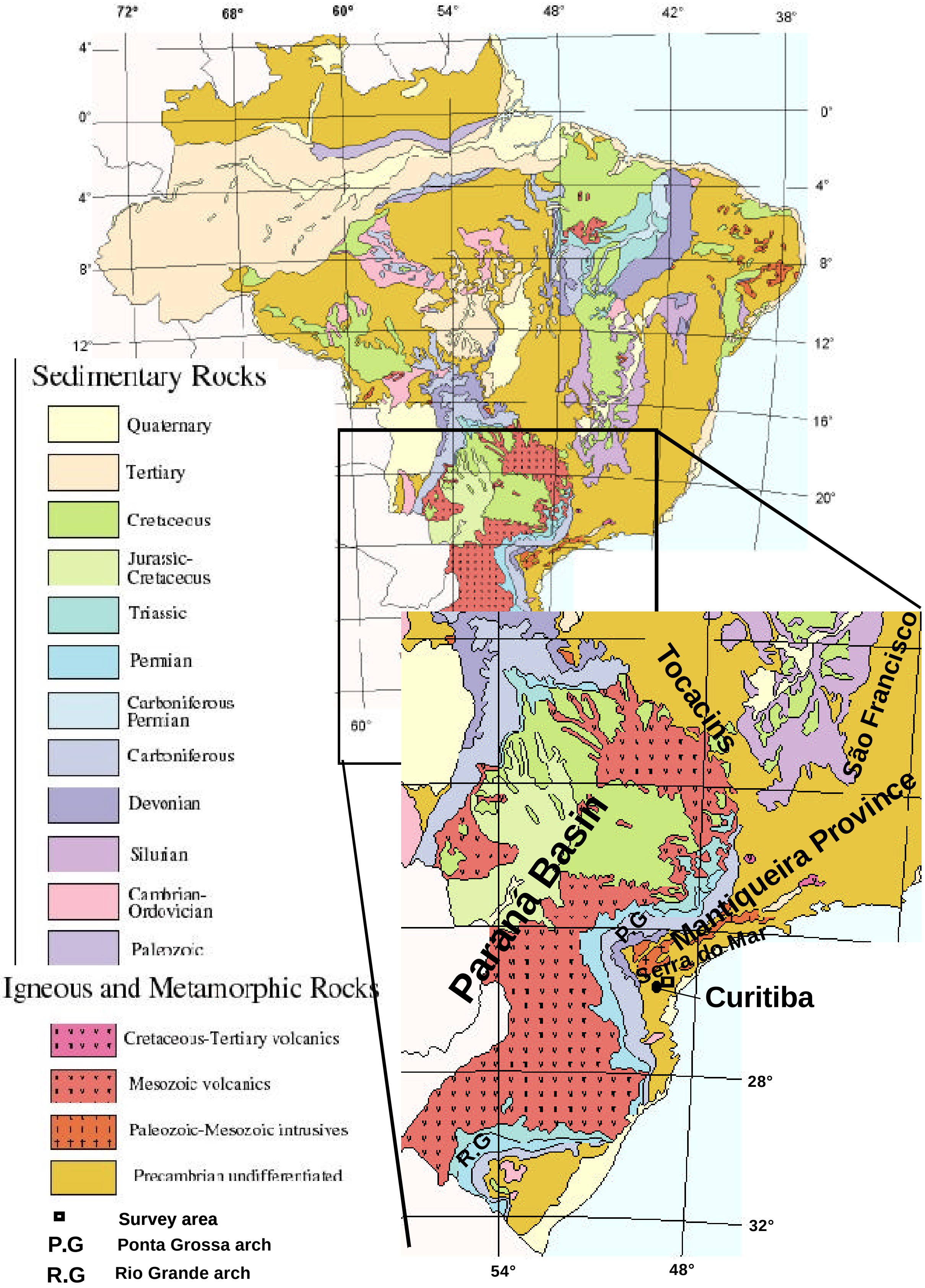


Figure 1: Geological map of Brazil with a detail of Southeast Brazil indicating the position of the structural provinces and the position of the survey area (changed from Alden, 2001).

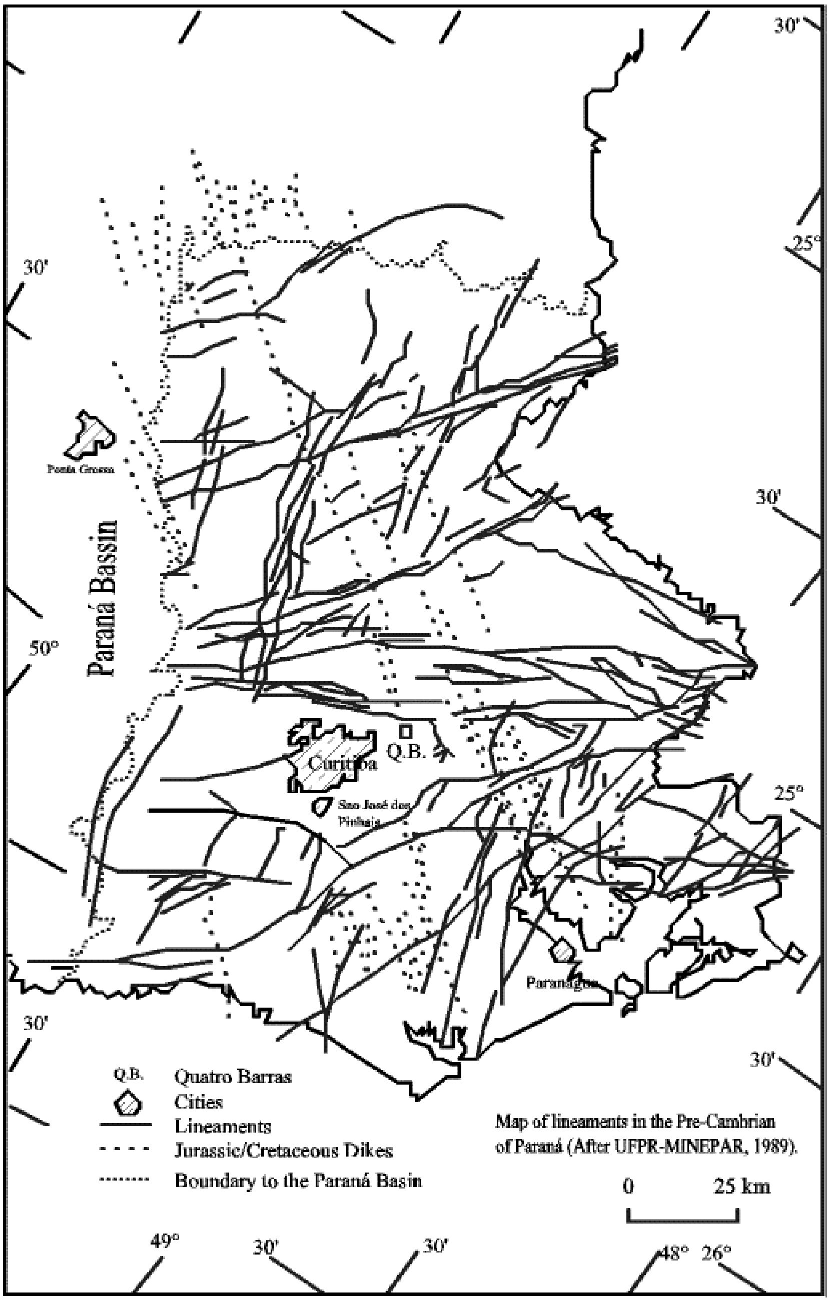


Figure 2: Map of tectonic lineaments in the Pre-Cambrian of Paraná (after UFPR-Mineropar, 1989).

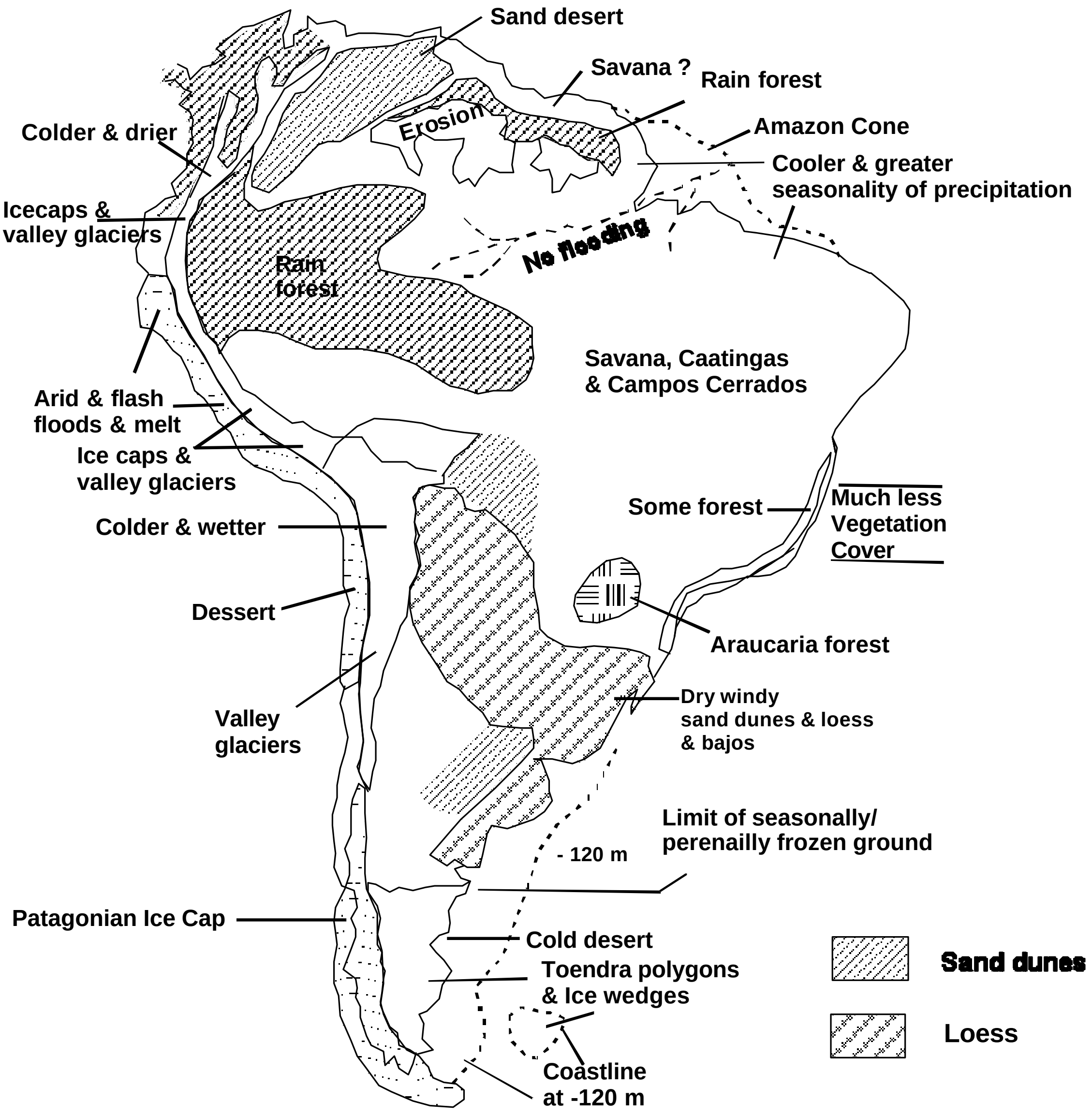


Figure 3: Probable distribution of the vegetation during the Last Glacial Maximum (after Clapperton, 1993).

The evidence for Quaternary climatic changes in the Brazilian Highlands is inferential rather than substantial.

The change from humid-dry climate caused a substantial change in the vegetation cover, together with a change in weathering environment.

A sub-tropical humid climate is characterised by deep chemical weathering. The crystalline basement rocks are decomposed in situ, commonly preserving crude elements of the original bedrock structure; residual zones of chemically inert quartz and quartzite may remain as hard clastic components.

Whereas in semi-arid conditions the landscape develops more by mechanical weathering and lateral degradation.

The change of climate was responsible for the removal of the regolith mantle to the depressions of the terrain. During heavy rains, the sediments were transported as mud flows, which would precipitate most of their load after the first break of gradient. Great amounts of clay and silt particles were taken to the depression in a playa-lake environment (bajada deposits).

In the case of the Plio-Pleistocene deposits of the Curitiba basin, the so called Guabirotuba Formation is proposed to have formed under such semi-arid conditions, in sites which favoured the development of extensive alluvial fans, as well as of playa lake environments (Bigarella, 1962).

The above described development of the geology of Southern Brazil formed the structure of the regional geology of the State of Paraná of which the city Curitiba, which is nearby the study area, is the metropolis.
The geology of the region of the study area is presented on the geological map of Eastern Paraná (fig. 4) which will be described in the following section.

2.1.2 Geological structure of the 1st plateau of Paraná

The crystalline/metasedimentary platform of Southern Brazil forms the Eastern edge of the Paraná Basin and consists of Precambrian rocks with acid and basic intrusions (Veit, 1985). Around Curitiba the crystalline is a to the West protruding arc. This area, also called the Primeiro Planalto (1st plateau) of Paraná, reaches heights around 900 m.a.s.l. In the East fringes the coastal mountain range Serra do Mar which reaches heights of 1950 m.a.s.l. (Pico do Paraná). This coastal range falls with a steep eastern flank to see level. At some places e.g. in the bay of Paranagua a narrow coastal plain has formed. From the crystalline/metasedimentary plateau going to the West soon follows the ascent to the 2nd plateau (plateau of Ponta Grossa) that is formed by a Devonian sandstone escarpment.

The crystalline platform has been formed by successive tectonic events and has developed since the Proterozoic. The tectonic events moulded pre-existent units so that these strike principally in a NE-E direction nowadays (Salamuni, 1998).
The Brazilian crystalline platform was ultimately consolidated in the Assyntic orogenesis. During the younger Paleaozoic sediments to 2000 m thickness were deposited because of subsidence. These epirogenic movements ended towards the end of the Permian. At the turn of the Jurassic/Cretaceous a reactivating of tectonics took place and volcanic activity began.
This new tectonic activity was induced by the opening and expansion of the South-Atlantic fissure.
In the Paraná Basin also fissures were opened and lava flows formed a closed cover. The fissures have a Northwest-Southeast to North-Southern strike. On the crystalline/metasedimentary platform in the region of Curitiba no plateau basalts are present, but appears as basaltic dikes on the surface.
The tectonic activity remains active until the Quaternary.

The Precambrian basement consists of Assyntic folded series and runs with a Northeast-Southwestern strike from Espirito Santo over Rio do Janeiro, São Paulo to the Curitiba elevated plain .
Roughly the Precambrian basement consists of following units: Pre-Setuva, Setuva, Acungui and Granitoides (Fig. 4). Further some units of the Archaic, and the Ordovician are present in this section of the Brazilian platform. The Pre-Setuva and Setuva Groups are of Lower Proterozoic age, as the Acungui Group is of Upper Proterozoic age. From the Granitoides most units have Cambrian ages and did not experience metamorphosis of any importance, as the Granite-Gneisses of Proterozoic age did experience metamorphosis to the grade of anatexis.

The units of the Cambrian/Ordovician present in the platform seem to be rests of the denudated sedimentary/pyroclastic rocks that used to cover the metamorphic units. They appear in units that seem to be graben-structures, West of Curitiba and in tectonical contact near the city of Ponta Grossa with the sedimentary units of the Paraná Basin.

Onlap appear deposits of Devonian ages curving around the Ponta Grossa Arch, representing the first sediments of the Paraná Basin.

In the same configuration sediments appear after a time gap of about the entire Carboniferous period with sediments of the Lower Permian to the Cretaceous (on the map the succession ends with sediments and flood Basalts from the Lower Permian to Jurassic-Traissic period in the Paraná Basin).

The crystalline/metasedimentary platform and the Paraná Basin contain numerous Basaltic dikes that generally strike Northwest-Southwest and are especially concentrated through the Ponta Grossa Arch. These dikes have an Jurassic-Cretaceous age and also appear in the study area.

Back to the platform: now the plutonic and metamorphic rocks form the land surface, but had a thick cover of rocks that all have been denudated.

The only recent sediments form the deposits in small intermontane basins like the Curitiba Basin with the Plio-Pleistocene Guabirotuba Formation and Holocene alluvial deposits, and the alluvium in several fluvial valleys.

2.1.3 Geological materials in the survey area

Migmatite

The migmatite of the Pre-Setuva complex of the “Primeiro Planalto” are of middle to upper Proterozoicum (Rosa Filho, 1991).

They have a rough texture and consist meanly of feldspar. They are irregularly banded, with a slight schistosity and a granite like texture.

The main mineralogical substances are quartz SiO_2, orthoclase (mikrocline) $K|AlSi_3O_8|$, oligoclase (Plagioclase with 10-30 % anorthite), and biotite.

A lesser part is formed by hornblende, augite and pyrop are sporadically found.

As accessory constituents pyrite FeS_2 , magnetite Fe_3O_4, ilmenite $FeTiO_3$, apatite $Ca_5(PO4)_3F$ and fluorite CaF_2 are found.

Often Mg(Fe),Al|OH|-chlorite is present as a conversion product of biotite and kaolinite as a conversion product of feldspars.

The migmatite has light and dark bands which have other dominating minerals. The dark bands have more plagioclase (Ca- and Mg-plagioclase), pyroxene and biotite, as the light bands have more orthoclase (alkali-feldspar).

These rocks were metamorphosed in the amphibolitic facies. The metamorphosis and migmatising probably occurred in the physical chemical environment of a developing geosyncline.

The age of the migmatite that has been dated by K/Ar is about 635 m.y. The migmatites formed probably during the Brasiliano Cycle and were derived from a sedimentary sequence.

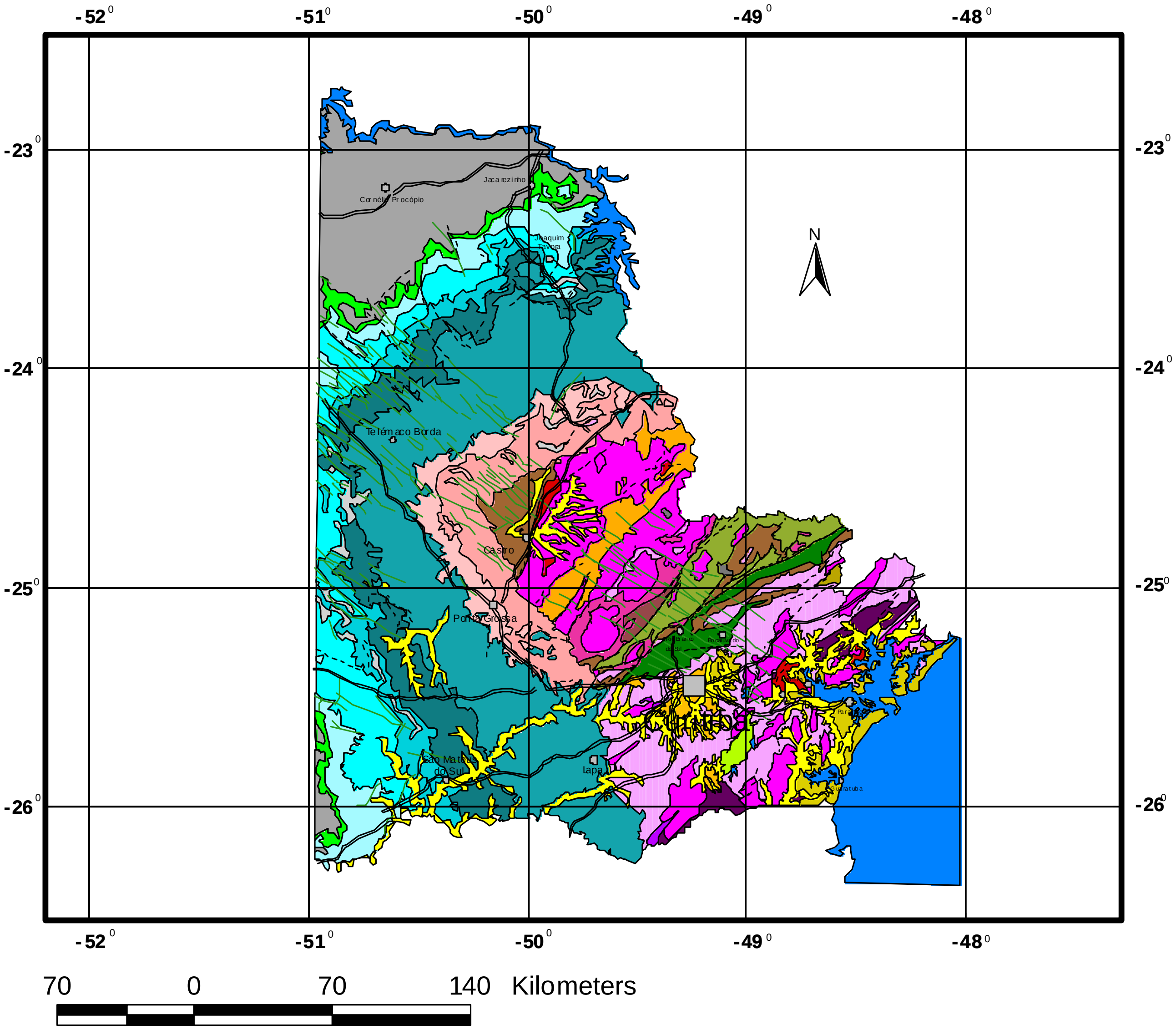
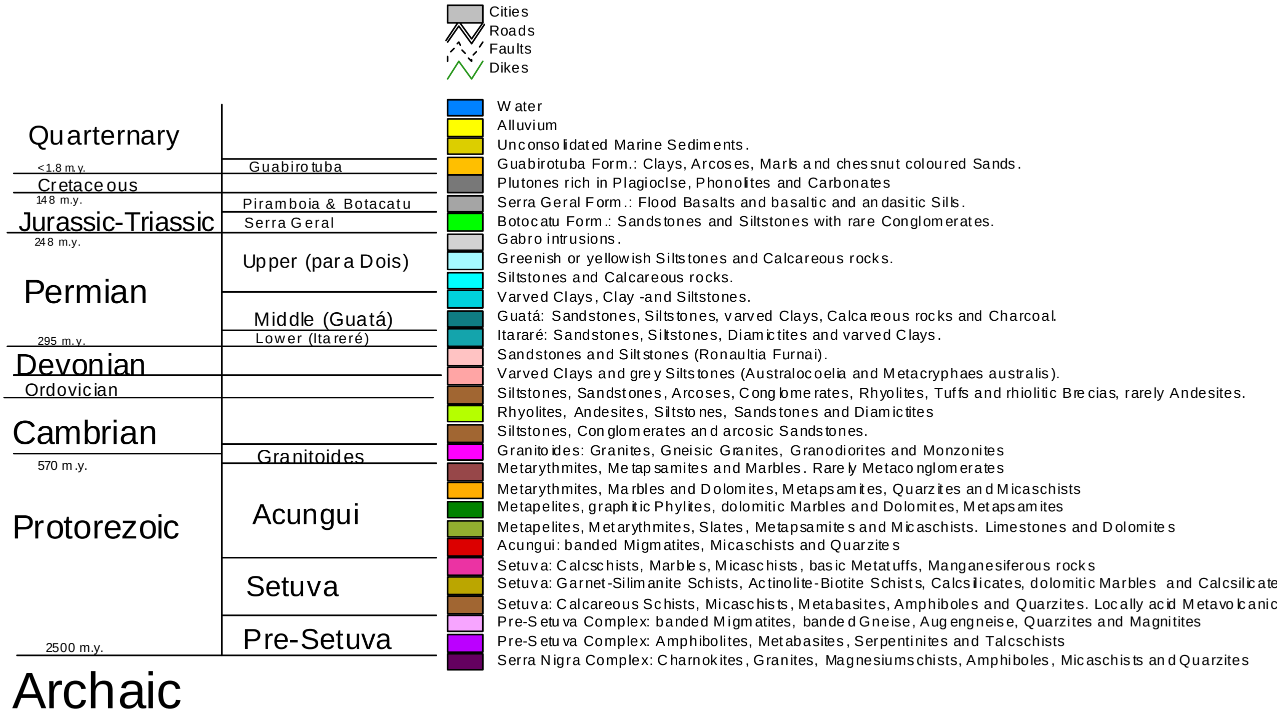


Figure 4: The Geological Map of Eastern Paraná (after Mineropar, 1986).

Legend:



Granite

At the Eastern border of the survey area a stock of granite (Anhangava granite) is present there where the Serra do Mar forms the boundary with the Curitiba-basin. The name for the Anhangava granite originates from one of the sites where this type was encountered, the Anhangava Hill, and is only a regionally used name for this kind of granite.

This stock is petrograficaly a rock with a medium to rough granulation, leucratic (the term signifies rich in light coloured minerals), coloured with light grey or grey-rose and sparkling green spots or black resulting of amphibole and biotite crystals. The rocks are isotropic and hypidiomorphic granulation, in some localities presenting a porphyric texture.

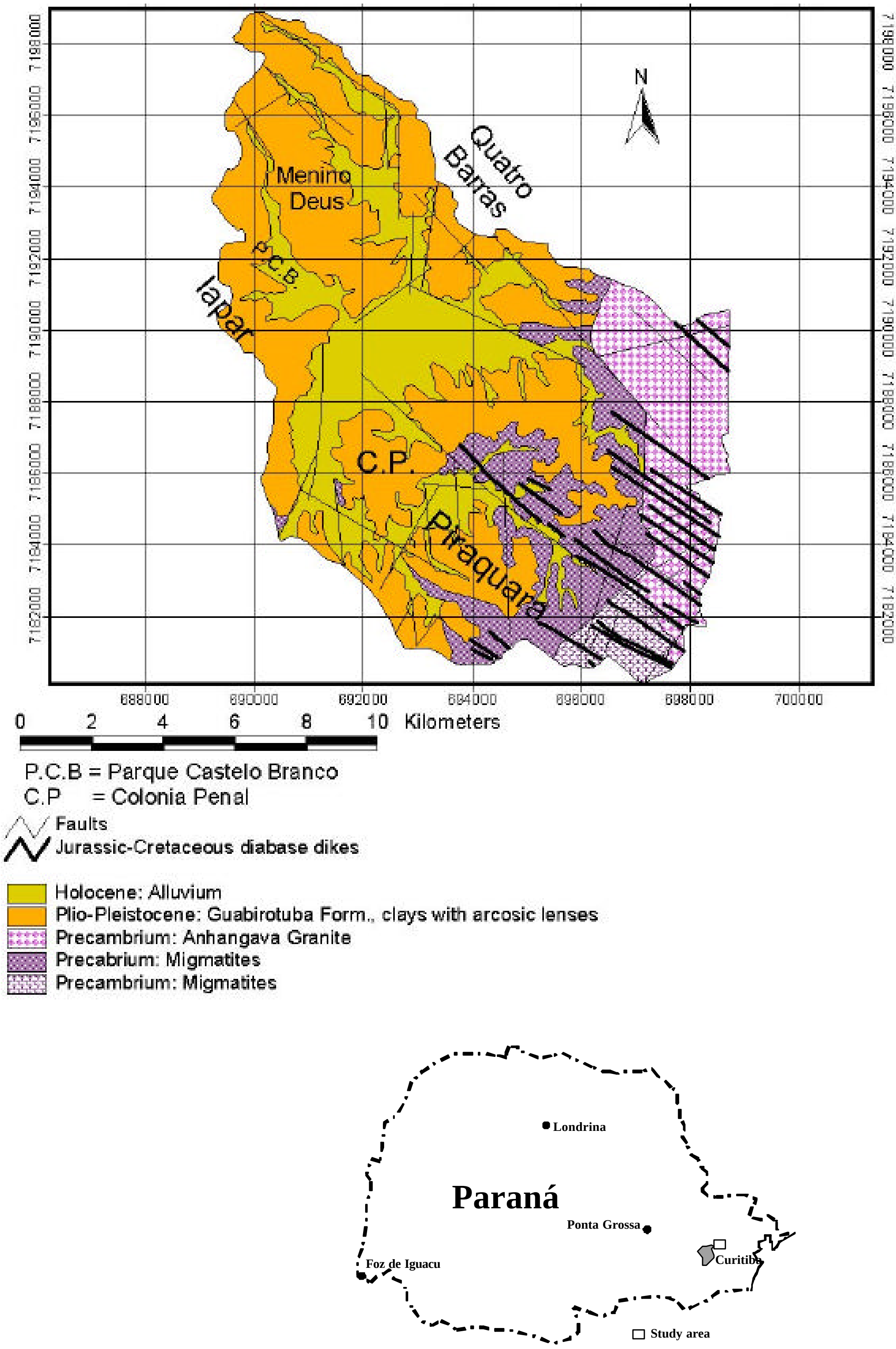


Figure 5: The Geological map of the Iraí-Basin (after Rosa Filho, 1998).

Mineralogically it is a alkali-feldspar granite consisting almost entirely of quartz and alkali-feldspar (orthoclase $KAlSi_3O_8$ and albite $NaAlSi_3O_8$ are the predominant feldspars), that contains alkali amphiboles and/or pyroxene, that may also be called an Alaskite (Le Maitre, 1996).

This granite also contains oligoclase.

Sporadically fluorite, zircon $ZrSiO_4$, opaque minerals, apatite and allanite (epidote group) are present.

This granite stock has been dated with Rb-Sr at 513 ± 13 m.y. making it a post-tectonic plutonic stock.

Basic intrusive rocks – Diabase

The diabase are rocks of jurassic-cretaceous age and are present in the area as dikes, having a predominant NW-SE direction. These diabase intrusions were formed during epigenetic movements which accompanied the rifting of Gondwanaland.

The main substances are labradorite, containing 50 - 60 % anorthite, augite and often quartz.

Secondary hornblende and biotite accompanied by magnetite, ilmenite, pyrite, apatite.

Chlorite is formed by weathering of pyroxene and biotite.

The Guabirotuba Formation

The Guabirotuba Formation is composed by a sequence of claystone, frequently interbedded by lens-shaped layers of arkoses (Bigarella, 1962). The material of the claystones and arkosic sands in the Iraí-basin are derived from (immature) weathering products of the granites and migmatites, which are present in the study area (fig. 4 and 5).

The clay stones are generally marked by a poor bedding, somewhat contrasting with the better stratification shown by the arkosic sediments. As was cited in section 2.1.1 these sediments have probably been deposited under semi-arid conditions, under a facies of coalescent alluvial fans, with an anastomatising drainage system at the side of extensive playas (Rosa Filho et al, 1996).

Another feature of former semi-arid conditions are stonelines that are found in soil profiles on slopes (as visible in the soil profile in figure 8). These stonelines were formed by the washing out of the fines at the surface so that an enrichment of pebbles occurred and the consequent transport and were later buried by finer material. These stonelines were not only observed in the study area, but is a feature that is widely observed in the tropics and subtropics.

In a geotechnical study, in which the ‘claystones’ of the Guabirotuba Formation were studied (Duarte, 1986) it has been determined that the clay is stiff and highly overconsolidated. The latter indicates that at least the sampled sites were buried and that the cover was eroded.

Several slope failures have been observed, occurring even in low-declivity slopes.

It has been suggested that the highly plastic character and low values of residual strength of the soil, play an important role in the previously mentioned instability problems. A triaxial pore pressure dissipation test showed that the soil is practically impermeable. The above mentioned characteristics and observations are evidence for the high erosivity of the Guabirotuba Formation.

Mineralogical analysis by X-ray difractometry revealed that montmorillonite is the predominant clay-mineral in the clay fraction of the soil and the high content of montmorillonite is made responsible for the low residual strength.

For the clay fraction the following fractions of clay minerals were found:

Kaolinite	10 %
Illite	10 %
Montmorilonite	80 %

Illites may form as a direct weathering product from micas, but also form feldspar weathering products. Montmorilonite is also formed from feldspar weathering products. Kaolinite is formed by further weathering of the montmorilonite and illite. The presence of illite and montmorilonite is a further indication of immature deposited weathering products.

The mineralogy of the arkoses consists of both primary and secondary minerals. The arkoses have according to their name a high feldspar content and contain both white and rose feldspars and their weathering product kaolinite, together with quartz.

As far as granulometry is concerned, both recent and older sequences show an outstanding variation in sorting and grain size distribution, owing to the competency fluctuation of the transporting agent.

Especially in the karst area Northwest of the survey area, much of the sediments have almost entirely been eroded, because of the solution of the underlying meta-dolomitic rocks. The only rests of these sediments are on phylites that were folded together with the dolomites.

Not so badly eroded sediments of the Guabirotuba Formation are present in the Iraí-basin, which is a sub-basin of the Curitiba-basin and North of the hydrographic basin which belongs to the Ribeira-basin.

Because several parallel faults are present near this northern border of the Iraí-basin it is thought that the hydrographic boundary may have shifted due to neo-tectonic uplift of the fault blocks (Lisboa, personal comm.). In these deposits in the North just outside the hydrographic basin, in the river valleys, the Guabirotuba Formation has been eroded to the migmatite in the stream valleys. These stream valleys seem to have their courses along faults.

In the Iraí-basin erosion took place mainly by the action of small streams that have their origin as springs directly from the Guabirotuba Formation. The erosion is so effective because of the large number of springs and the large number of gullies originating from them.

The course of the main tributaries of the Iraí-river, the Canguiri river and the Timbo river seem to have been determined by parallel faults, actually the same faults that determine the above mentioned Northern basin boundary and some faults more or less parallel to them.

The trunk valley of the Iraí-river seems to have been determined by faults and to the Northwest tilted fault blocks. Figures 5 and 6 perfectly illustrate this structural control. In the Southeast the migmatite outcrops and to the Northwest the fault blocks are subsequently covered by the Guabirotuba Formation and Holocene alluvial sediments. Subsequently the alluvial plain is followed by the hills build of the Guabirotuba Formation in the Northwest. This boundary probably coincides with a fault.

All these observations are strong arguments for the in section 2.1.1 mentioned neo-tectonic activity.

2.2 Geomorphology

Much of the geomorphology seems to have been determined by faulting. The geological map gives this indication but also the topography of the terrain supports this. As described in Section 2.1.2 the position of the trunk valley and the Iraí-river seems to be determined by fault blocks that are tilted to the Northwest.

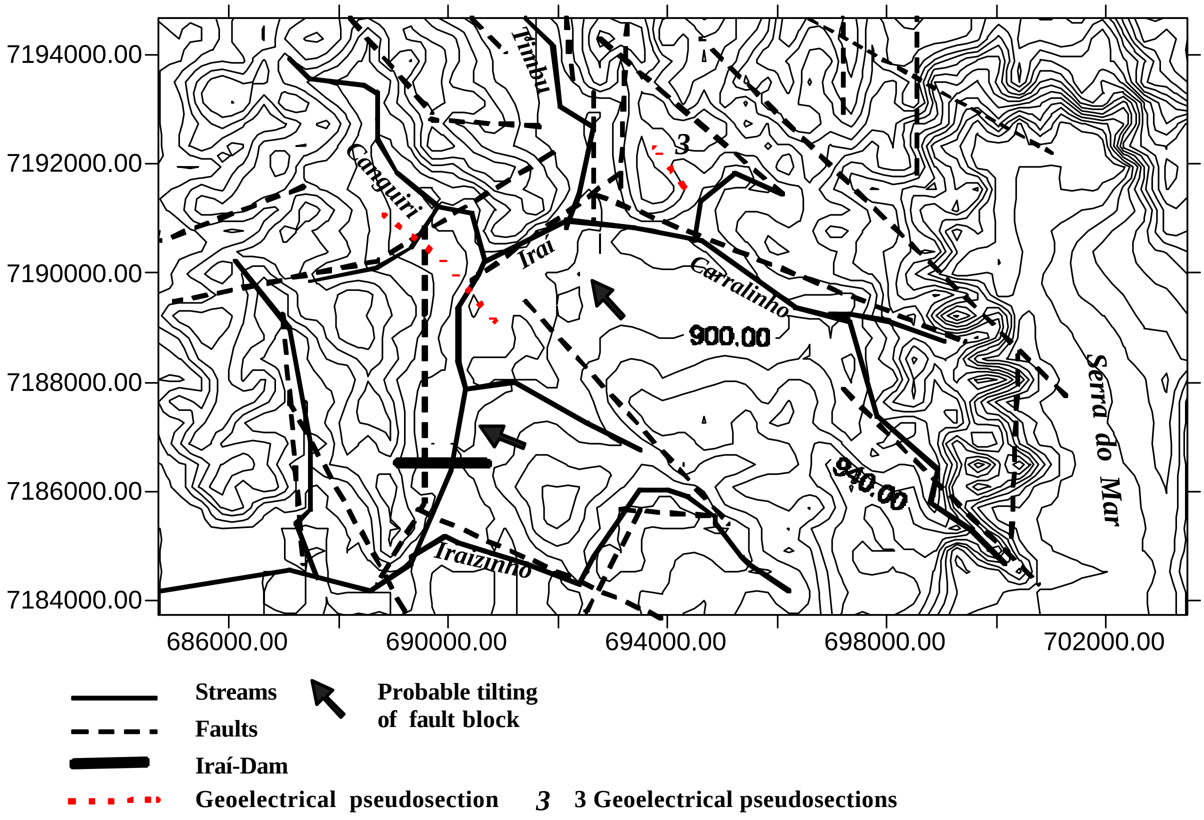


Figure 6: Schematic drawing of the course of streams and faulting on the height contour map

The course of the Iraí-river may support this view of tilted fault blocks (fig. 6).

There are both erosive and depositional landforms in the Iraí-basin. The erosion takes place in the hills and at the mountain slopes of the Serra do Mar, as deposition takes place in the lower parts of the basin (the so called várzea). In general where the alluvium is present the deposition takes place, forming a plain in the central part of the basin and along the tributaries of this central trunk plain.

This central trunk plain widens when the Curralinho (whose name changes later to the Iraí-river) enters this valley from the Serra do Mar and is at its broadest where the Canguiri tributary flows into the Iraí-river.

This central plain grows narrower downstream until the Rio Iraizinho flows into the Rio Iraí were the plain is at its narrowest. About 1 km upstream from were the floodplain is at its narrowest the so called Iraí-dam has been planned, so that the water may collect in this valley, which will be used as a drinking water reservoir.

The pros and contras for this approach for water supply will be discussed in section 2.5.2.

Where the valley narrows the depth to the bedrock gets shallower in the flood plain (Sanepar, 1996).

In figure 17 the isoline contours of hydraulic heads show that the groundwater flow is across the western hydrographic boundary so that it is possible that downstream the axis of the trunk valley may develop in a western direction by lateral fluvial erosion. It is an indication that the Iraí-valley in this reach is geomorphologically not in equilibrium. This may be explained by neotectonic activity that raised the blocks East of the Iraí.

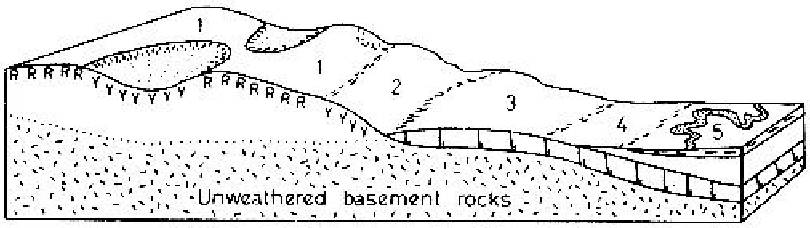
The mayor part of the survey area (where the Guabirotuba Formation predominates) has an asymmetric relief, consisting of broad levelled ridges whose sides are gentle and with gentle sloping escarpments. Those escarpments are most steep where they are probably along faults.
The height of this relief varies between 890 and 950 m. The slope angles of this relief vary mostly between 6 and 12 %, with lengths often larger than 1 km, and for angles larger than 20 % the extensions are in general smaller than 500 m.
The inundation areas along the streams are rather flat plains (várzeas). The flood plain is a large swamp apart from the areas that are drained by ditches.
At the east side of the basin, where the Serra do Mar stands out, the altitudes vary between the 900 to 1200 m. In this area slopes larger than 45 % predominate.

The weathering in the area is predominantly chemical weathering, but often on cleared land erosion during storm events takes place especially when the soil is less permeable. Observations of intensively (chemically) weathered rocks (in all cases migmatites) the rock structure was still visible but from the rock only clay with quartz veins remained. When land is cleared or under a changed climate these weathering products are easily eroded.
In the following paragraph soil formation is discussed which is actually important for chemical weathering.

2.3 Soils

What type of soils are available in the study area depends much on the climate but also on the lithology, the duration soil formation took place and the topography.
The climate may laterally be seen as a constant (wet subtropical) and is described in the next section. The characteristic fully developed soils of the wet tropics and subtropics are red or yellow in colour, old and strongly leached (Driessen and Dudal, 1991). They are deep, finely textured, contain no more than traces of weatherable minerals, have low-activity clays, less than 5 percent recognisable rock structure and gradual soil boundaries. The differences among the soils in the (sub)tropics may be largely attributed to differences in lithology (e.g. Plinthosols, FAO-classification commonly in weathering material of basic rock, essential is that sufficient iron is present as Ferralsols may be pre-weathered material from a wide variety of rocks) and (past) moisture regime (e.g. Plinthosols from Gr. plinthos, brick) common were the water table is fluctuating as Ferralsols are on level to undulating land). For clarity the fluctuation of the water tables (near) the surface is not so extreme that Plinthosols are formed in the area because the drier season in winter is not so pronounced.
The lithology is geochemically not very different for the rocks in the study area so that it is not an important factor for the distribution of the different soil units, which as described in section 2.1.2 consist of migmatites and granites or their weathering products. Generally in the study area under well drained conditions deep and intensive weathering takes place and resulted in a residual concentration of resistant primary minerals, and the formation of kaolinitic clays and iron and aluminium oxides and hydroxides. This mineralogy and the low pH account for the

stable microstructure (pseudo-sand) and yellowish (goethite) and reddish (hematite) colours of Ferralsols (Latosols for the Brazilian Soil Survey EMBRAPA).
Probably important for the differentiation of soil units present are the age of the soils (stage of development) and the topography (water table and relief as illustrated in figure 7). Especially in the near vicinity of the flood plain and small tributary valleys younger soils are present that have still not evolved to a mature soil (Cambisols) or which have on the same time an impeded drainage (hydromorphic gleyic soils and organic soils).

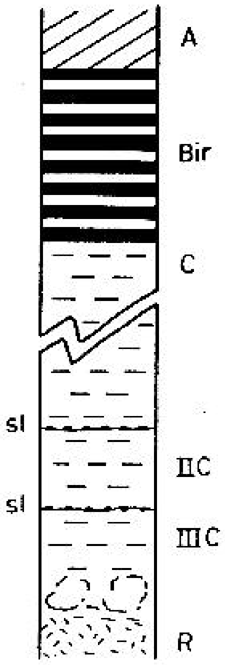


1. Ferralsols
2. and 3. Ferralitic Cambisols
4. Gleysols
5. Histosols

Figure 7: A soil catena of the humid tropical and subtropical regions, changed to represent the situation in the study area and named after the FAO-classification (after Bridges, 1978).

The most important occurring soils in the survey area are Latosols, Cambisols and organic soils. Further soils that occur in the area are hydromorphic gleyic soils and Lithosols.
All the soils in the area are acid, with a low base saturation and a high aluminium content indicating a low natural fertility.
The above mentioned soil names are according to the taxonomy of the Soil Survey Staff adapted to the Brazilian situation (EMBRAPA, 1984). For clarity with the class description of the soils, the FAO-UNESCO and the Soil Taxonomy (ST) names will be given as well (Driessen and Dudal, 1991; Schroeder, 1992). The soils and their possible influences on the groundwater quality will be discussed.

Latosols (FAO: Ferralsols; ST:Oxisol): this class covers the soils that are not hydromorphic, that have a latosol B equivalent to a ferralic B-horizon (FAO-UNESCO) or an oxic horizon according to classification of the Soil Survey Staff (fig. 8). For a definition of the diagnostic B-horizon see Driessen and Dudal, 1991. The Latosols are present on the migmatites and the Guabirotuba Formation. The environment is typically level to undulating land of Pleistocene age or older; perhumid or humid tropical to subtropical climates.



A: A-horizont
Bir: B-horizont with accumulation of illuvial iron (ferralic B-horizon), may be meters thick.
C: C-horizon, the parent material; IIC and IIIC is for layers.
sl: layer with pebbles a socalled stoneline
R: rock

Figure 8: Diagrammatic profile of a Ferralsol (after Bridges, 1978).

The name for this kind of soil formation is because of the ferralitisation, which is equivalent to hydrolysis in an advanced stage.

Water affects primary minerals through the processes of ‘hydration’ and ‘hydrolysis’. Hydration is water absorption by solid particles. In hydrolysis, H^+-ions penetrate the structures of minerals such as feldspars which then release cations (K, Na, Ca, Mg). As the hydrogen ion is much smaller than any of the cations it replaces, the structure of the mineral is weakened. This accelerates the dissolution of Si and Al.

The combination of (slow) release and leaching of Si, K, Na, Mg and Ca keeps the concentrations of these ions in the soil solution low. If the soil temperature is high and percolation intense, all weatherable primary minerals will ultimately dissolve and be removed from the soil mass. Less soluble compounds such as iron and aluminium oxides and coarse quartz grains, remain (enrichment of Fe- and Al-oxides). Although most silica disappears through leaching, some silica combines with aluminium to the 1:1 clay mineral Kaolinite. Impeded internal drainage may enhance kaolinitization because silica in solution is less quickly removed.

Indeed, the clay fraction consists predominantly of kaolinite and sesquioxides (EMBRAPA, 1984).

Ferrihydrite ($Fe(OH)_3$) forms if the iron concentration of the weathering parent material is high. Hematite (Fe_2O_3), the mineral which lends many tropical soils their bright red colour may form out of ferrihydrite, if the content of organic matter is low, the temperature is high (accelerates dehydration of ferrihydrite and decomposition of organic matter) and the soil pH is higher than 4.0.

Because the organic matter is rapidly decomposed, chelation is not possible so that no iron-mobilisation takes place unless the redox-potential is sufficiently lowered.
The temperature amplitude at depth is substantially less than at the surface, so that at some depth no more hematite is formed.

Ferralitization should be taken into account in the tropics and subtropics when building a well because it has a direct influence on the iron-content in the water. That is why a well is normally cemented to a depth of at least 12 meters (where the temperature amplitude is damped and no soil formation takes place). This depth is normally determined by regarding the colour of the rock by the geologist in the field.

Cambisols (FAO: Cambisol; ST: Ochrept, Umbrept): cover non-hydromorphic soils, with a cambic B. The soils are in a transitional stage of development (Driessen and Dudal, 1991) from a young soil to a mature soil, with in this case a ferralic B-horizon which corresponds to a Latosol. The soil still contains primary minerals that are relatively easily weatherable, which do not have significant accumulation of iron-oxides, humus and clay that would permit an recognition of a textural B or a podzol B. Very often similar characteristics to a latosol B horizon, but less evolved, and less deeply developed. The Cambisols are found in the Holocene alluvial deposits along the tributaries of the Iraí-river where the land is relatively well drained and former erosion surfaces that have stabilised..
The same ferralitization processes take place in these soils but because they are still relatively young , they are not so far evolved.

Organic soils (FAO, ST: Histosols): This are hydromorphic soils that are essentially organic, little evolved, arising from plant remains with varying grade of decomposition, accumulated in a flood plain environment, forming a black coloured upper horizon (EMBRAPA, 1984; Schroeder, 1992; Driessen and Dudal, 1991).
The (organic) A-horizon possesses a thickness of at least 40 cm. The texture may vary from one locality to another locality.
As the conspicuous characteristics of the soils are the acidic nature, the low base saturation, the high saturation of exchangeable aluminium, and the high Cation Exchange Capacity (CEC), all in relation with bad drainage.
Because the decomposition of organic matter is retarded, chelation is possible so that iron-mobilisation is possible together by reduction of Fe^{3+} with the lowered redox-potential.
That is why iron is almost always a problem for the water quality when wells are developed in badly drained areas in this region.

Hydromorphic gleyic soils (Gleysols: FAO; prefix Aqu: ST): soils in unconsolidated materials, exclusive of coarse-textured materials and alluvial deposits showing at least some stratification; showing gleyic properties within 50 cm of the surface; having no diagnostic horizons other than an organic A-horizon or a histic (more than 20 cm but less than 40 cm thick) H-horizon.
So long the (organic) A-horizon possesses a thickness thinner than 40 cm a hydromorphic soil may be called a Gleysol, otherwise it should be called an organic soil.
The formation of Gleysols is conditioned by excessive wetness at shallow depth (less than 50 cm from the surface) in this case throughout the year. Low-redox conditions, brought about by prolonged saturation of the soil material in the presence of organic matter, result in the reduction of ferric iron compounds to (mobile) ferrous compounds. This explains why the permanently saturated subsoil layers of Gleysols have grey, olive or blue colours: with the iron compounds mobilised and removed, the soil material shows its own colour.

Subsequent oxidation of transported ferrous compounds (back) to ferric oxides can take place near fissures or cracks in the soil and along former root channels where is a supply of oxygen. Hysteresis between (comparatively rapid) oxidation and (slow) reduction processes leads to a net accumulation of ferric compounds near such aerated spots in the otherwise reduced soil matrix: the subsoil develops a pattern of mottles (around air pockets) and ‘root prints’ . Such ‘gleyic properties’ are strictly associated with movement of the groundwater table.

The same problems as in the case of organic soils may arise here when wells are developed, because iron may be mobilised by chelation and reduction.

2.4 Climate and meteorological data within the study area

Because the Southern Hemisphere is dominated by oceans, atmospheric circulation is primarily zonal (Clapperton, 1993). Air flows generally from East to West in equatorial-tropical latitudes and from West to East in temperate-subpolar latitudes. This is controlled by the semi-permanent pressure fields established in the inter-tropical (low pressure), sub-tropical (high pressure), temperate (low pressure) and polar (high pressure) latitudes (fig. 9). This simple pattern of circulation is disrupted in the Southern Hemisphere by the Southward penetration of the South American landmass to latitude 55°, and by the North-South continuity of the Andes mountains. Thus the massive band of sub-tropical high pressure is broken into two discrete cells on either sides of South America.

Air mass movement associated with seasonal fluctuations of these pressure systems is mainly responsible for the various climatic types over the continent (fig. 9). In tropical latitudes, equatorial air flows from either side of the equator to the inter-tropical convergence zone (ITCZ) which migrates in position north and south with the annual passage of the overhead sun from tropic to tropic. In Southern latitudes, temperate and polar air converge along the atmospheric polar front. This does not migrate far from its average position around latitude 55°-60°, but it generates frontal systems which, in winter can penetrate into tropical South-America. This is because the Andes barrier creates a pronounced ‘gap’ in the zonal continuity of the subtropical high pressure belt.

In addition to these primary atmospheric pressure cells, which generate the easterly and westerly air flow dominating South-American climates, secondary circulation is caused seasonally by strong insulation in subtropical latitudes; this heats the land surface and

produces thermal low pressure cells. Other influences on the continent’s climate include land area, topography, biomass and sea surface temperatures.

Because the continent becomes very narrow in temperate latitudes, the extremes of temperature of ‘continental interior’ climates typical of the Northern hemisphere are absent.

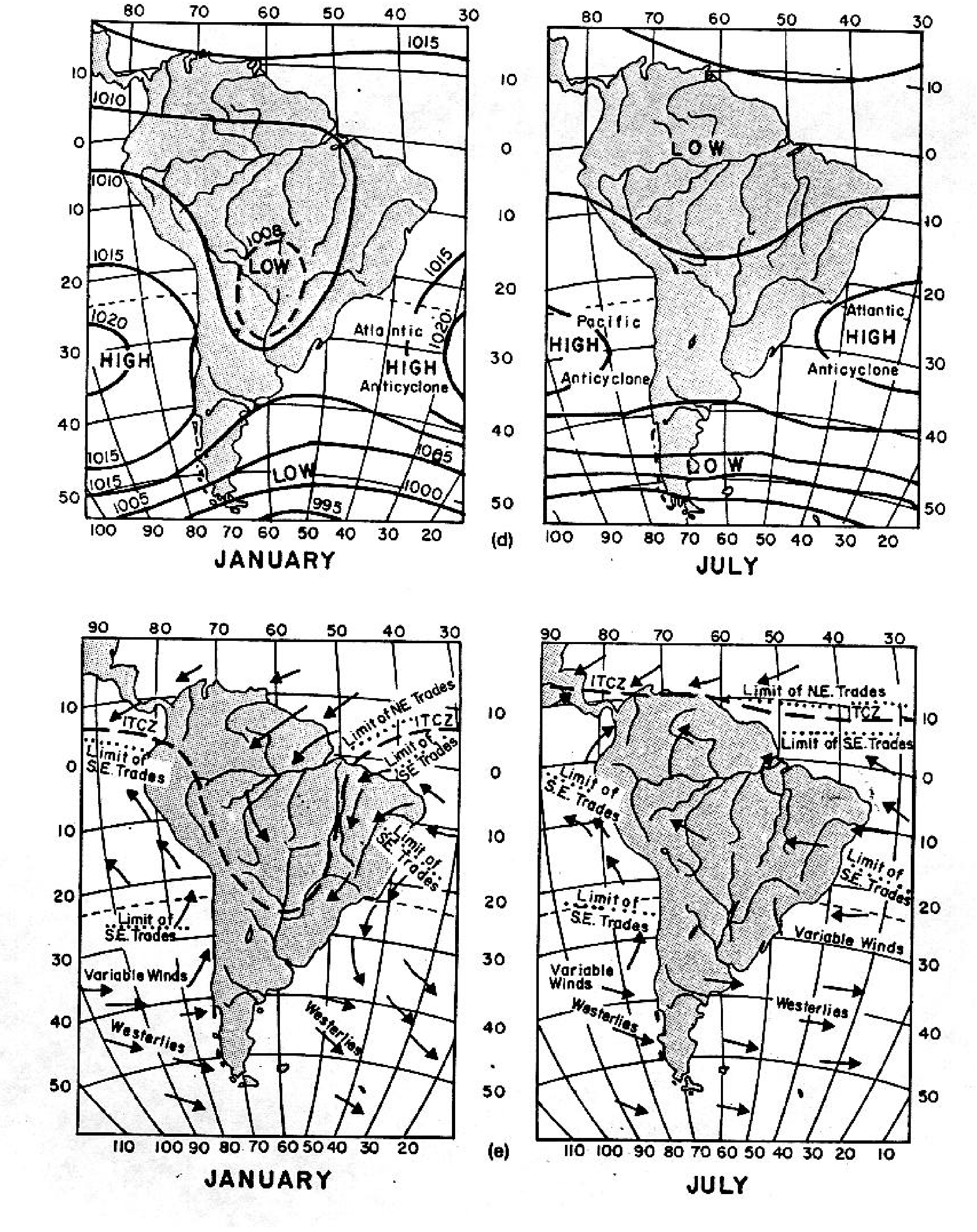


Figure 9: Average atmospheric pressure (sea level) patterns for January and July and the average airflow for January and July (After Clapperton, 1993).

The sub-tropical zone in which the survey area is situated, the mean annual temperature varies seasonally from 27°C in summer to 15°C in winter. An important control on climate here is the greatly increased width of the continent north of 40°S which means that more land area lies under influence of the upper atmospheric low pressure trough in the lee of the Andes (which are also much higher in these latitudes). Over the Argentine Pampa, the south-westerly airflow from

Patagonia gradually curves round to flow from the West and Northwest, becoming cyclonic in a zone of converging air. Cold polar maritime air pushed North from the Southern Ocean (South-Atlantic) makes contact with the warm tropical air of subtropical latitudes, thereby initiating cyclogenesis. Frontal weather systems associated with these bring precipitation to the eastern part of the continent. Because much of the airflow sweeps in from the Southeast, rainfall is highest near the coast and decreases inland to very low totals. Rainfall throughout most of the subtropics is highly seasonal, occurring mostly in summer.

The type of climate on the smaller regional scale of the survey area (EMBRAPA, 1984) falls into the Cfb-class of Köppen; mesothermic, moist, without a dry season, with a mean temperature in the hottest month of less than 22°C and with frequent frosts.

From the climatic station at the IAPAR, Piraquara in the survey area meteorological measurements are made since 1970. In the graphs (fig. 10 and 11) the mean values are plotted from the mean monthly temperatures at 15:00 hours (!) and the mean monthly precipitation. The values of the mean monthly precipitation, the mean monthly evaporation and the effective precipitation in the period of 1970 to 1997 are presented in Table 1. The evaporation is actually the evaporation from a free water surface (pan evaporation), but is the only value available.

But it gives some indication of what the magnitude of evaporation or even evapotranspiration may be.

Though to quantify the evapotranspiration may be very dangerous with the available data.

The effective precipitation is the water that may flow as surface water and groundwater (total runoff).

In this case the effective precipitation is said to be the difference between the precipitation and the evaporation, which does not necessarily conform with the official terminology which is actually the difference between the precipitation and evapotranspiration (Ward, 1999). Because the evapotranspiration can not be determined with the available data (pan evaporation), the evaporation is used to get at least a possible magnitude of the evapotranspiration so that the effective precipitation can be estimated. The yearly effective precipitation is 712.1 mm according to table 1, with minimum effective precipitation in August and maximum in January.

In the conceptual model the volume of the surface flow and the groundwater recharge will be the same quantity as the yearly total effective precipitation which corresponds to $2.26 * 10^{-5}$ mm*m^2/s, for the Iraí drainage area of 163 km^2 is equal to 3.749 m^3/s. For the summer the mean distribution of wind-directions for January is given, as for the winter the mean distribution of July is given (fig. 12 and 13). The directions are given in degrees. In table 2 the total yearly precipitation is given for the period of 1970 to 1997 to give an indication how it may vary.

In summer the prevailing wind comes from the East, while the frequencies from the other wind directions seem random.

In winter the prevailing wind direction comes from the North, with higher frequencies from the Northeast and East. In winter it is very rare that the wind comes from the South. In summer the prevailing wind direction seems to correspond with the larger scale average air flow (fig. 9), but in winter the regional wind direction seems to slightly deviate from the larger scale average air flow. Probably the Sierra do Mar has some influence.

Table 1: Mean Precipitation, Evaporation and Effective Precipitation in the period from 1970 to 1997.

	Precipitation [mm]	Pan Evaporation [mm]	Effective Precipitation [mm]
Jan.	189.3	61	128.3
Feb.	140.3	53.3	87
March	120.2	52.8	67.4
April	79.4	55.9	23.5
May	110.1	49.2	60.9
June	97.8	45.4	52.4
July	91.5	55.8	35.7
Aug.	71.6	60.1	11.5
Sept.	82.9	55.9	27
Oct.	129.8	62.1	67.7
Nov.	116.3	62.2	54.1
Dec.	157.4	60.8	96.6
Yearly Total:	1386.6	674.5	712.1

Table 2: Total Yearly Precipitation for 1970 to 1997; * for 1970 and 1993 January is missing.

Year	precipitation [mm]	Remarks
1970	1134	*
1971	1211.2	
1972	1366.1	
1973	1370.9	
1974	1345	
1975	1303.7	
1976	1786.9	
1977	1239.4	
1978	1073.2	
1979	1249.1	
1980	1535.5	
1981	1249.1	
1982	1538.3	
1983	2009.1	
1984	1458.9	
1985	936.1	
1986	1528.1	
1987	1275	
1988	1309.3	
1989	1439.6	
1990	1770.8	
1991	1134.9	
1992	1419.3	
1993	1193	*
1994	1400.6	
1995	1610.2	
1996	1892.8	
1997	1603.1	

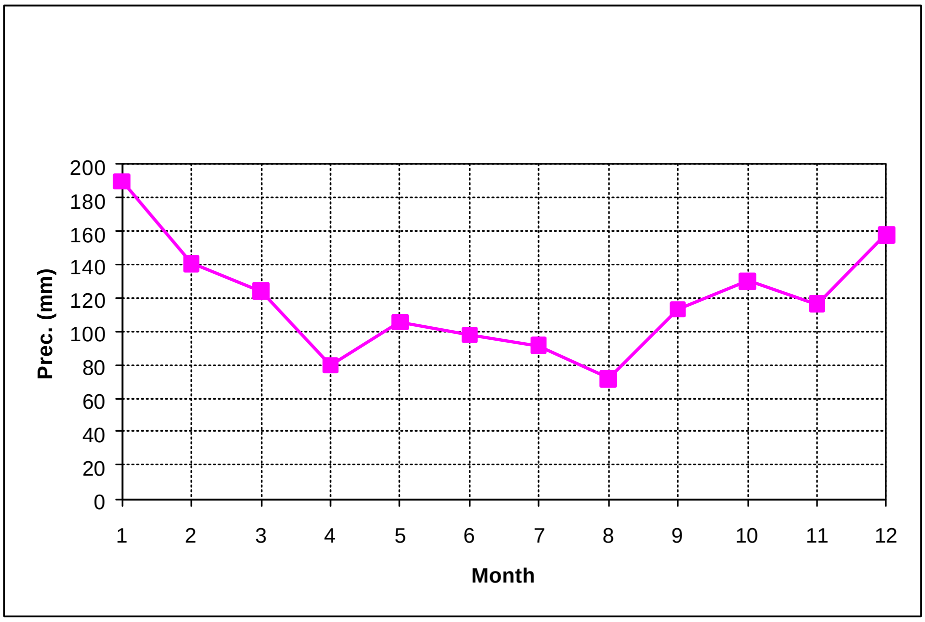


Figure 10: Iapar, Piraquara: Mean monthly precipitation from 1970 to 1997.

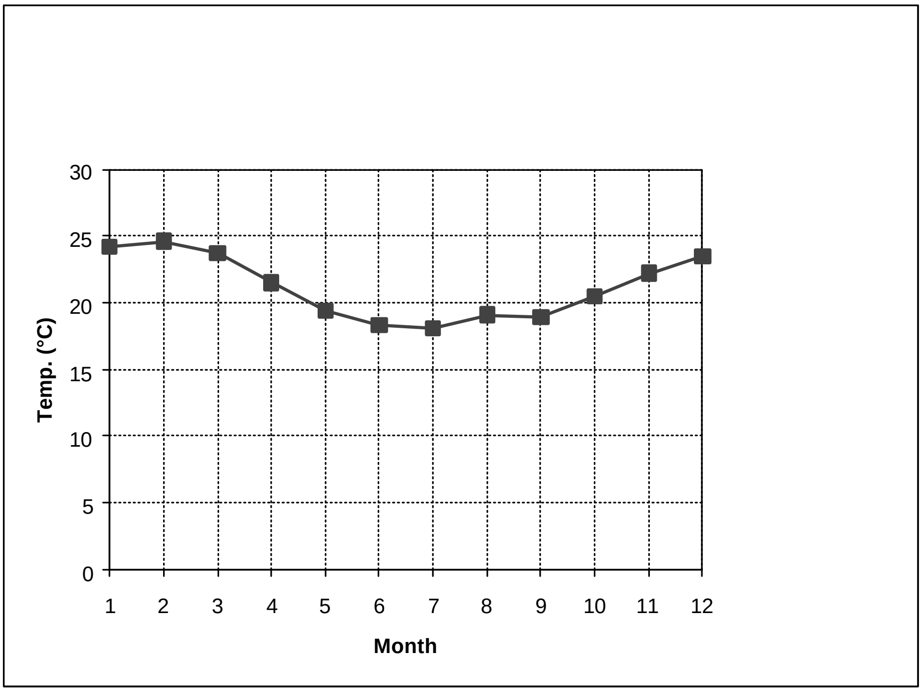


Figure 11: Iapar, Piraquara: Mean monthly temperature from 1970 to 1997.

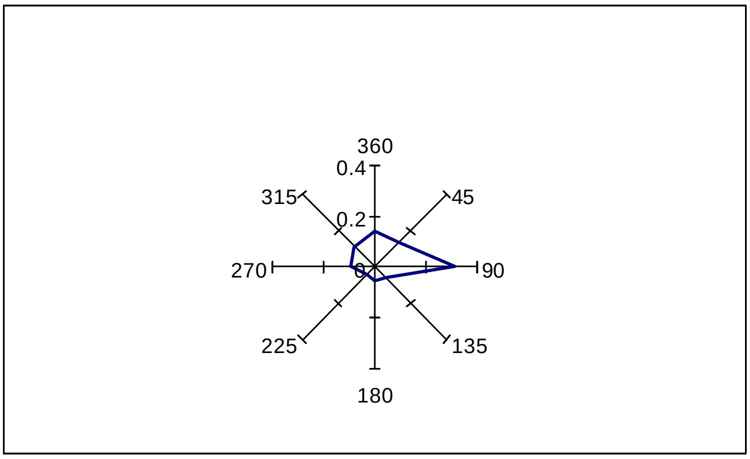


Figure 12: Iapar, winddirections in January (summer).

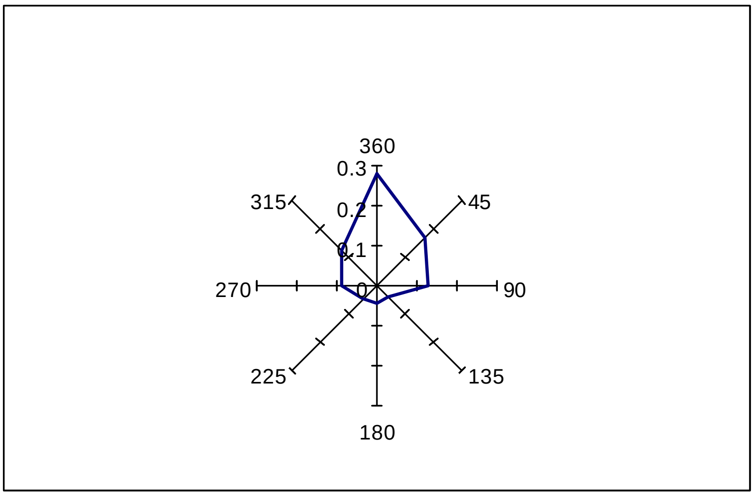


Figure 13: Iapar, winddirections in July (winter).

2.5 Possible stresses on the water resources in general in the Metropolitan Region of Curitiba, with emphasis on the study area

Several stresses act upon the water resources, which may be quantitative and/or qualitative, and may act on both surface and subsurface waters. The large population of the Metropolitan Region of Curitiba (MRC) needs a lot of water and on the same time poses a large environmental stress on the limited resources. This environmental stress is induced by the large quantities of water needed, the large volumes of sewage waters, uncontrolled littering of waste and the use of herbicides, pesticides and fertilisers by the agriculture. These anthropogenic influences on the water resources will be described below, containing a description of these influences on the surface waters, their possible influence on the groundwater, the water supply of the MRC, the development of the MRC, and the necessity for the development of new drinking water facilities. The planning of these facilities in the form of reservoirs (from which the Iraí-reservoir is one) or other alternative measures to be taken to secure the water supply is described. With the discussion of the pros and contras for the planned reservoirs.

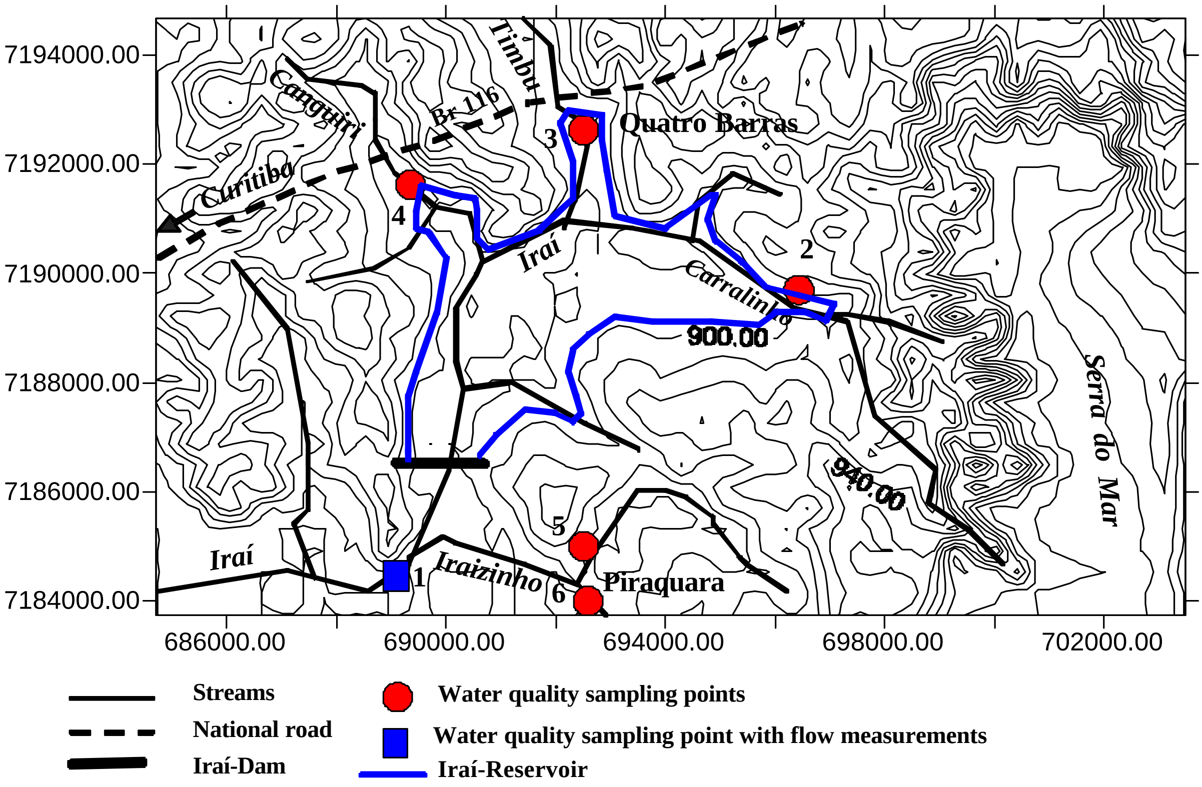


Figure 14: Water quality sampling points: 1. Rio Iraí, Olaria do Estado; 2. Rio Carralinho; 3. Rio Timbo; 4. Rio Canguiri; 5. Rio Iraizinho; 6. Rio do Meio (after Suderhza, 1997).

2.5.1 The surface waters and their possible influences on the groundwater

The sewage waters in Brazil are mainly released without any treatment. In the RMC only 41 % of the population is linked to the sewage system and taking in account the sewage waters that are actually treated, the percentage falls to 16 % (COMEC, 1997). In the survey area absolutely no purification of the sewage waters takes place. This will probably not change in a short time because the majority of the households in the study area are not even connected to the sewage system (e.g. in Quatro Barras 755 of 12215 inhabitants corresponding to ± 6 % in 1991; Sanepar 1991).

In addition about 3000 tons of agrochemical are used around the RMC (Edinei Bueno do Nascimento, personal commun.), which form a diffuse source of pollution.

Water quality data taken from Suderhza (1997) at the water quality sample points from the Iraí-basin and Iraizinho-basin are presented in appendix A.

The flow of the Iraí was measured at water quality point Olaria do Estado.

Unfortunately this measuring point was chosen past the confluence of the Iraí –and Iraizinho rivers outside the drainage area of the Iraí-reservoir, so that these data represent the flow volume of the Iraí downstream the Iraizinho (fig. 14). The Iraizinho is draining an area from outside the study area. From other points within the study area and the area corresponding to the Iraizinho drainage area, only water quality data and no flow data were determined. This is why the flow data from Olaria do Estado can be seen as the maximal possible discharge as a member in the water balance of the surveyed drainage area, and its water quality data as a mixed sample of both basins. As the mean discharge at Olaria do estado a value of 2.29 m^3/s has been calculated.

About 20 to 30 % of this quantity belongs to the Iraizinho drainage area, which leaves about 1.6 m^3/s as the mean discharge for the Iraí-basin, when the Iraizinho drainage area delivers 30 % of the discharge measured at Olaria do estado.

The data available within the survey area are from the Curralinho, Rio Timbo and the Rio Canguiri from which the Rio Timbo and Rio Canguiri have higher values of faecal coliforms , BOD_5, total nitrogen and phosphorus than those of the Rio Carralinho. The higher values of the Rio Timbo and Rio Canguiri may be explained by the fact that they stream through urban developed areas as the Rio Carralinho originates from the little populated Serra do Mar. The values of faecal coliforms, BOD_5, total nitrogen and phosphorus of the Rio Timbo and Rio Canguiri are higher than those of the Rio Iraí at Olaria do Estado, which has been mixed with the waters of the Rio Iraizinho and the Rio Iraí. Another striking feature is the slightly lower pH of the Rio Carralinho water which is flowing straight from the Serra do Mar and through a not so densely populated and cultivated area, compared with the other tributaries. The other tributaries have slightly higher pH’s, which are probably more influenced by human activities (higher phosphorus, nitrogen and total dissolved solids).

In general for the study area the total phosphorus values and nitrogen values fall within the range of eu- to polytroph (Heitfeld, 1991), which means that there exists a high risk for eutrophication of the water. Another striking feature is that the pH and conductivity vary much for surface waters in time. The reason for these variations is unclear.

The parameters that may influence the groundwater are probably not the faecal coliforms and the organic matter but nitrate, ammonia, and phosphorus.

Typically, phosphorus contamination of groundwater is considered together with nitrogen. However, it is less important because of the low solubility of phosphorus compounds in groundwater, the limited mobility of phosphorus due to its tendency to sorb on solids, and the lack of proven health problems. Ammonia may only be used as indication for possible contamination by surface waters provided that the soils are highly permeable and no adsorbing agent like clays are present. Another problem with ammonium and phosphorus is that the aquifer may underlying an agricultural area so that these compounds do not necessary originate from infiltrated surface waters.

Because of the better solubility and mobility of nitrogen in the form of nitrate, this compound may be used as indicators in the groundwater to trace infiltration of surface waters, provided they are eutrophic.

But nitrate may also originate from agricultural activities.

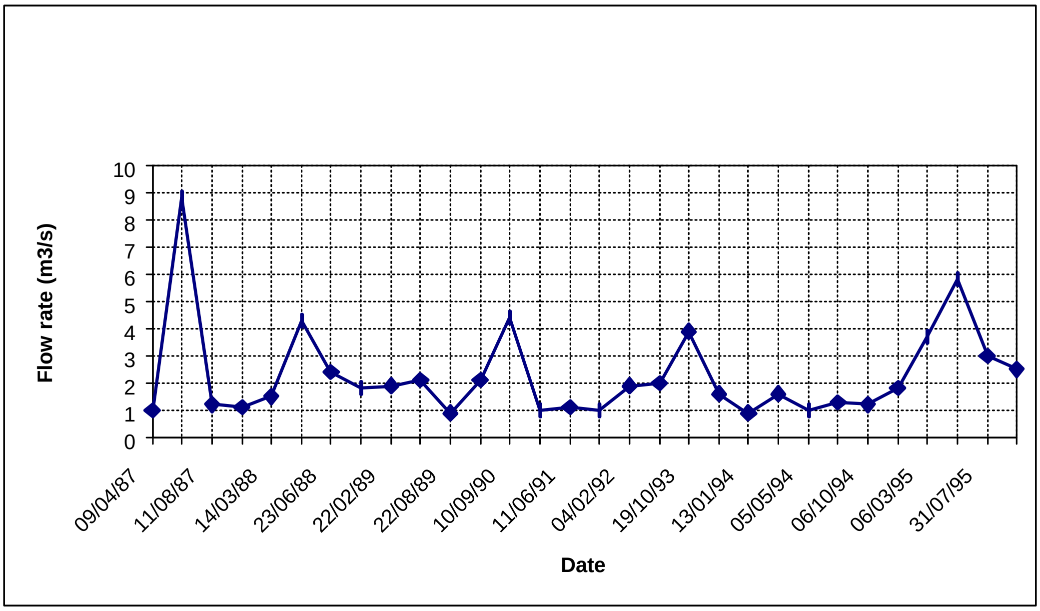


Figure 15: flow rate of the Iraí-river at Olaria do estado from 1987 to 1995 (after Suderhza, 1997).

2.5.2 The development of Metropolitan Region of Curitiba (MCR)

Curitiba is nowadays the fastest growing metropolitan region of Brazil (Wilhelmy, 1985; Ernani, 1991). Although the city of Curitiba is the one before last of the nine largest cities in Brazil with 1.4 million inhabitants (1991), it will soon pass the cities Fortaleza and Salvador in numbers. As the Metropolitan Region of Curitiba has 5.8 million inhabitants nowadays (Dalarmi, 1995).

The capital city of Paraná is situated at 900-950 m above sea level on an elevated plain and was surrounded by woods.
1654 it was founded as a settlement for gold miners and was until the 19th century a small rural town, which developed to a centre of the yerba-mate trade (mate tee) and cattle transport.
1854 it became the capital city of the newly founded Federal State of Paraná.
Curitiba prospered from the European immigration in the hinterland predominantly by German, Polish and Italian immigrants.
With the arrival of European immigrants the first agricultural colonies were founded in this region.

Since 1941 the city grew to over 100,000 inhabitants, as 1960 it had 345,000 inhabitants.
The relative young economical grow of the small rural –and administrative town really started with the Southern shift of the coffee-frontier as far as on the territory of Paraná, based on a global coffee boom.
During the 50s and 60s Curitiba accommodated mainly immigrants, who settled the rural areas. As new agricultural colonies arose nearby places like Almirante Tamandaré, Araucária and Campo Largo, which are nowadays the most significant satellite cities of Curitiba.

The beginning of the 1960s was the beginning of a tremendous boom of the population of Curitiba, that had 1.025 million inhabitants in 1980.

Because of the concentration of the urban population on one city centre, Curitiba has a centre of high-rise buildings which skyline is as large as the city of Pôrto Alegre that has double the population of the city of Curitiba.
The effect of the skyline is raised by the plain surroundings and that the centre with adjacent neighbourhoods is surrounded by favelas. The high-rise buildings stand out as an islands of economic prosperity and modernity.
A contrast of this prosperity and modernity of the centre of Curitiba, forms the ring of marginal settlements.
These favelas are illegally build on speculating grounds and are tolerated for the present by the municipal administration. These favelas are crowded by people from whom most of them came from the country fleeing unemployment (due to mechanisation of the agriculture) hoping to find employment in the city of Curitiba.

With the gaining importance of Paraná Curitiba grew together with Pôrto Allegre to the most important centre of industry for Southern Brazil.
A refinery of Petrobras provided by a pipeline belongs together with the Volvo factory and a branch from the German company Bosch to the most important employers in the MRC.
About 120 industrial corporations produce steel, iron, machinery, fertilisers, petroleum derivatives, cement, sugar and alcohol. The MRC also draws new investors like Renault.
This concentration of industries draws a lot of people from weaker developed regions.
This explosive expansion of the population raised a high increase in the demand for water resources and the uncontrolled settlement poses a large problem for the environment.

2.5.3 Water supply of the Metropolitan Region of Curitiba, necessity for the Iraí-reservoir

The population of the MRC is at present about 5.8 million people who need approximately 6400 l/s. The total available at the moment is 5800 l/s. This deficit of approximately 600 l/s leaves about 320.000 people without water during about 60 hours in a week, equivalent to 2.5 days per week or 10 days in a month (Ernani F. da Rosa Filho and Udluft, P., 1998; Dalarmi, 1995). Given the substantial demographic growth of the MRC, the region is facing an enormous difficulty in the utilisation of its water resources for the public water supply.
To eliminate the drinking water deficits, a planning is made (SANEPAR, 1992) for the construction of 5 dams for capturing the Iraí, Piraquara, Pequeno, Miringuava and Cotia/Despique rivers (fig. 16).
Three systems for the water supply are planned, namely Iraí (comprising the Iraí-, Piraquara II and Pequeno dams), and respectively, the Miringuava -and Cotia/Despique systems which have the same name as the captured rivers from which they extract their water. The maximum possible volume of the water captured in the Iraí-basin will be 1120 l/s (COMEC, 1997).

Another target is to avoid the frequent floods in various more or less densely populated areas, causing much damage and even loss of lives (SANEPAR, 1991) by controlling the river discharges.
The prediction for the water supply is that with the development the yield of these systems until the year 2020 will be 12.74 m^3/s, including a karst aquifer providing 600 l/s that will be used in emergencies. This quantity may provide a population in Curitiba of 5.8 million inhabitants.

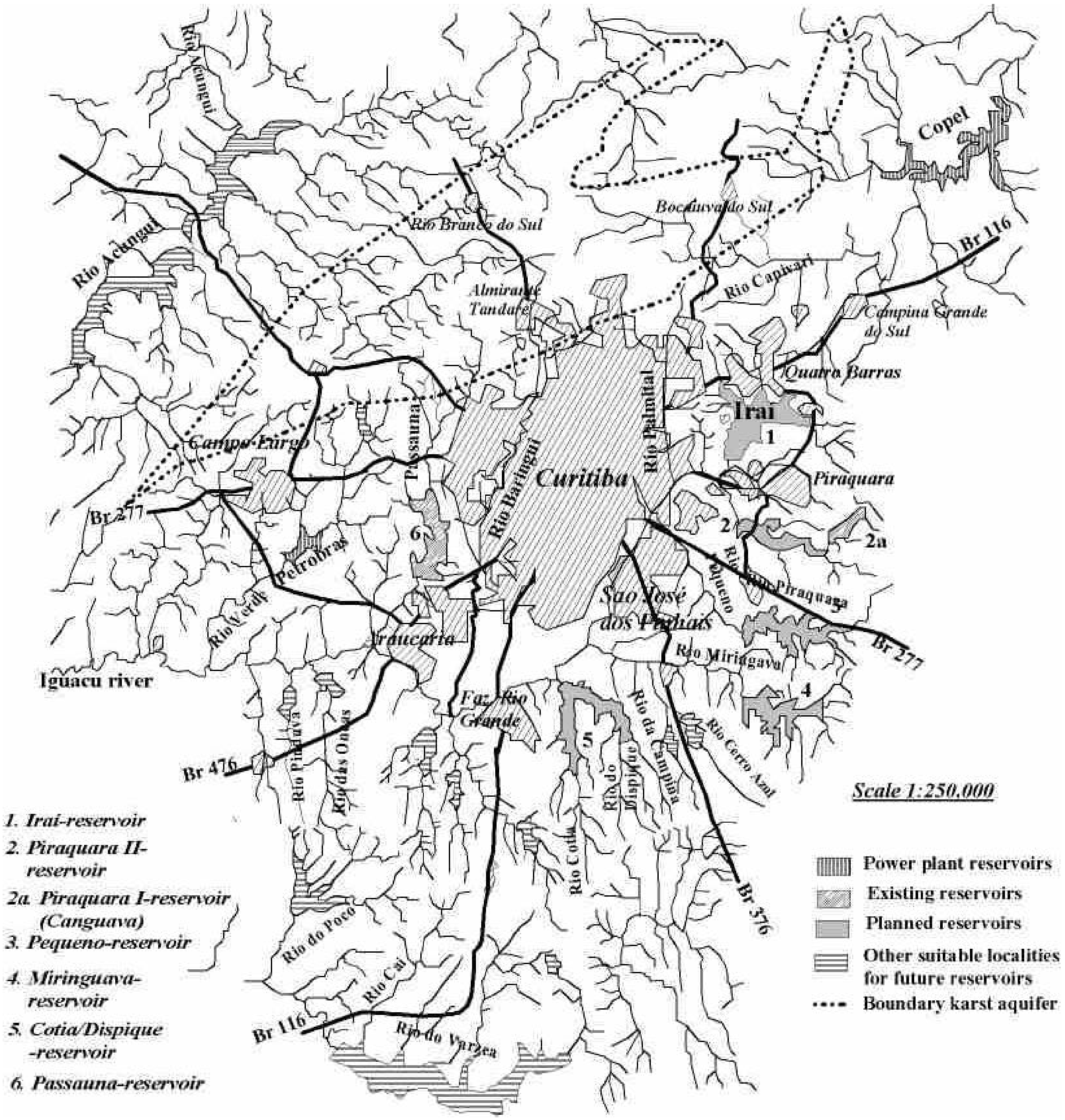


Figure 16: Water resources for the Metropolitan Region of Curitiba (after Dalarmi, 1995).

With the utilisation of the Iraí-basin for the purpose of public water supply, it is necessary to get control for inhibiting or reducing water pollution. To solve this problem it is necessary for the inhabited areas to receive a sewage system which have a treatment station for the sewage waters and the garbage collecting should be improved.

Not only may the garbage pollute the water but also may block the channels so that floods may be more disastrous.

The greatest menace to the water supply sources of this region is the urban occupation (invasion) into the areas that contain these resources. This occupation continues with its slow, silent, although progressive march, threatening precious and irreplaceable resources (Dalarmi, 1995).

Controlling the pollution may be the weakness for this system of reservoirs. The Iraí-reservoir even though an area around the lake will be protected may be polluted by two tributaries which flow through more or less densely populated areas. The water quality data of these two tributaries (Rio Canguiri and Rio Timbu) have higher values of faecal coliforms, BOD_5, total nitrogen and phosphorus.

In general for the study area the total phosphorus values and nitrogen values fall within the range of eu- to polytroph (Heitfeld, 1991), which means that there exists a high risk for eutrophiering of the water.

Because nitrogen in the form of nitrate has a much better solubility and mobility than the other compounds and the coliforms that probably not even reach the Guabirotuba aquifer, this compound may be used as parameter for calibration of the transport model and as indicator for contamination of nutrients.

This contamination of the Guabirotuba aquifer may be another disadvantage of building reservoirs for the water supply, also because this aquifer is already in use for the water supply. In general the groundwater is better protected so that it is more sensible to use more of the groundwater resources instead. On the other hand the groundwater resources in the region may not be sufficient to provide the MRC so that it is then simply necessary to build the reservoirs.
The influence that the Iraí-reservoir may have on the Guabirotuba aquifer, will be described with the help of a groundwater transport model a socalled particle tracking model.
Another disadvantage is that a larger area will be flooded, though this depends on the economical value of this area. Though this area probably does not have a very high economical value, because the area is a rather marshy area, environmentalists may find it a disadvantage in an ecological point of view.

2.6 The groundwater system

2.6.1 Recharge (hydrological balance)

To make a quantitative assessment of the groundwater resources may be considered in two ways: the total volume of water stored in an aquifer, or the long-term average recharge (Brassington, 1998). The more significant figure in terms of groundwater resources is the long-term average recharge, and it is usual for this value to be regarded as the available resources. Groundwater recharge to an aquifer cannot be measured directly, but only inferred from other measurements. As groundwater is part of the hydrological cycle, measurements of other components of the cycle can be used to estimate the value of the resources, using a technique called a water balance. In this type of calculation it is assumed that all the water entering an aquifer system is equal to the water leaving it, plus or minus any change in groundwater storage.

In this study the available data for the computation of water balance consist of precipitation, evaporation, river discharge and well abstraction data. The average monthly precipitation P, the average monthly evaporation E are presented in the section 2.4 and the river discharge data are presented in the section 2.5.1 and Appendix C. In section 2.4 the term effective precipitation P_e which is here the difference between precipitation and evaporation was introduced. So that P- E = P_e , which is equal to 712.1 mm/year. R_o is the total surface runoff, Q_p is the pumping withdrawal and R_r is the groundwater recharge. The river discharge at 'Olaria do Estado' is actually the flow of the basin were the Iraí-reservoir is developed and the Iraizinho that is a tributary of the Iraí that joins the Iraí-river downstream where the dam is build. That is why the flow data from Olaria do Estado can be seen as the maximal possible discharge as a member in the water balance of the surveyed drainage area. Because the area of the Iraizinho river is assessed as a fraction of about 30 % of the recharge area of Olaria do Estado, 30 % of the mean discharge at Olaria do Estado is subtracted so that the discharge of 1.6 m^3/s is taken for the Iraí-basin above the confluence.

All the data will be calculated for a period of at least a day, because the wells from which the pumping rate is known are only used for 20 hours per day. The total pumping rate per day is 1080 m^3/day, the P_e for the drainage area of 163 km^2 is $3.18 * 10^5$ m^3/day and R_o is $1.95 * 10^5$ m^3/day (437 mm/y*m^2).

The hydrological balance may be written as:

$$P_e - R_o = R_r \qquad \text{(Eq. 2.1)}$$

Which is a very simple equation in this case because of the very limited data available.

Inserting the above given terms in the formula gives $1.79 * 10^5$ m^3/day (275.1 mm/y* m^2) as the mean groundwater recharge.

The quantity of the subsurface outflow is the unknown parameter but should normally be equal to $R_r - Q_p$ on the long term.

The quantity pumped by wells is a bit less then a hundredth of the probable groundwater recharge. This will therefore probably have a larger influence on the modelling result. When pumping wells it will cause some local lowering of the water table levels in order that groundwater will be induced to flow towards the wells.

Because some of the terms (R_o and E) are only known in magnitude (the evaporation cannot be measured exactly and it is better to calculate P_e with the evapotranspiration) and the soil evaporation a comparison with an other water balance should be made.

The results of the water balance are compared with the results derived from the Water Balance Model MODBIL which is described in chapter 4. Because the principles, execution and the data processing need a more extensive explanation.

2.6.2 Groundwater hydraulics data, pumping tests, wells, groundwater system

The type of well used in the survey area are lined with a casing and sealed into the ground with concrete grout in the upper part. This design serves two main purposes: it provides support through unconsolidated or weathered materials near ground level, and also prevents surface water from entering the well and possibly contaminating the supply. In the survey area the wells have to be cemented to a depth of at least 12 meters, because of the possible contamination of iron as described in section 2.3.

The wells in the survey area all have filter screens in all the suitable aquifers penetrated to allow groundwater to flow into the well, so that the water level in the well represents the water pressure in all the aquifer material penetrated by the filters. So that the hydraulic head may represent the combination of hydraulic heads of several different aquifers.

The piezometers are build according to the same design which actually means that they are according terminology no real piezometers (CHO, 1986; Brassington, 1998). For simplicity all wells and piezometers will be called wells in the text.

From the hydrostatic levels of the wells (i.e. the water level in the well, before the pumping of a well test or pumping test of a new well took place) a isohypse map is constructed of hydraulic heads (fig. 17), the hydraulic data and technical data of the wells are presented in appendix B and from topographic features like wetlands or streams.

In the area of Parque Castelo Branco and Iapar where the most wells are constructed the isohypses in the isoline map correspond more or less with the topography, in the not so well covered area a general trend is visible. Figure 17 gives a very rough picture of the isolines of hydraulic heads, because the range of the interpolated data is very wide by the integration of the valley and the mountains in the recharge area. That is why an additional (zoomed) isoline map of hydraulic heads is given for the Iraí-valley, which is not used in the simulation model, that gives a better view of the hydraulic head surface (fig. 18). On this map also the wells, piezometers, (stream levels) and geotechnical drillings of the Iraí-dam are marked.

Additionally the course of the Iraí and the most important tributairies that are present in the zoomed area are drawn on the map.

Immediately in the area of the wells at Iapar, although the isolines have been constructed of the static levels of the wells, the influence of pumping wells is visible in the isoline map.

This general trend follows more or less the trend of the surface drainage, which means that the hydraulic head is decreasing from upstream to downstream in the hydrographic basin.

This general trend is the best result one can get in the not so well covered area. Probably the boundaries with the bedrock and its depth have to be taken into account. This is for example obvious for this general trend in hydraulic head which is from east to west nearby Parque Castelo Branco and the mouth of the basin, instead of the expected downstream gradient. This is probably because the depth of the bedrock is at Parque Castelo Branco about 50 m depth and according geotechnical studies for the Iraí-dam (Sanepar, 1996) more downstream this depth has been reduced to much shallower depth. The section of the Iraí-dam shows from east to west: bedrock (or its residual soil) at the surface that is gradually covered by drift in the floodplain to a depth of 5 m, to about a depth of 30 m were the land surface is elevated (fig. 19) so that it may be concluded that the hydraulic gradients are partially determined by the through-flow surface. The hydraulic heads near the dam indicate that the aquifer is probably not confined because the hydraulic heads more or less correspond to the water level in the Iraí. That is why for the area some measured in points in the floodplain were taken as additional points for the isoline map.

Another reason to take the topography of wet areas for the isoline map is that the hydraulic head (achieved by interpolation of scarce well heads) in a phreatic aquifer cannot be higher as the height of the land surface. It should be noted though, that the integration of stream levels in the isoline map of hydraulic heads is very dangerous and indeed did not make the calibration of the flow model very simple.

Additionally, near Iapar in the alluvial flatland geoelectrical pseudo-sections were measured in (Sanepar/GEA, 1998). The arrangement of the electrodes was Dipole-Dipole. This section was measured in along the road between Iapar and Colonia Penal (NW-SE) and suggests that

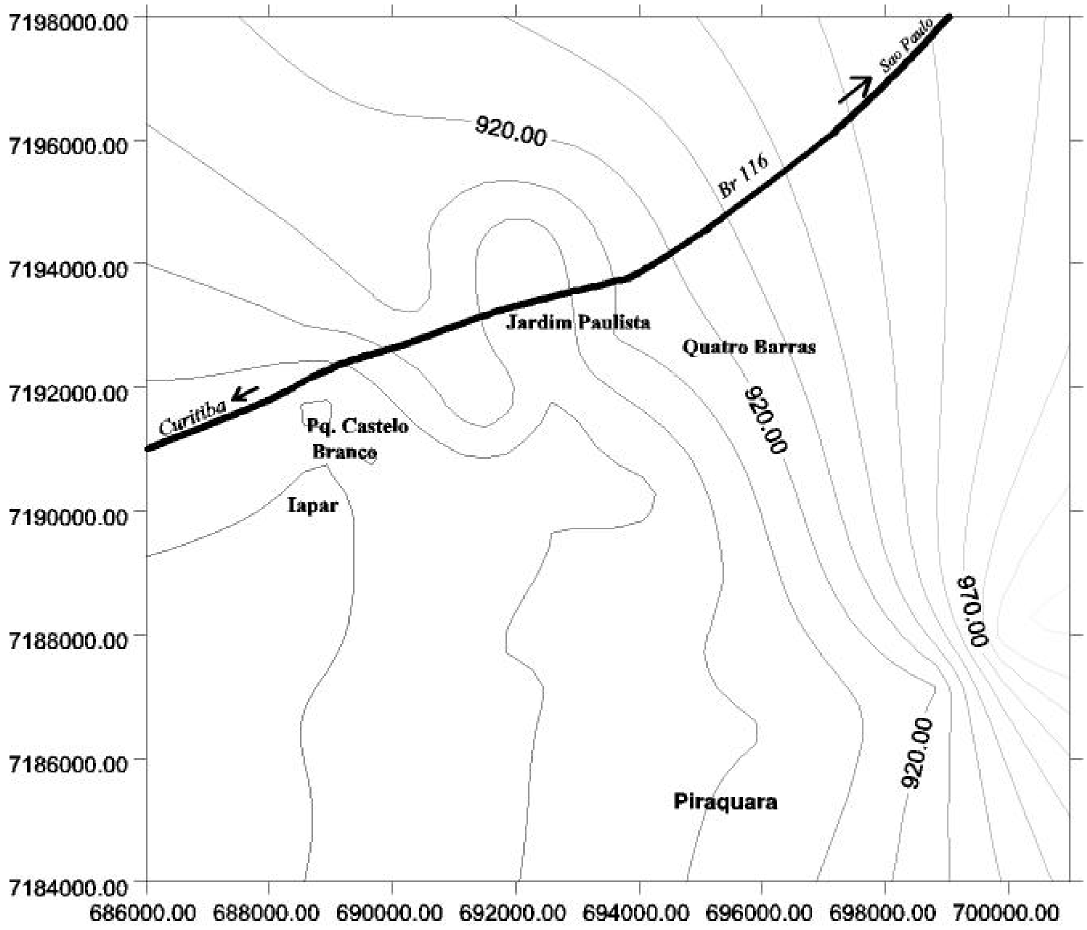


Figure 17: isoline map of hydraulic heads in the study area

bedrock of high resistivity lies under a clayey sediment cover that is highly conductive (see figure 6). The pseudo-section shows that about 100 m across the Iraí-river in the Southeast direction, the bedrock is at once much shallower. From the topography it was not clear how far from Colonia Penal the bedrock was that shallow, because there were the shallow bedrock protrudes it is covered by alluvium in the floodplain. These findings however are very important for the shapening of the model.

In general during the pumping tests, only the level of the pumping well was measured, no other levels of adjacent wells were measured.

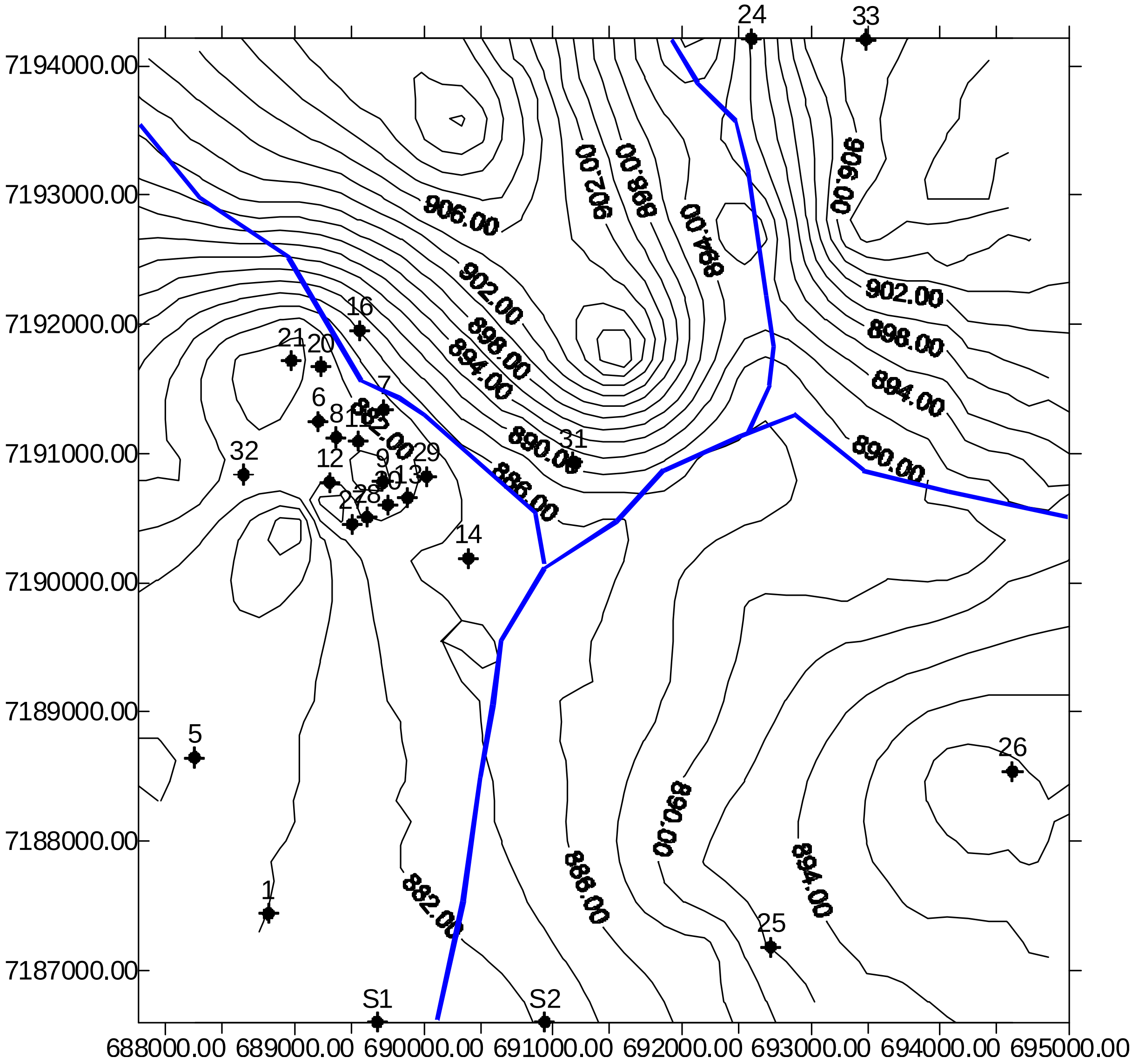


Figure 18: Detailed isoline contours of hydraulic heads in the direct vicinity of the Iraí-reservoir: numbers are for wells and piezometers, S for soundings of site investigation for the Iraí-dam (appendix B), blue is for the most important streams.

To get an idea of the magnitude and variations of the permeability of aquifers in a relatively large area, for e.g. planning of a new well field or modelling studies (de Ridder, 1977), this is appropriate. Requirement is that after some time with a constant pumping rate permanent flow conditions are achieved i.e. when stationary conditions are achieved. This is when no measurable fall of the water level has been established and the maximum fall of the water level of the well and the flow rate during the test have been measured.

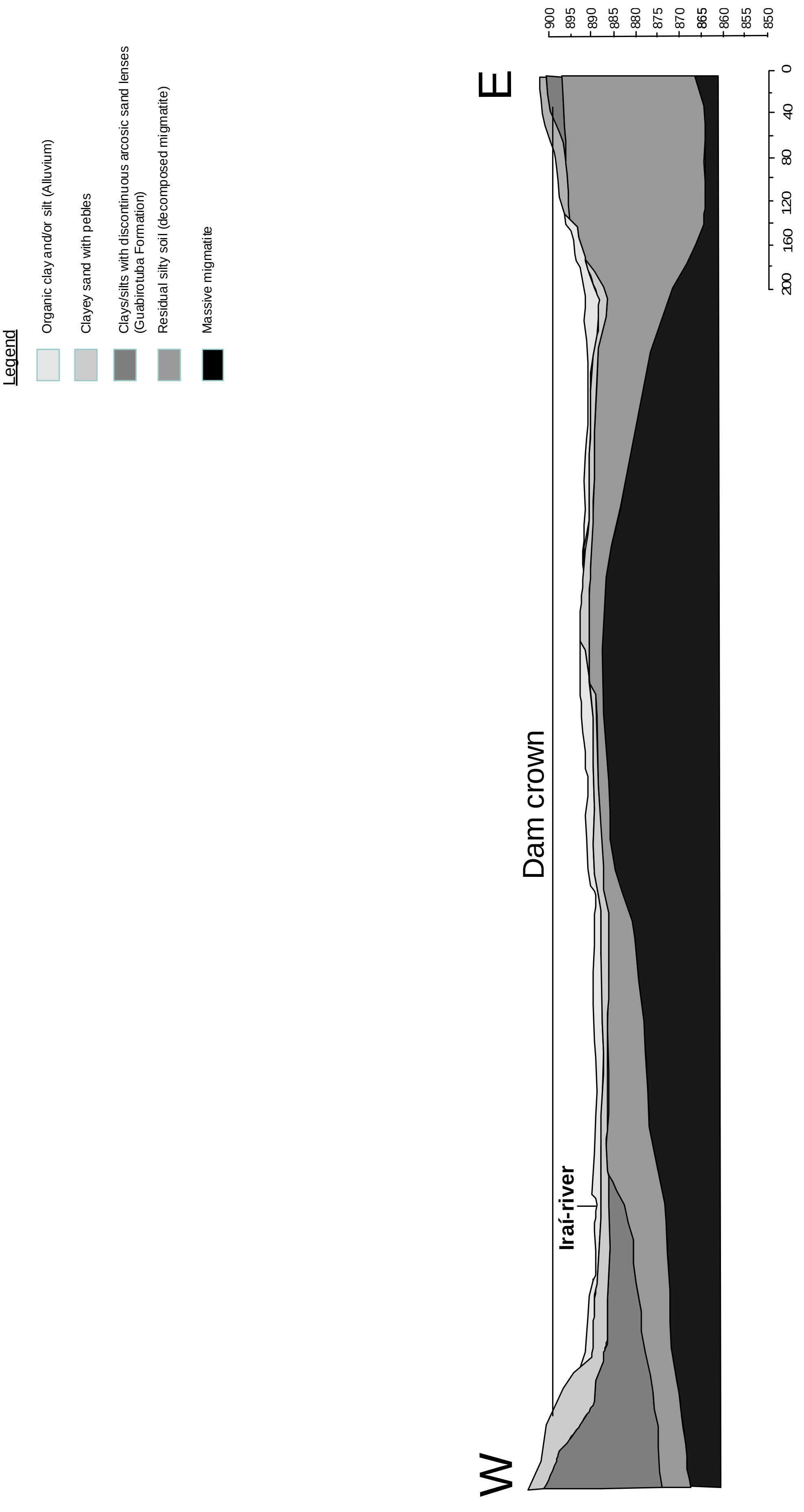


Figure 19: Section at the location of the Iraí-dam (derived from Sanepar, 1992).

When stationary conditions are achieved after a given period of time t and the pumping is then shut down, the residual drawdown (the original water level minus the water level at any time after shutdown) can be approximated as the numerical difference between the drawdown in the well as if the discharge had continued and the recovery of the well in response to an imaginary recharge well, of the same flow rate, superimposed on the discharging well at the time it is shut down (fig 20).

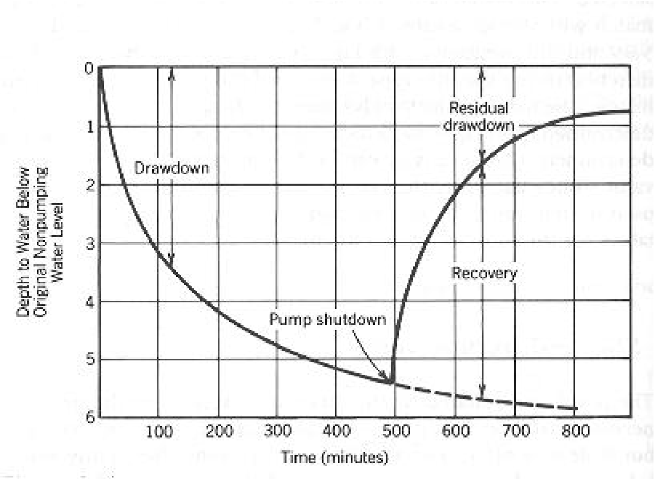


Figure 20: Arithmetic plot of drawdown and recovery curve versus time (after Domenico and Schwartz, 1990).

Designating original head as h_0 (the static level) and the recovered head at any time as h’, residual drawdown is expressed from the modified Eq. of 2.2 from Cooper and Jacob:

$$s = \frac{2.3Q}{4\pi T}\log\frac{2.25Tt}{r^2\,S} \qquad \text{(Eq.2.2)}$$

$$h_0 - h' = \frac{2.3Q}{4\pi T}\log\frac{2.25Tt}{r^2 S} - \frac{2.3Q}{4\pi T}\log\frac{2.25Tt'}{r^2 S} \qquad \text{(Eq.2.3)}$$

where $\Delta s'$ is residual drawdown, t is the time since pumping started, t’ is the time since pumping stopped and r is the distance of the well used for monitoring the drawdown at that distance of the pumping well. This equation reduces to

$$\Delta s' = \frac{2.3Q}{4\pi T}\log\frac{t}{t'} \qquad \text{(Eq. 2.4)}$$

so that this equation may be used for the well that was pumping after the pumping stopped.
The test carried out is actually a recovery test (recovery of the hydraulic head to static level).

Field procedure requires a drawdown measurement at the end of the pumping period (t) and recovery measurements during the recovery period (t’). The graphic procedure is to plot residual drawdown on the arithmetic scale and the value of t/t’ on logarithmic scale (Fig. 21). The time t includes the interval over the pumping plus recovery period whereas the time t’ includes the recovery interval only. If calculations are made over one log cycle of t/t’,

$$\Delta s' = \frac{2.3Q}{4pT} \qquad \text{(Eq. 2.5)}$$

where Δs’ is the residual drawdown per log cycle. Δs’ is computed from the regression line of the graph (e.g. from fig. 21, Δs’= 0.5881 (Ln t/t’- Ln t/t’) = 0.5881 (Ln (1000)-Ln(100) = 1.354), with this number and the known parameters the transmissivity can be computed.
The storativity is not determined directly with this method, but may be calculated with Eq. 2.2 by taking the well radius.

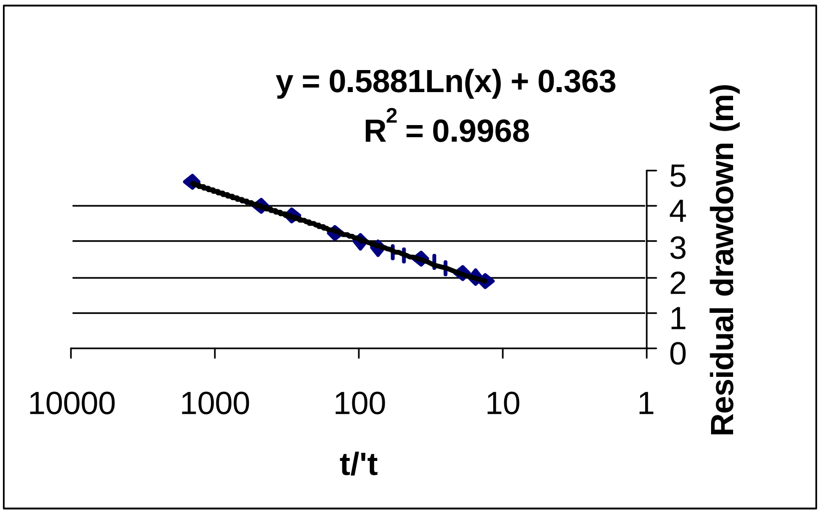


Figure 21: Single bore-hole production test at the well Iapar 4.

Other computational methods for single-borehole production tests may also be used as a recovery test (de Ridder, 1977; Udluft, 1998), but they compute the transmissivity from the drawdown during the pumping which is not necessarily at a constant pumping rate as the recovery of the well probably corresponds more with the natural well characteristics.
Another point is requirement e.g. for the Depuit-Thiem method is two different pumping rates (Udluft, 1998), which the available data rarely satisfy.
The wells and their hydraulic data are presented in Appendix B.

2.6.3 Groundwater chemistry

In general the wells presented in Appendix B have been sampled for hydrochemical analysis, though some of the wells were not sampled because during the construction it was clear that the water was chemically not suitable. In general not suitable because of probable formation of iron hydroxide deposits in the water conduit-pipes. One well could not be used because of faulty construction.

The analyses of the samples have been done by different laboratories for often various purposes. Some laboratories make their analyses so that the water is tested on specific substances as is required on legal directive, or as is important for the maintenance of the waterworks and conduit-pipe system. A laboratory like for example that of the Hydrogeological Department of the Federal University of Paraná makes it's analyses on a combination of such purposes together with scientific purposes.

Probably these various purposes resulted in the varying usefulness of the data. Additionally the groundwater has generally a low mineralisation (TDS have magnitudes 75 to 276 mg/l). That is why small errors of the analysis may have a large effect on the ionic balance of the sampled water.

The substances that could not be traced are written as zero in appendix B, as substances that were not analysed are left as blanks. Actually samples that had species which were not traced or analysed are also 0 in the Piper-diagram (fig. 22) and should be considered with some doubt.

Looking at the Piper-diagram the bad quality of the analyses is evident. But on the same time it is not impossible to make a characterisation of the type(s) of water by looking at the dominant species and the few analyses that seem right.

While the modelling study will take into account both the situations before and after the construction of the Iraí-reservoir it should be noted that all the hydrochemistry data were analysed before finishing its construction.

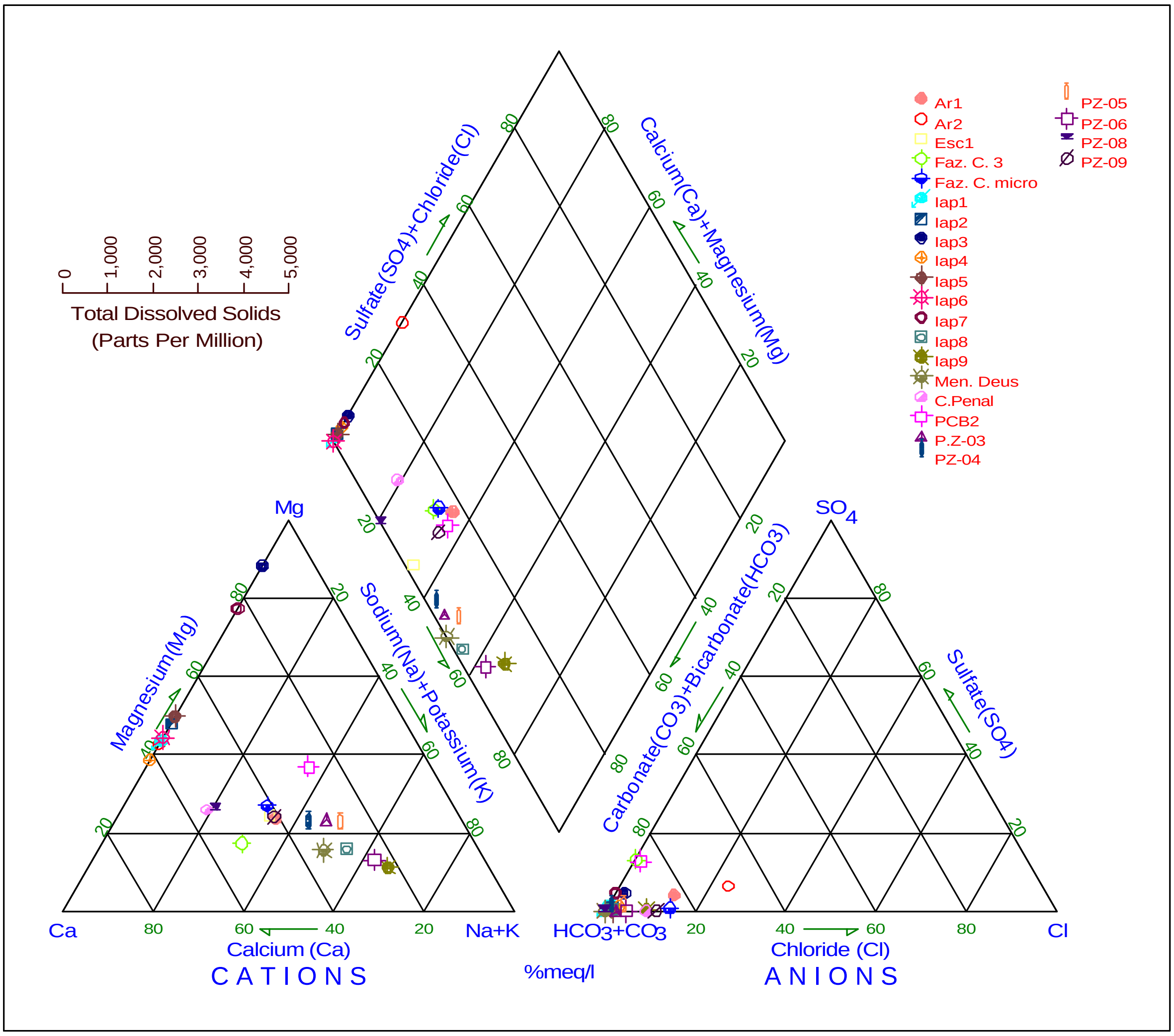


Figure 22: Piper-diagram of the groundwater analysis.

The possible influences of the surface water chemistry to the groundwater chemistry were discussed in the sections 2.5.1 and 2.5.2 from which it was concluded that of pollutants analysed from the surface water, only nitrate flows more easily to the groundwater.

Some pollutants were not analysed because of their complexity, additional costs, the possible number of pollutants is too large or simply because the lack of knowledge or interest.

The surface water and groundwater analyses unluckily do not match at all except that for both analyses the pH was determined. The pH may be used to make a comparison between the surface water and the groundwater. The pH's of the various wells show larger differences as that of the surface water in time. Though in the case of the wells the pH-data concern a random test of several points, the pH-data of the surface water concern a random test at some points through time. The wells with higher pH's are probably influenced by agricultural land use (possibly Calcium-rich fertilisers e.g. $CaHPO_4$) and settlement. A Piper diagram was constructed for classification and comparison of the groundwater chemistry from the available data that were suitable. It was hoped for that a possible differentiation in the Piper diagram may identify possible infiltration areas and possible pollution. Especially the anions Cl^-, HCO_3^- and the cations Ca^{2+} , Mg^{2+} and Na^+ may be of value in this case.

In the modelling study the transport of dispersible substances will be modelled, but this study is not based on sound data.

With the available data no real conclusions may be drawn for the future but several scenarios may be played with the help of transport modelling (particle tracking). This modelling study must be seen as the testing of varying scenarios of transport.

Table 3: Representative examples of the two types of groundwater within the Iraí-basin

	Cluster 1: Iapar 9		Cluster 2: Piezometer 9	
pH	6.28		7.86	
EC (ìS/cm)	81.7		208	
Alkalinity (mg/l CaCO3)	38.76		181.6	
	(mg/l)	(meq/l)	(mg/l)	(meq/l)
Ca (mg/l)	3.83	0.19	29.41	1.47
Mg (mg/l)	1.16	0.1	10.52	0.87
Na (mg/l)	12.17	0.53	27	1.17
K (mg/l)	1.45	0.04	2.8	0.07
Fe (mg/l)	0.68	0.04	0.09	0
NH4 (mg/l)	0	0	0	0
HCO3 (mg/l)	47.29	0.78	162.26	2.66
SO4 (mg/l)	0.14	0	0	0
NO3 (mg/l)	0.08	0	14	0.23
CL (mg/l)	2.75	0.08	12.16	0.34
PO4 (mg/l)	0.145	0	0.041	0
CO2 (mg/l)	20.24		27.82	
SiO2 (mg/l)	47		34.02	

The groundwater in the Iraí-river basin may be subdivided in two types of water (cluster 1 and cluster 2 in table 3) according to all the available analysis, the groundwater not under agricultural/anthropogenic influence ($NaHCO_3$-type) and the probably agricultural/anthropogenic influenced groundwaters ($Ca(Na)HCO_3$-type with a higher Mg-content).

It seems that the redox-potential is probably more in a oxidative range taking into account the chemical analysis (low Fe^{2+}, SO_4^{2-}, low Mn^{2-} and presence of NO_3^-). Both nitrate and organic species have only been found in negligible amounts. The amounts of nitrite are negligible in all wells. This could be expected because the water is more in the oxidative range. The Guabirotuba aquifer is a relatively shallow confined (at least in some places phreatic) aquifer that is generally low in organic matter that could be responsible for a reductive environment .

Excess iron in some of the wells can be explained by the soil formation (as described in section 2.3) and exfiltration areas as in one case has been encountered in the field survey. In this case a drill-hole was drilled at 50 m distance of a spring and the first 24 meters of the profile showed brownish mottles of rust. The excess iron in the case of soil formation plays a role in the ferrallic B-horizon of Latosols and the ferallic Cambisols and in the case of Organic soils and Gleysols. In the ferrallic B-horizon of Latosols and the ferallic Cambisols may play a role when wells have to shallow filters. Below Organic soils and Gleysols the environment may be more reductive. The SO_4^{2-} may be a product of pyrite-weathering that is present in migmatite as an accessory constituent.

The hardness of the water is all because of carbonates.

The data have been subdivided between 2 clusters; cluster 1 smaller than 10 mg/l Ca^{2+} and cluster 2 larger than 10 mg/l Ca^{2+}. This was done because it was clear that some waters clearly showed a Calcium content that was about 4 times higher as that for most samples. Also showed these samples higher Na^+-contents. Table 3 shows the analyses of these two types of water.

The higher amounts of Calcium in some waters relative to the “natural chemical characteristics” of water is probably by Calcium-rich fertilisers ($CaHPO_4$) and also the samples higher Na^+-contents are waters that are probably anthropologically influenced.

Phosphorus concentrations in natural water are normally no more than a few tenths of a mg/l (Hem, 1988). This form of phosphorus has a low solubility and is an element essential as a nutrient used by biota and a major cause of eutrophication. Higher values have been found in almost all wells that were analysed on phosphate. All these wells lie on or near the property of Iapar were the soil is fertilised by artificial fertilisers for at least since 30 years. Higher amounts of calcium and phosphate indicate that these fertilisers probably consisted of calcium phosphate

Ammonium is normally not present in natural groundwater, but may be present because of dunging, sewage waters or because of moors. Only some of the wells had NH_4^+, but this never exceeded 0.07 mg/l and than in agricultural areas (Castelo Branco/Iapar) and settled areas (Menino Deus). NH_4^+ is preferentially adsorbed by clay-minerals.

Chloride values higher than 2 mg/l may be coupled to anthropogenic influences.

F^- is normally $\leq$ to 0.05 mg/l but in alkaline waters pH ≥ 8 or thermal waters it may be a higher quantity.

In this study fluoride was found in waters with pH ≥ 7.3 with values mainly below 0.2 mg/l.

3 The methodology and construction of the flow and transport model

3.1 Introduction

In this chapter the methodology of the modelling study is discussed. How is it designed and what kind of software were applied. What kind of algorithms were used (e.g. finite differences), where choices (solution method) could be made and why were these particular choices made ?

A model is a simplification of the reality to get a better understanding of the system. The art of making a model is not to oversimplify the modelled situation and on the same time keep it simple. The situation is modelled with MODFLOW model which is a finite difference groundwater model to simulate two-dimensional areal or cross-sectional, and quasi- or fully three-dimensional, transient flow in anisotropic, heterogeneous, layered aquifer systems (HR Wallingford, 1995).

A transport model is made in conjunction to make scenarios how the quality of the groundwater resources will be influenced by the building of the Iraí-reservoir. For these scenarios the modelling system MODPATH was used that uses particle tracking to represent particle transport across flow lines.

The construction of the MODFLOW-model and the software used for the construction will be discussed in this chapter. Finally the construction of a particle tracking model with MODPATH will be discussed.

In this chapter the finite differences and the solution methods that are available in the used graphical interface (Groundwater Modelling System) for the analysis codes MODFLOW and MODPATH will be discussed.

Finally MODFLOW and MODPATH are presented shortly in connection with the problem that is modelled.

3.2 Design and construction of the model

The land surface elevation data were digitised from the map ‘Bacia do Iraí área de influência do reservatório’ map of 1:20,000 with Polyplot (digitalisation program Polyplot) for the elevation model for the hydraulic model. Every contour line was drawn in a separate layer. Other attributes that are needed were also digitised in Polyplot. With these attributes the geology, the watercourses and lakes, and the infrastructure are meant.

Values were assigned to the contour line layers from Polyplot with a program ‘DXF zu XYZ’ written by Dipl. Geol. R. Barthel in Visual Basic. Interpolation of the contour line data by the gridding method Kriging was executed with the SURFER software package. The interpolation was actually done to assign data between the contour lines.

Georeferencing of the map has been carried out in Idrisi and preparation of a geological map, and a map of watercourses and infrastructure was also carried out.

The UTM-coordinates of the wells with hydraulic heads are the basic data for the isoline map of hydraulic heads that has been used for the groundwater flow model and its conjugate particle tracking model.

The input of the hydraulic head data has been done manually in SURFER and the interpolation to a grid has been done by Kriging.

The model has been constructed with Groundwater Modeling System (GMS) that functions as the user interface for the MODFLOW and MODPATH programs. But can also be used for modelling itself (The Department of Defense Groundwater Modeling System, 1996), while it also contains a number of analysis codes (MODFLOW, MT3D, MODPATH, FEMWATER).
With the construction in GMS the following steps were followed:
A conceptual model was constructed in the Map Module (section 3.3.2) in which 3 layers of units of varying hydraulic properties have been assigned according to the geologic map and observations in the field, well and geotechnical data and information from geoelectrical lines for exploration. Additionally streams as drains, recharge and for the 3 layers specified heads for the Eastern boundary of the basin and bedrock units were added in the Map Module as layers. The units of hydraulic properties and the boundary conditions (drains, specified heads) are presented in the figures 34 and 35.
Having the 3D-grid ready and MODFLOW initialised all layers of the Map Module have been assigned to MODFLOW and also the SURFER-grids that have been imported in GMS and have been assigned to the 3D-grid of the MODFLOW-model.
After execution and calibration of the conceptual model in MODFLOW, the MODPATH interface has been used for modelling contaminant transport by particle transport or advective transport of particles or dissolved chemicals. This is a simplification of the transport process because apart from advection as is taken into account with particle tracking dispersion, diffusion, retardation, mineralisation, etc. may take place depending on the type of matter transported. Advection is the movement of a solute at the speed of the average linear velocity of groundwater, as dispersion is the process whereby solutes are mixed during advective transport caused by the velocity variations at the microscopic level, diffusion is the movement of dissolved matter driven by the difference in concentration. Retardation may take place by e.g. absorption of the matter on clay minerals or by filtering out. In aquifers the processes that have the larger impact on transport velocity of matter are advection and dispersion, as diffusion has a larger impact on transport velocity in an aquitard. The MODPATH-model only takes advection into account. By not taking dispersion into account the modelled transport may be to slow when retardation may be neglected in the aquifer.

For the construction of a MODPATH-model a MODFLOW simulation is preliminary because it uses the flow field of the simulation result. After initialising MODPATH the layer data have to be assigned for the model which was done by the Map Module. The following step is to set the particle starting locations and then the simulation can be executed. The tracking of the path of particles may be done forward or backward i.e. respectively from the starting point or from the end point.
Providing the layout is satisfactory the results from the MODFLOW and MODPATH simulations are now ready for publication.
In the following section the GIS-program IDRISI, GMS, MODFLOW and the module MODPATH will be discussed, while they are really vital in making this modelling study.

MODBIL that was used to make an additional water balance model as a comparison of the water balance in section 2.6.1 is discussed in chapter 4.
A more thorough description of the construction and calibration of the groundwater flow model will be discussed in chapter 5, as the Particle Tracking Model will be discussed in chapter 7.

3.3 Description of the used software

3.3.1 Use of a Geographical Information System (GIS)

The nature of a groundwater modelling exercise such as that being undertaken is that it has to handle a large amount of spatially varying data (HR Wallingford, 1995). During both model development and operation it is efficient to enter this data directly into the modelling software. Such a procedure would be time consuming and, potentially, subject to a large degree of error. The best way to handle such spatial data is by using a GIS which has a link to the modelling software. Such a system will allow visualisation of input data, manipulation of data and rapid modification of inputs during calibration and model operation.
For the purpose of this study IDRISI, which was developed at Clark University in the USA, was selected as the most suitable GIS for reasons of ease of use and the inclusion of tutorial.

IDRISI is a grid-based geographic information and image processing system. It is designed to provide professional level geographic research tools on a low cost, non-profit basis. IDRISI is used in over 80 countries around the world by a range of research, government, local planning, resource management and educational institutions.

IDRISI is not a single computer program, but a collection of over 100 program modules that may be linked to a unified menu system. These modules fall into one of three broad groups,

- Core modules, providing fundamental utilities for the entry, storage, management and display of raster images
- Analytical Ring Modules, providing major tool groups for the analysis of raster image data
- Peripheral modules associated with data conversion utilities between IDRISI and other programs and data storage formats.

By using independent modules linked by a set of simple data structures, the system allows users to develop their own modules with minimal regard for the internal workings of IDRISI modules in the core set. Furthermore, these modules can be developed in any computer language, and still maintain a simple compatibility.

One extremely important peripheral module for IDRISI is a program which allows conversion from IDRISI format to AUTOCAD DXF-format. This is important since GMS is able to handle input data in AUTOCAD DXF-format. This peripheral module allows the GIS and GMS to be linked.

3.3.2 The graphical user interface GMS

The Department of Defense Groundwater Modelling System (GMS) is a comprehensive graphical user environment for performing groundwater simulations (The Department of Defense Groundwater Modelling System, 1996). The entire GMS system consists of a graphical user interface (the GMS program) and a number of analysis codes (MODFLOW, MT3D, MODPATH, FEMWATER). The GMS interface was developed by the Engineering Computer

Graphics Laboratory of Brigham Young University in partnership with the U.S. Army Engineer Waterways Experiment Station.

GMS was designed as a comprehensive modelling environment. Several types of models are supported and facilities are provided to share information between different models and data types. Tools are provided for site characterisation, model conceptualisation, mesh and grid generation, geostatistics, and post-processing.

The interface of GMS is subdivided into ten separate modules. A module is provided for each type of the basic data types supported by GMS. By switching from one module to another module allows the user to focus only on the tools and commands related to the data type the user wishes to use in the modelling process. Generally there are modules that may handle data that are meant for models that are discretised according the finite difference method (MODFLOW, MODPATH, MT3D) or the finite element method (FEMWATER). From these modules there are modules to interpolate point data (e.g. well heads to isolines of hydraulic heads by the 2D Scatter Point Module), to visualise and interfaces to the models (e.g. the 3D Grid Module that acts as an interface to the models MODFLOW, MT3D and MODPATH) and to manipulate objects (the Map Module e.g. to draw polygons and assigning them hydraulic characteristics defined by layer attributes).
Now the modules in GMS used for this study are presented.

The 2D Scatter Point Module

The 2D Scatter Point Module is used to interpolate from groups of 2D scattered data to any of the other data types. For example, hydraulic conductivity or porosity can be interpolated from the sampling locations to the cells in a layer of a 3D grid for use in a MODFLOW/MT3D/MODPATH simulation. A variety of interpolation schemes are supported.

The 2D Grid Module

The 2D Grid Module is used for surface visualisation. For example, you can interpolate from a set of 2D scatter points to a 2D grid. The grid could then be contoured or displayed with hidden surface removal and colour fringes to display the variation in the interpolated data

The Map Module

The Map Module is used to manipulate four types of objects: DXF objects, image objects, drawing objects and feature objects. The first three objects: DXF objects, image objects, drawing objects are primarily used as graphical tools to enhance the development and presentation of a model. DXF objects consist of drawings imported from standard CAD packages such as AutoCAD or Microstation. Drawing objects are a simple set of tools that are used to draw text, lines, polylines, arrows, rectangles, etc. to add annotation to the graphical representation of a model. Image objects are digital images representing aerial photos or scanned maps in the form of TIFF files. The fourth type of object, feature objects, are used to construct conceptual models (e.g. the units representing specific hydraulic properties of the model, these were digitised in the Map Module and then the polygons were assigned hydraulic properties). Feature objects are patterned after the data model used by geographic information systems (GIS) such as ARC/INFO. Once a conceptual model is constructed, it can automatically be converted to a numerical model.

The 3D grid Module

The 3D grid module is used to create 3D Cartesian grids. These grids can be used for 3D interpolation, iso-surface rendering, cross sections and finite difference modelling. Complete interfaces to the models MODFLOW, MT3D and MODPATH are provided in this module.

In this modelling study the interpolation was executed in the 2D Scatter Point Module, the 2D-grid for the interpolation was constructed in the 2D Grid Module and the data that were used in the models were assigned and manipulated in the Map Module. Before the data from the Map Module and the interpolated data were assigned to the 3D Grid Module that acts as the interface for the MODFLOW -and MODPATH-models.

Further details on the construction of the model are discussed in section 5.2.

3.3.2.1 The simulation program MODFLOW

MODFLOW is a finite difference groundwater model to simulate two-dimensional areal or cross-sectional, and quasi- or fully three-dimensional, transient flow in anisotropic, heterogeneous, layered aquifer systems (HR Wallingford, 1995). The model uses the block centred finite difference approach for spatial discretisation. Aquifer layers may be simulated as confined, unconfined or convertible between the two conditions. The model can also handle layers which pitch out such as where a multi-layered system meets a single layered aquifer of i.e. outwash fans. The model allows for analysis of external influences such as wells, areal recharge, drains, evapotranspiration and streams (rivers). Solution techniques available in GMS for the finite difference equations are the Strongly Implicit Procedure (SIP), the Slice Successive Overrelaxation (SSOR) or Pre-conditioned Conjugate Gradients (PCG). Finite differences and the mentioned solution methods will be discussed in section 3.4.

MODFLOW has a modular structure which consists of a Main Program and a series of highly independent subroutines or modules. The modules are grouped into packages. Each package deals with a specific feature of the hydrological system which is to be simulated, such as flow from rivers or flow into drains, or with a specific method of solving the linear equations which describe the flow system. The division of the program into modules permits the user to examine specific hydrological features of the model independently. It also facilitates the development of additional capabilities since new packages can be added without modifying the existing packages.

The available packages in MODFLOW in GMS may be subdivided in the flow model, areal sources/sinks, point sources/sinks and the solver. The flow model that is used in the groundwater flow model is BCF3, which has additionally to the original BCF1 flow model the capability to rewet cells and compute conductance. For the areal sources/sinks the packages recharge and evapotranspiration are available, but only recharge because the value used is the value of the water balance that was computed by precipitation minus the pan evaporation. For point sources the packages river, drain, general head and well are available in GMS. For the streams the package drain was used because nothing was known about the quantitive characteristics of the stream channels needed for the flow hydraulical computation. For the solver (solution methods) the packages Strongly Implicit Procedure, Preconditioned Gradient method, and the Slice Successive Over-relaxation are available in GMS. For the solver the package strongly implicit procedure (SIP) is used. The solution methods available in GMS are discussed in section 3.4.

A major consideration in selecting MODFLOW was that it is simple to handle and that the finite difference method that is used by MODFLOW for the computation of the groundwater flow modelling is easy to understand. Further MODFLOW is very widely available and very widely used; across the world it is probably the most widely used groundwater flow modelling package.

MODFLOW was originally developed by McDonald and Harbaugh in the United States Geological Survey in the early 1980's. This was prior to the huge explosion in the use of micro-computers and also before the advent of user friendly user interfaces. The original version of MODFLOW was written for a mainframe computer and input was from data files. Because of the popularity of MODFLOW a number of user interfaces for the software have been developed; in addition to providing the software a user interface (mask) was provided. The interface selected is the Groundwater Modelling System (GMS) as is described above.

3.3.2.2 MODPATH

A complete interface to MODPATH is included in the 3D Grid module of GMS. MODPATH is a particle tracking code that was designed to work with MODFLOW (The Department of Defense Groundwater Modeling System, 1996). After running a MODFLOW simulation, the user can designate the location of a set of particles. The particles are then tracked through time assuming they are transported by advection using the flow field computed by MODFLOW. Particles can be tracked either forward in time or backward in time. Particle tracking analysis are particularly useful for delineating capture zones or areas of influence for wells. In our case particle tracking is used to make an estimation of the residence time from possible dissolved contaminants in the water, that is recharged from the future Iraí-reservoir to the aquifer of the Guabirotuba Formation, towards the wells at Iapar.

MODPATH was developed by the U.S. Geological Survey. Version 3.0 of MODPATH is supported in GMS. The version of MODPATH distributed with GMS is the original public domain version distributed by the USGS.
Output from steady-state or transient MODFLOW simulations is used in MODPATH to compute paths for imaginary "particles" of water moving through the simulated ground-water system. In addition to computing particle paths, MODPATH keeps track of the time of travel for particles moving through the system. By carefully defining the starting locations of particles, it is possible to perform a wide range of analyses such as delineating capture and recharge areas or drawing flow nets.

Contaminants are transported in groundwater by advection in MODPATH (Anderson, 1991; Pollock, 1994), i.e. the movement of a solute at the speed of the average linear velocity of groundwater (**v**):

$$\vec{v} = -\frac{\vec{K}}{n_e} grad(h) \qquad \text{(eq. 3.1)}$$

where $\vec{v}$ is a vector; $\vec{K}$ is the hydraulic conductivity tensor and n_e is the effective porosity. There are, however, two other processes that affect contaminant movement, namely dispersion and chemical reactions. Consideration of all three processes requires solving a solute transport model for concentrations in space and time may be done with the transport simulation model MT3D. In our case is this task simply impossible because of the lack of data and additionally for

a regional modelling study the discretisation of the modelling grid is to rough for an advective-dispersive -and additionally chemical transport modelling (taking into account adsorption and degradation of matter), because the model would be unstable during simulation.
This discretisation may only be appropriate for local studies when using MT3D.
Another additional restriction because of the lack of data is that only a stationary simulation in MODPATH is possible in this case.

3.4 Finite differences and the solution methods

3.4.1 Finite differences

When the groundwater flow equation is solved with finite differences the discretisation of the model follows by a rectangular net which is a block-centred or mesh-centred grid, depending on the position of the nodes (in the centre of the cell or centred on the grid). In this case the cell centred discretisation is used because MODFLOW uses this kind of grid (Anderson and Woessner, 1992). Corresponding to the grid a rectangular of Nx cells in the x-direction and Ny cells in the y-direction forms the modelled area. All the nodes in this rectangular but outside the modelled area will have a transmissivity value of zero, so that these nodes do not contribute anything to the water balance of the modelled area. For each individual element the Darcy-equation is calculated.
For this purpose, the partial derivatives are replaced by an algebraic equivalent, with a quotient of two finite differences of the dependent and the independent variable replacing the differential quotient (Bear and Verruijt, 1987). The basic idea is that the derivative df/dt of a function f(t) is defined as

$$\frac{df}{dt} = \lim_{\Delta t \to 0} \frac{f(t+\Delta t) - f(t)}{\Delta t} \qquad \text{(Eq. 3.2)}$$

and that an obvious approximation of the derivative can be obtained by the simply omitting the limiting process, $\Delta t \to 0$.
It may be noted that in the definition (Eq. 3.2) it was tacitly assumed that the limit does exist, and that the same limit is obtained for positive and negative values of the step Δt. When using finite differences, the limit is replaced by some value for a finite value of Δt and the actual value may depend upon the magnitude of Δt, and also upon its sign.
The derivative f' may be approximated by the finite difference suggested by omitting the limit operation in (Eq. 3.2), the differential equation is replaced by the equation

$$\frac{f(t+\Delta t) - f(t)}{\Delta t} = f' \qquad \text{(Eq. 3.3)}$$

Equation 3.3 is said to be the forward finite difference approximation (downstream) of the derivative. Another type of derivation the backward finite difference (upstream) may be chosen as a solution method in the transport modelling. In the upstream finite difference the numerator is $f(t) - f(t+\Delta t)$.
The approximation of the differential equation by a quotient of finite differences may lead to a very simple numerical algorithm.

The simplicity and power of the finite difference method become evident when considering problems of non-steady flow. The basic partial differential equation for unsteady flow in an aquifer, with the possibility of water supplied to the aquifer by infiltration, is

$$S\frac{\partial h}{\partial t}=T\left(\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}\right)+I \qquad \text{(Eq. 3.4)}$$

where I is a given source function, representing the net infiltration, due to natural or artificial replenishment of the aquifer, T is the transmissivity and S is the storativity. The complete formulation of the problem requires the specification of boundary conditions, and in this case of unsteady flow, of initial conditions. It is assumed that along part of the boundary the head is given, and that the rest of the boundary is impermeable, i.e.

$$h = f$$

$$Q=-T\frac{\partial h}{\partial n}=0$$

with n is groundwater flow direction normal towards the boundary (normal component).
The initial condition is assumed to be

$$t=0:h=h_0$$

where h_0 is a known function, specified throughout the entire domain. The spatial derivatives in the right-hand side of equation 3.4 can be approximated by expressions in the form of

$$\frac{\partial^2 f}{\partial x^2}\approx\frac{f(x+\Delta x,y)-2f(x,y)+f(x-\Delta x,y)}{(\Delta x)^2}=\frac{f_{i+1,j}-2f_{i,j}+f_{i-1,j}}{(\Delta x)^2} \qquad \text{(Eq. 3.5)}$$

The form is converted in global indices (*x*=*i*,*y*=*j*). It seems most natural to approximate the time derivative by a forward finite difference, because the problem actually is to predict future values of the head from the initial values. Accordingly, we introduce the approximation

$$\frac{\partial h}{\partial t}\approx\frac{h'_{i,j}-h_0}{\Delta t} \qquad \text{(Eq. 3.6)}$$

with $h_0=h_{i,j}$ at $t=0$ and $h'_{i,j}$ is the value of the head at the end of the time step.
Equation 3.6 contains two values of the head, at node *i*,*j* of the mesh. It is not immediately evident, however, which of these values should be used in the spatial approximation. In fact, there exist several solution methods in finite differences of which one has to be chosen. The choice of which solution method will be discussed in the following paragraph.

3.4.2 The choice of the solution method

To solve the groundwater flow equation by finite differences several existing solution methods are based on the explicit and implicit methods. In GMS the Strongly Implicit Procedure (SIP) method, Preconditioned Gradient method, and the Slice Successive Over-relaxation method may be used. All methods used in GMS are implicit methods.

The choice of implicit methods for MODFLOW is probably because implicit solution methods are expected to be fast, accurate and particularly suitable for large scale phenomena (Rijo and Pereira, 1988).

Explicit methods will be unstable when the time-steps are to large (Kinzelbach and Rausch, 1995) and also the size of the cells have be taken large enough.

After temporal finite differentiation and spatial discretisation have been done, the partial differential equations are transformed into a system of simultaneous linear algebraic equations or a matrix equation in the form

$$[A]\{f\}=\{F\} \qquad \text{(Eq. 3.7)}$$

The size of the matrix depends on the number of nodes, the number of variables, and the solution schemes. The solution for the unknown nodal values in $\{f\}$at time $t+\Delta t$ can be obtained through the use of either direct elimination methods or iterative methods (Javandel et al, 1984).

All methods available for solving finite differential equations in GMS solve the equations iterative. Iterative methods may offer certain advantages over direct methods, if the matrix is sparse and large. An iterative method starts from a first approximation which is successively improved until a sufficiently accurate solution is obtained (Smith, G.D., 1978; Javandel et al, 1984). The iterative procedure is said to be convergent when the differences between the exact solution and the successive approximations tend to zero as the number of iterations increase. In general, the exact solution is never obtained in a finite number of steps, but this does not matter. What is important is that the successive iterates converge fairly rapidly to values that are correct to a specified accuracy.

Implicit methods approximate the flows between cells by gradients at the end of the time interval, instead of the beginning of the time interval which is approximated in explicit solution methods.

3.4.2.1 The Preconditioned Conjugate Gradient method

The Preconditioned Conjugate Gradient method utilises the fact that every solution problem can be defined as an optimisation problem (Kinzelbach and Rausch, 1995) e.g. ax=b or ax-b=0.
Equivalent to the task is find the minimum of

$$y=\frac{1}{2}ax^2-bx \qquad \text{(Eq. 3.8)}$$

This can be found easily by derivation and setting to zero of this equation. The same follows with the equation system of the discretised flow equation (e.g. in stationary conditions)

$$Ah=q \qquad \text{(Eq. 3.9)}$$

to a more dimensional optimisation problem of the form: define the vector of the unknown hydraulic heads h, so that

$$y=\frac{1}{2}h^TAh-h^Tq \qquad \text{(Eq. 3.10)}$$

is minimised. Originating from a starting vector rises the condition of the initial point of the gradient following the descents of the more dimensional surface y to a local minimum. The steps follow for the acceleration of the descents in so called conjugate directions which does not make the reached minimisations insignificant.

The method needs to accelerate the convergence a preconditioning of the matrix A. This preconditioning exists of a identical conversion of the equations system so that the maximal distance of the eigenvalues of the matrix A are reduced.

The Preconditioned Conjugate Gradient method is very suited for problems with a very high number of nodes. The Preconditioned Conjugate Gradient method requires that the matrix A is symmetric which is always so in the case of flow problems.

3.4.2.2 The Slice Successive Over-Relaxation method

If one splits a matrix $[A]$ into diagonal $[D]$, lower $[L]$, and upper $[U]$ triangular systems, $[A]=[D]+[L]+[U]$. The matrix equation $[A]\{f\}=\{F\}$can be rewritten as

$$([D]+[L])\{f\}=-[U]\{f\}+\{F\} \qquad \text{(Eq. 3.11)}$$

An approximate solution from the *k*th iteration step to the (*k+1*)th step is

$$\{f\}^{k+1}=([D]+[L])^{-1}\left(-\left|U\right|\{f\}^{k}+\{F\}\right) \qquad \text{(Eq. 3.12)}$$

This is the matrix form of Gauss-Seidel's method. In this method starts from the principle that the hydraulic heads are guessed. This is not met by the flow equation, but is improved when every node is made consistent with it's neighbours node with the help of the water balance equation. After several passes through the matrix the result converges to the correct solution. This convergence may be accelerated by relaxation. The inverse of the lower triangular matrix $([D]+[L])$ can be handled by forward substitution. If the residual from the *k*th to the (*k+1*)th iteration is denoted

$\{r\}^{k}=\{f\}^{k+1}-\{f\}^{2k}$, the generalised iterative method $\{f\}^{k+1}=\{f\}^{k}+w\{r\}^{k}$ is the Successive Over-Relaxation (SOR) method. In matrix form the new solution is

$$\{f\}^{k+1}=([D]+w[L])^{-1}\left[((1-w)[D]-w[U])\{f\}^{k}+w\{F\}\right] \qquad \text{(Eq. 3.13)}$$

The relaxation factor *w* should be chosen so that the rate of convergence is optimised. For real, symmetric, and positive definite matrixes, $0 < k < 2$.

The Slice Successive Over-relaxation method is an extension for 3-dimensional problems (Huyakorn and Pinder, 1983).

3.4.2.3 The Strongly Implicit Procedure method

The strongly implicit procedure (SIP) is one of a class of incomplete factorisation methods (Huyakorn and Pinder, 1983).

To understand the fundamental ideas behind this approach we first write the matrix equation arising out of a standard five-point difference approximation of a second-order equation which is applicable to a two-dimensional flow problem. Consider the regular nodal arrangement of figure 23.

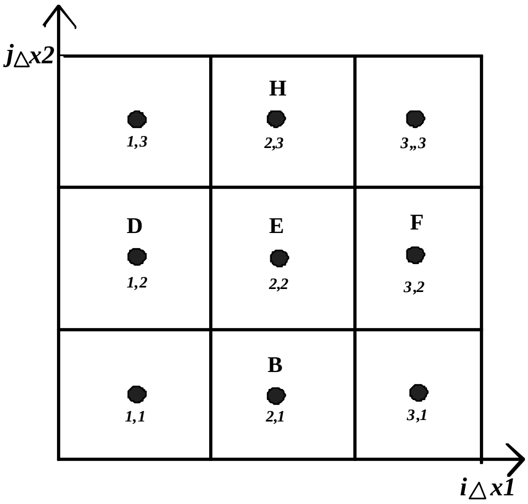


Figure 23: Finite difference net used to describe the strongly implicit procedure. The symbols B, D, E, F, and H are displayed for node (2,2), after Huyakorn and Pinder, 1983.

The coefficients for our problem are derived from the basic balance equation. As an example for the aquifer confined conditions are assumed.

$$S\frac{\partial h}{\partial t} = T\left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right) + I \qquad \text{(Eq. 3.14)}$$

$$HK\left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right) + I = HS_s\frac{\partial h}{\partial t} \qquad \text{(Eq. 3.15)}$$

with S_s as specific storativity. Because in the matrix equation the coefficients are expressed so that the thickness H of the aquifer is not taken into account the expression can be written as

$$K\left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right) + I = S_s\frac{\partial h}{\partial t} \qquad \text{(Eq. 3.16)}$$

The coefficients of matrix equation 3.25 are

$$B_{ij} = \left(\frac{-1}{(\Delta x)^2} K_{22} \right)_{i,j-\frac{1}{2}}, F_{ij} = \left(\frac{-1}{(\Delta x)^2} K_{11} \right)_{i+\frac{1}{2},j}, D_{ij} = \left(\frac{-1}{(\Delta x)^2} K_{11} \right)_{i-\frac{1}{2},j},$$

$$H_{i,j} = \left(\frac{-1}{(\Delta x)^2} K_{22} \right)_{i,j+\frac{1}{2}}, E_{i,j} = -(B_{ij} + D_{ij} + F_{ij} + H_{ij}) + \left(\frac{S_s}{\Delta t} \right)_{i,j}, \qquad \text{(Eq. 3.17 – 3.24)}$$

$$Q_{ij} = \left(\frac{S_s}{\Delta t} \right)_{i,j} h_{i,j,s+1},$$

$$h_{ij}^* = h_{i,j,s+1}$$

Equation 3.25 of the matrix is written as:

$$\begin{bmatrix} E_{11} & F_{11} & 0 & H_{11} & & & & & \\ D_{21} & E_{21} & E_{21} & 0 & H_{21} & & & & \\ 0 & D_{31} & E_{31} & 0 & 0 & H_{31} & & & \\ B_{12} & 0 & 0 & E_{12} & F_{12} & 0 & H_{12} & & \\ & B_{22} & 0 & D_{22} & E_{22} & F_{22} & 0 & H_{22} & \\ & & B_{32} & 0 & D_{32} & E_{32} & 0 & 0 & H_{32} \\ & & & B_{23} & 0 & 0 & E_{13} & F_{13} & 0 \\ & & & & B_{23} & 0 & D_{23} & E_{23} & F_{23} \\ & & & & & B_{33} & 0 & D_{33} & E_{33} \end{bmatrix} * \begin{Bmatrix} h_{11}^* \\ h_{21}^* \\ h_{31}^* \\ h_{12}^* \\ h_{22}^* \\ h_{32}^* \\ h_{13}^* \\ h_{23}^* \\ h_{33}^* \end{Bmatrix} = \begin{Bmatrix} Q_{11} \\ Q_{21} \\ Q_{31} \\ Q_{12} \\ Q_{22} \\ Q_{32} \\ Q_{13} \\ Q_{23} \\ Q_{33} \end{Bmatrix} \qquad \text{(Eq. 3.25)}$$

The matrix can be rewritten as $[A]\{f\} = \{F\}$. We now assume that there exists a matrix $[A']$ which is very similar to $[A]$ but is easily factorised. $[A']$ is factorised in the upper and lower triangular matrices $[L']$ and $[U']$ which contain only three elements per row. For how the matrixes $[L']$ and $[U']$ look like, Huyakorn and Pinder, 1983, may be referred.
To utilise $[A']$ in an effective iterative scheme equation 3.26 may be employed:

$$[A']\{h\}^{k+1} = [A']\{h\}^k - \boldsymbol{b}\left([A]\{h\}^k - \{q\} \right) \qquad \text{(Eq. 3.26)}$$

where $\boldsymbol{b}$ is an iteration parameter and the superscript k is denoted for each iteration step. While the solution method is an implicit method the increment is defined by $\{\mathrm{H}\}^{k+1} = \{h\}^{k+1} - \{h\}^k$ so that equation 3.26 becomes

$$[A']\{\mathrm{H}\}^{k+1} = \boldsymbol{b}\left([A]\{h\}^k - \{q\} \right) \qquad \text{(Eq. 3.27)}$$

Recall, however, that we defined $[A']$ so that it factored into the upper and lower triangular matrixes $[L']$ and $[U']$ so that equation 3.27 may be rewritten as

$$[L'][U']\{\mathrm{H}\}^{k+1} = \boldsymbol{b}\left([A]\{h\}^k - \{q\} \right) \qquad \text{(Eq. 3.28)}$$

3.4.3 The tracking method of MODPATH

Several methods may be used (Anderson, 1991) as a particle tracking method (e.g. linear, bilear, bicubic interpolation schemes, semianalytical, Euler, Range-Kutta, and Taylor series expansion). MODPATH uses a linear interpolation scheme (Pollock, 1994).
In order to compute pathlines, a method must be established to compute values of the principal components of the velocity vector at every point in the flow field based on the intercell flow rates from the finite difference model. The algorithm described, uses simple linear interpolation to compute the principal velocity components at points within a cell.

Linear interpolation produces a continuous velocity vector field within each cell that identically satisfies the differential conservation of mass equation 3.29 everywhere within the cell.
The fact that the velocity vector field within each cell satisfies the differential mass balance equation assures that pathlines will distribute water throughout the flow field in a way that is consistent with the overall movement of water in the system as indicated by the solution of the finite difference flow equations.
The partial differential equation describing conservation of mass in a steady state, three-dimensional groundwater flow system can be expressed as

$$\frac{\partial}{\partial x}(nv_x)+\frac{\partial}{\partial y}(nv_y)+\frac{\partial}{\partial z}(nv_z)=W \qquad \text{(Eq. 3.29)}$$

where v_x, v_y and v_z are the principal components of the average linear groundwater velocity vector, n is porosity, and W is the volume rate of water created or consumed by internal sources and sinks per unit volume of aquifer.
Using simple linear interpolation, the principal velocity components can be expressed in the form

$$v_x=A_x(x-x_1) + v_x \qquad \text{(Eq. 3.30)}$$

$$v_y=A_y(y-y_1) + v_y \qquad \text{(Eq. 3.31)}$$

$$v_z=A_z(z-z_1) + v_z \qquad \text{(Eq. 3.32)}$$

where A_x, A_y and A_z are constants that correspond to the components of the velocity gradient within the cell

$$A_x=\frac{(v_{x2}-v_{x1})}{\Delta x} \qquad \text{(Eq. 3.33)}$$

$$A_y=\frac{(v_{y2}-v_{y1})}{\Delta y} \qquad \text{(Eq. 3.34)}$$

$$A_z=\frac{(v_{z2}-v_{z1})}{\Delta z} \qquad \text{(Eq. 3.35)}$$

The results of the particle tracking simulation will be described in chapter 7.

3.5 The hydraulic model

In section 3.2 the design and construction of the model were discussed shortly. Just as a reminder: from the grid data interpolated in SURFER and layers constructed in the Map Module of GMS containing the hydraulic properties and boundary conditions were assigned to the 3D-grid of the MODFLOW model so that a simulation may be executed.
For the simulation stationary conditions are assumed. Meaning that equation 3.4 may be written as

$$S\frac{\partial h}{\partial t} = T\left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right) + I = 0$$

That means that no change in head in time appears according to the model. A stationary model is may be the basis for a transient groundwater flow model that may be calibrated when monitoring data of wells are available. Unfortunately this is not the case in this study.

After constructing the simulation model, MODFLOW has been ran to see how the model input behaves. Is it stable in other words does the model converse ? Does it correspond more or less to the real live situation ?
The steps taken to make the model stable and fit to the real live situation as good as possible fall under the calibration step of the model construction.
To make the model fit to the real live situation the simulation will first be executed as an inverse stationary model, minimise the number of uncertain parameters. This means that on the base of the data of the well heads an approximation is made of the conductivity distribution by considering the hydraulic gradient. This is done by defining map units with expected magnitudes of conductivity with the help of some fixed points from wells and the spacing of the isolines of hydraulic heads (Fig. 17).
The distances between the isolines make it possible to discriminate between zones of higher and lower conductivity.

To approximate the change of conductivity the principle of refraction of stream lines is used (Langguth and Voigt, 1980). With the assumption that the groundwater water streams perpendicular to the isolines of hydraulic heads. The change in flow direction may be approximated from the isoline map. With this change in flow direction the change in conductivity may be approximated by

$$\frac{\tan \boldsymbol{a}_1}{\tan \boldsymbol{a}_2} = \frac{K_1}{K_2} = \frac{T_1}{T_2} \qquad \text{(Eq. 3.36)}$$

This so called stream line refraction law is used here in a semi-quantitative way.
Taken the gradient of the isolines and the refraction of isolines on the interface of different units into account when constructing a groundwater flow model, a simulation run may be carried out and with a (hopefully) good result that is close to the real situation.
The running of the groundwater model and its improvement (e.g. by changing hydraulic properties, configuration of units representing hydraulic properties, changing boundary conditions, etc.) all belong to the step of calibration.

The calibrated flow simulation model is the base for modelling changes in the hydraulic environment like the building of the Iraí-dam. For the different hydraulic environments scenarios of groundwater transport may be constructed using a particle tracking simulation so that an approximation may be made on the influence of the groundwater quality by the Iraí-reservoir.

Further details on construction and calibration together with the results will be discussed in chapter 5.

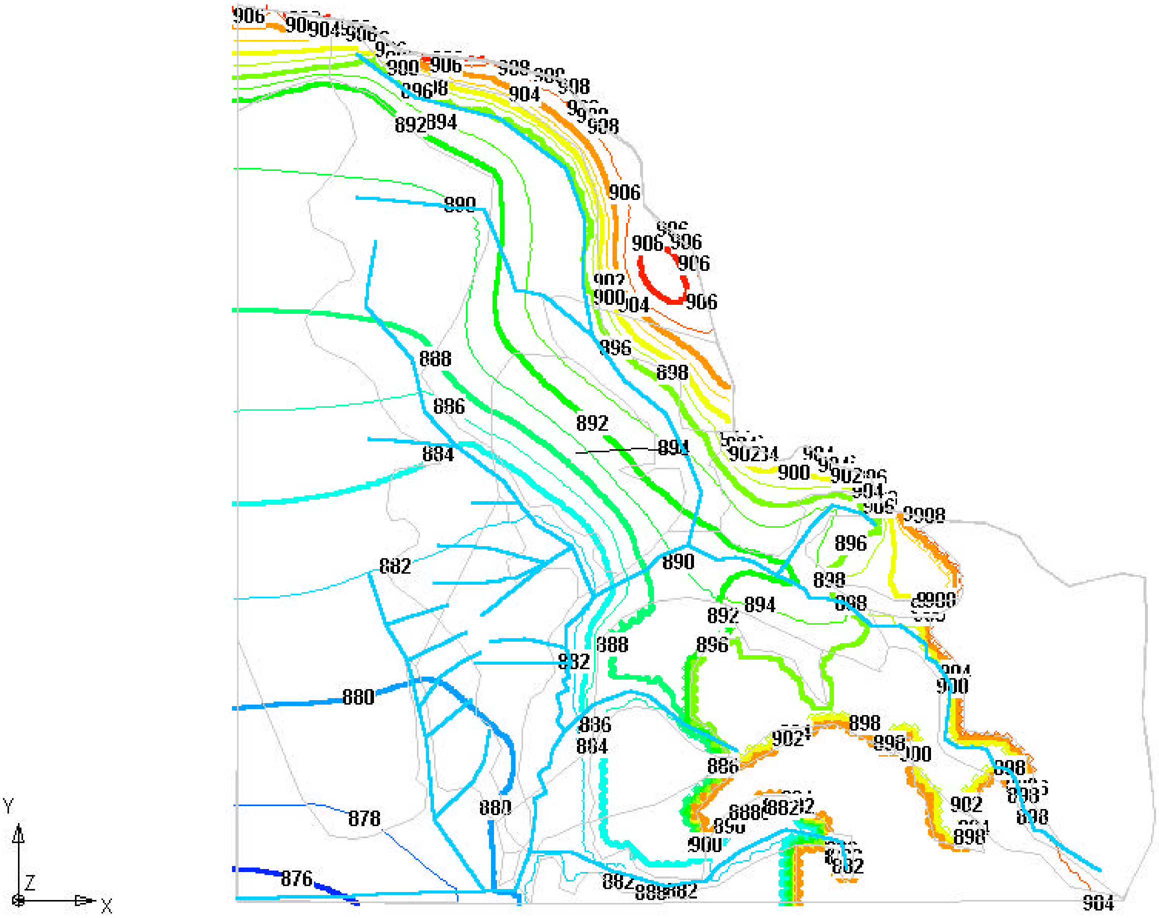


Figure 24: An effort to calibrate the model; visible are the hydraulic isolines and the streams, the grey lines are from other layers in the simulation model (e.g. the hydrographic basin boundary, boundaries between the various hydraulic units).

3.6 The particle tracking model

The groundwater flow field computed by simulation of the hydraulic flow model is used by the particle tracking algorithm of MODPATH. In chapter 5 the hydraulic model of the situation before and after the construction of the Iraí-dam is described. With the hydraulic model corresponding to the situations before and after the dam construction the MODPATH simulation is carried out.

A MODPATH simulation is carried out because two tributary streams of the Iraí-reservoir are polluted by flowing through populated areas and the hydraulic gradient towards the aquifer in which the wells at Iapar have been constructed increased (Chapter 5). So that probably the transport velocity of the groundwater increased and possibly the direction of the streamlines has changed. The time that the reservoir water can reach the wells should be taken into account because of a possible bacteriological contamination and a change of flow direction will influence other parts of the aquifer.

The description of the particle tracking model follows in chapter 7.

4 The computation of the recharge by the Water Balance Model MODBIL

4.1 Introduction

Several methods exist to make a hydrological model. Decisive is what the target is. Originally hydrological modelling was made to determine runoff of catchment areas with emphasis on flooding forecasting. The MODBIL hydrological model has been constructed for another purpose namely to determine the recharge together with the other water fluxes. To make the distinction between MODBIL and other hydrological models it is necessary to get an idea of the several methods used. To make the distinction between several hydrological models the way to classify the various forms of hydrological models is described first.

MODBIL is a hydrological model for the computation of the water balance written by Prof. P. Udluft of the Department of Hydrogeology and Environment at the University of Würzburg. It uses daily climatic data, soil physical data, topography and land use to calculate the groundwater recharge together with other components of the water balance.

Our main interest is the groundwater recharge because that is the parameter that is needed for the groundwater flow modelling with MODFLOW as the other components are needed to compare the water balance described in section 2.6.1.

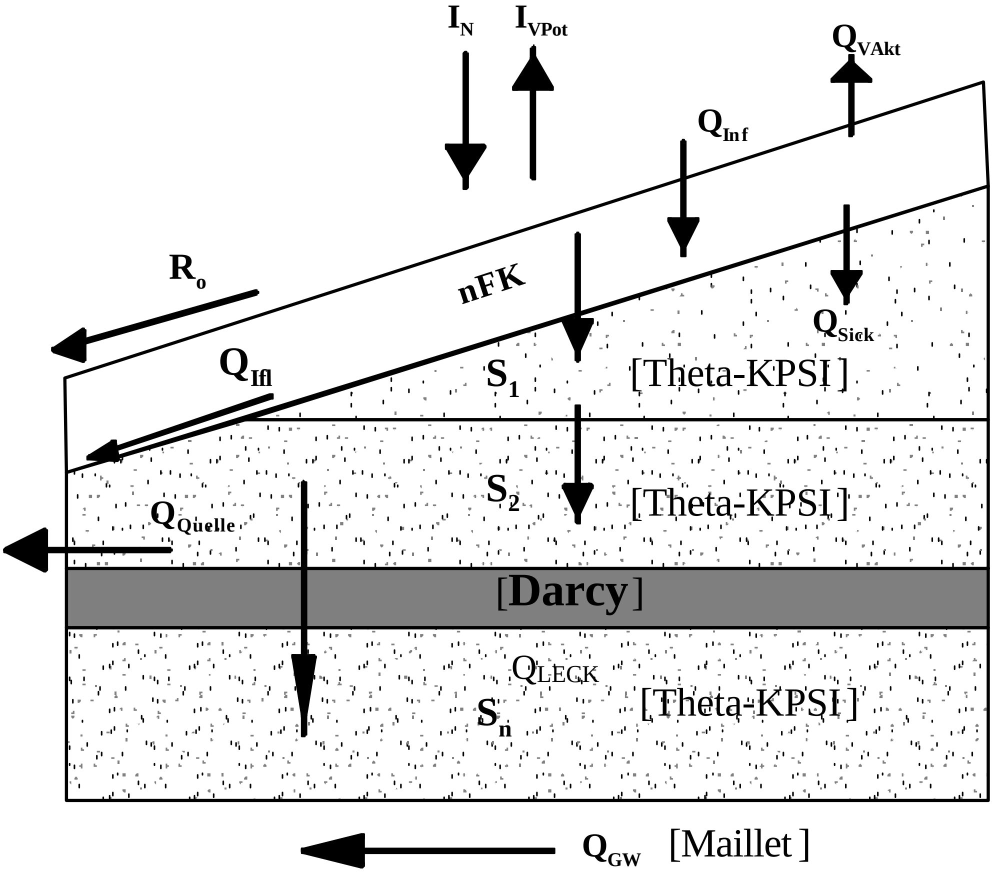


Figure 25: Blockdiagram of the water balance components modelled with the MODBIL Water Balance Model; I_N: precipitation, I_{VPot}: potential evapotranspiration, Q_{Vakt}: actual evapotranspiration, Q_{Inf}: maximum infiltration rate, R_o: surface runoff, Q_{Ifl}: Interflow, [Theta-KPSI]: water content/permeability relationship in the unsaturated zone, nFK: effective field capacity S_1, S_2 and S_n: layers , Q_{Sick}: percolation rate, Q_{LECK}: leakage, Q_{Quelle}: spring flow, Q_{GW}: groundwater recharge (Udluft, 2001).

4.2 Hydrological modelling, which position has MODBIL

Originally in hydrology hydrological models were often constructed to estimate runoff (Singh, 1992, Watson, 1993). Runoff is a general term used to indicate the accumulation of precipitation excess. Of greater interest is either runoff volume from a storm event or for some other time period or peak discharge for the event.

Nowadays hydrological models are used for a range of other purposes like water balances, water resources or water protection.

Modelling systems may be classified by several criteria. These classifying criteria basically can not always be separated. The classification based on the process-description is closely connected to the spatial -and time scales, that at the same time are classification criteria themselves (Lempert, 2000).

The same is valid for the process description and the chosen solution method.

The classification of the process description models may be subdivided in very simple models, which processes are summarised (black box models) and in detailed models, with separate processes and partially their interactions.

The process description can be merely deterministic, stochastic or a combination of both.

The transition of this classifying criterion is mostly fluid, because not all models that are denominated as detailed are really detailed.

Additionally deterministic process descriptions of physically based computational approaches may be put oppositely to empirical approaches.

Conceptual approaches are used a long time to illustrate hydrological processes.

Simple linear approaches like the single linear storage or unit hydrograph (fig. 26) were first used to compute the runoff together with an integral representation of the catchment basin.

With the introduction of serial and parallel storage cascades and the extension to non-linear storage cascades of varying forms the black box models became refined.

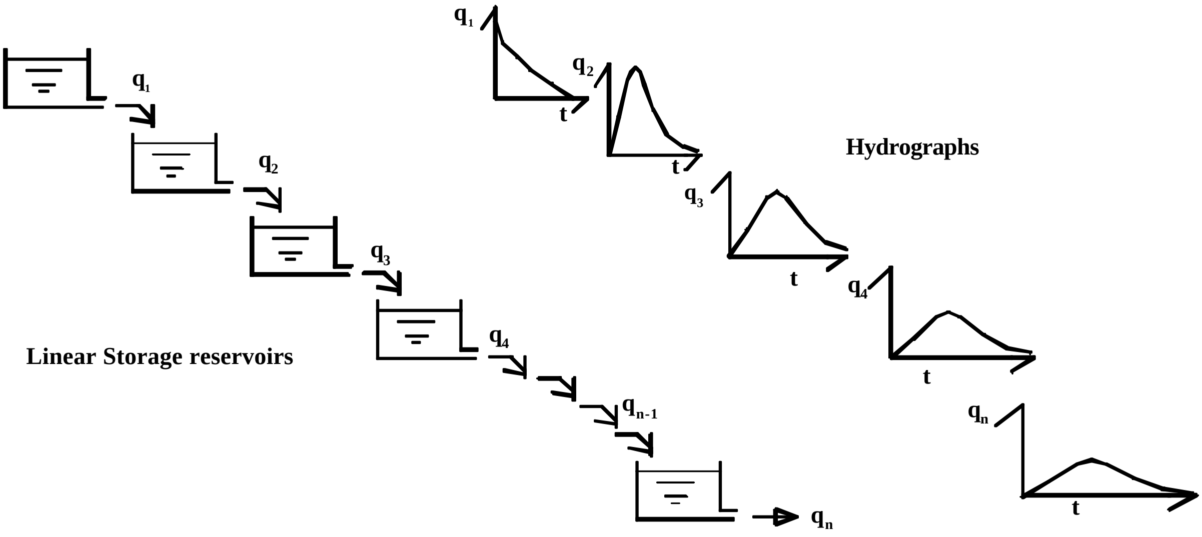


Figure 26: Single linear storage or unit hydrograph (After Dyck, 1978).

With the assignment of conceptual approaches like surface runoff (on the surface and in channels), interflow etc. the first step to detailed model description were made.

The precise description of individual processes by physical equations is until now the most detailed representation of hydrological processes.

Another means of classification as described above is the means of spatial discretisation. This is closely connected to the detail of the process description. Black box models with a simple spatial representation often have as the smallest represented unit the catchment basin or sub-basin. Another but not so widely used more detailed representation of the land surface is by TIN's (Triangulated Irregular Network).

Detailed hydrological modelling systems have a high spatial resolution with e.g. raster units as smallest spatial units. This is also the case with MODBIL, that may be seen as a detailed meteorological-soil physical modelling system.

4.3 The execution of the Water Balance Model

The water balance model uses meteorological variables, soil and vegetation parameters for the prediction of fluxes within the soil and into the aquifer. Input data consists of daily values of temperature at 14:00 hours [°C], mean daily temperature [°C], relative humidity at 14:00 hours [%] and precipitation I_N [mm].

Potential evaporation I_{vpot} is derived from temperature and relative humidity or can be entered directly (if data on pan evaporation are available). The main soil parameters are slope, effective field capacity nFK and the infiltration capacity of the soil that is a maximum infiltration rate Q_{INF}. Surface runoff Q_{Ob} is produced if the intensity of rainfall events exceeds this threshold. The movement within the soil is controlled by evapotranspiration (upward movement) and percolation. Percolation rates are modelled as a function of the soil moisture state.

In the model two different layers S_1 and S_2 are implemented. For each of them a saturated hydraulic conductivity can be entered. The model provides the possibility to calculate the seepage through sediments and bedrock of variable thickness, for the latter case leakage through an aquitard can be simulated as Darcy-flow Q_{LECK}. For the simulation of spring flow Q_{QUELLE} the percolating water can be routed through a Maillet-type reservoir.

The water balance modelling with MODBIL is not only carried out at a point scale but maps of input parameters can be processed (Idrisi or Surfer format) for distributed modelling.

It should be noted that the output is based on the input of the separate cells, and that the output are members of the water balance of the separate cells for one year.

The daily climatic data are data sets in ASCII-files without extension which are derived from monthly data as described below, as the soil physical data, the topography (digital elevation model, slope map derived from the DEM) and land use are in the form of raster maps of ASCII-format derived from Idrisi.

The Program MODBIL (Udluft, 2001) calculates only with daily data, but monthly data may be randomised from monthly data. The daily data necessary for computation are the date, the temperature at 2 p.m. (T14(i)) [°C], the mean temperature (Tm(i)) [°C], the relative 2 p.m. relative humidity (F14(i)) [%], the daily precipitation (N(i)) [mm] and optionally the pan evaporation [mm]. For (F14(i)) [%] unfortunately the measurements were not taken at 2 p.m. but at 3 p.m. but there are no other data that may be used for the hydrologic model.

Daily data are available only for some of the above mentioned parameters of the meteorological station Iapar in the study area and then with many gaps.

Monthly data for Iapar for February 1970 to December 1997 are available for the relative humidity (F(i)) [%], the precipitation (N(i)) [mm] and the pan evaporation. For the daily mean temperature (Tm(i)) [°C] unfortunately no data are available, only the mean monthly temperature data are available.
That is why temperature data of other nearby stations are taken. Data of two stations are taken because none of the records is complete, so that to fill in the gaps those two stations have to be correlated. Then the station that has the best correlation (0.994) with the mean monthly temperatures at Iapar is used to calculate the daily mean temperatures of the station Iapar at Piraquara. Unfortunately these data that are from Aeroporto range only from January 1981 to October 1990. The data from the station Curitiba range from January 1885 to December 1993 but has many gaps and has only a moderate correlation (0.852) with the mean monthly temperatures of Iapar. Between January 1970 and November 1991 it was possible to fill in the gaps for Iapar by calculating a regression function between consequently Iapar-Aeroporto and Iapar-Curitiba. This means that the data used are from the period January 1970 to November 1991.

When the computation (with the help of the correlation factors) for the monthly data is finished a daily data file is calculated with the help of the program *"Month to Days"* in MODBIL.
Now the data are ready to compute the precipitation distribution and the quasi-potential evaporation after Haude with the meteorological basis-program. The arithmetic-base of Haude uses the 2 p.m. temperature as well as the 2 p.m. relative vapour pressure. The potential evaporation is directly as well indirectly proportional to these two values. The program uses the barometric height-formula so that the height is taken into account when the precipitation and potential evaporation is calculated.
For the Haude factors in Paraná different factors are used as for Central Europe for which the Haude-method was originally developed. MODBIL tries to describe the maximum evaporation-values with modified Haude-factors for the different land uses. A land use map is constructed with the GIS-system Idrisi which is illustrated in figure 27.

Interception storage values are based on land use values for Central Europe for various land uses. The intercepted precipitation is subject to the evaporation and will be reduced with this amount. The rest arrives in the next time-step as through-fall on the ground. In the forest the precipitation occurs under certain conditions as wet fog on the ground. If the measured precipitation is less than 0.5 mm/day and the saturation deficit is less than 0.15 Torrs, the fog precipitation becomes 1.5 mm/day.
As a result the snow storage is 0 during the full time that was computed. This was expected because temperatures below 0 °C and snow are very rare. Around 1975 there was a rare occasion that snow had fallen and this melted very rapidly.

MODBIL is a detailed meteorological-soil physical modelling system that computes the precipitation, Haude (potential) –and effective evapotranspiration, interflow and groundwater recharge. The following description is actually from a previous version of MODBIL, but this describes the principles of the computation of the hydrologic water balance for only one cells as the advantage of the new version is that the output are raster maps. In Version MBC the topography, spatial distribution of the soil physical parameters and land use is taken into account.
The following equations are written in the by the MODBIL program used symbols.

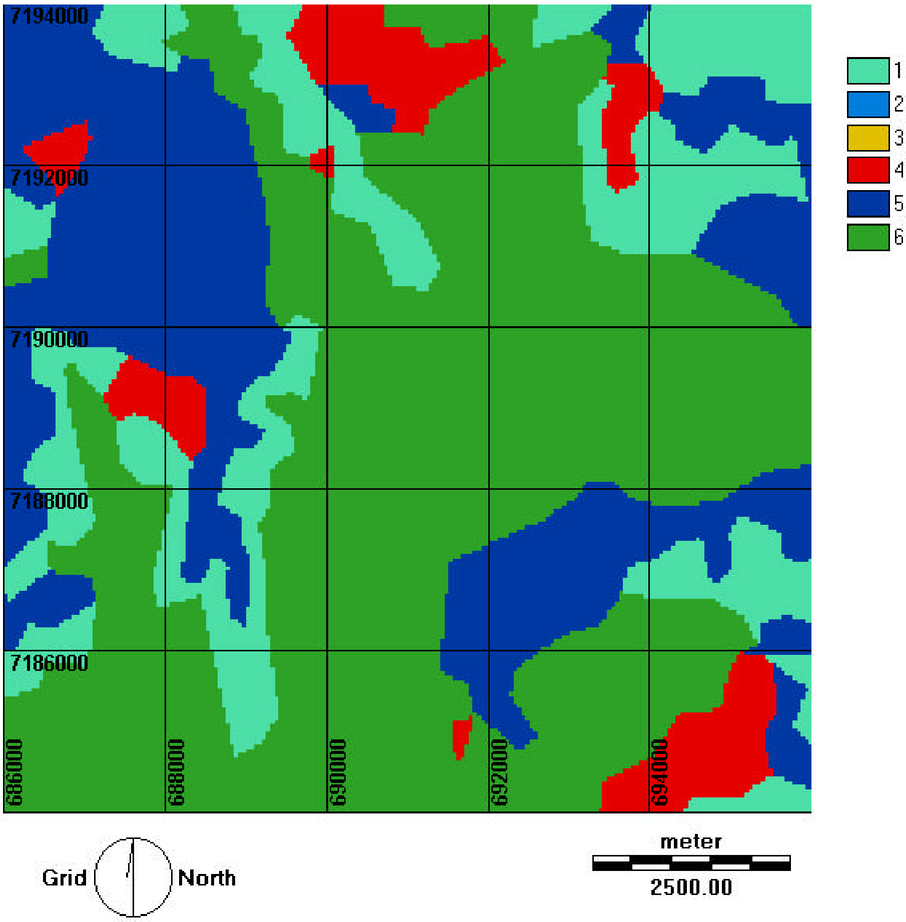


Figure 27: the land use map of the survey area; legend: 1. deciduous forest 2. mixed forest 3. coniferous forest 4. settled surfaces 5. farmland 6. grassland

The effective precipitation falls on the ground surface (1st Border surface) defined by the value of the border-permeability GD. The border permeability depends on the ground permeability (KFBOD1) and the land use (TYPE) and is additionally steered by the slope of the land surface (NZ) and the saturation state (HP) of the soil. The soil physical units are illustrated in figure 28. In this map soil physical units are illustrated though some of these units also represent soil type units this is no soil type map.

Draining on the surface originates then when the precipitation value (NWIRK) is higher than the real border permeability (DURCH1). The reduction (NRD) is dependent on NZ:

NRD=1/1-Tan(PI/180*NZ) valid for slope inclinations below 45°

DURCH1=GD*NRD

The permeability of the boundary increases when the soil water content increases, provided the soil is not saturated.

FTOR=1/(0.2+0.008*PS) with a limitation at 10 % saturation.

DURCH1=DURCH1*FTOR

Before the latter computation the DURCH1 is the saturated permeability of the border permeability. PS is the water content in %.

Because frost events are very rare in the region the reduction of the permeability by frost is not taken into account.

The next boundary condition for a division of the fluxes in "deeper percolation" or "interflow" is the permeability of the soil itself (KFBOD1) which is estimated with the "Bodenkundige Kartieranleitung (1994)" The matrix values for the soil map (fig. 28) may have a value from 1 to 6 and may be coupled to a k_f-value with $X := -8 + 0.5 * \text{Matrix-value}$
$k_f := 10^X$.
Now the water content of the soil will be increased by the gain of infiltration INF. If the field capacity is reached the surplus continues to the next barrier that exists at the boundary of the soil to the subsoil (C/C_v). Where interflow may appear if the permeability of the subsoil (KFBOD2) is smaller than the infiltration from KFBOD1. In general a factor 0.5 is taken that reduces between the root zone and the unweathered soil zone (C) in crystalline rocks like the migmatites in the study area this reduction factor equals 10.

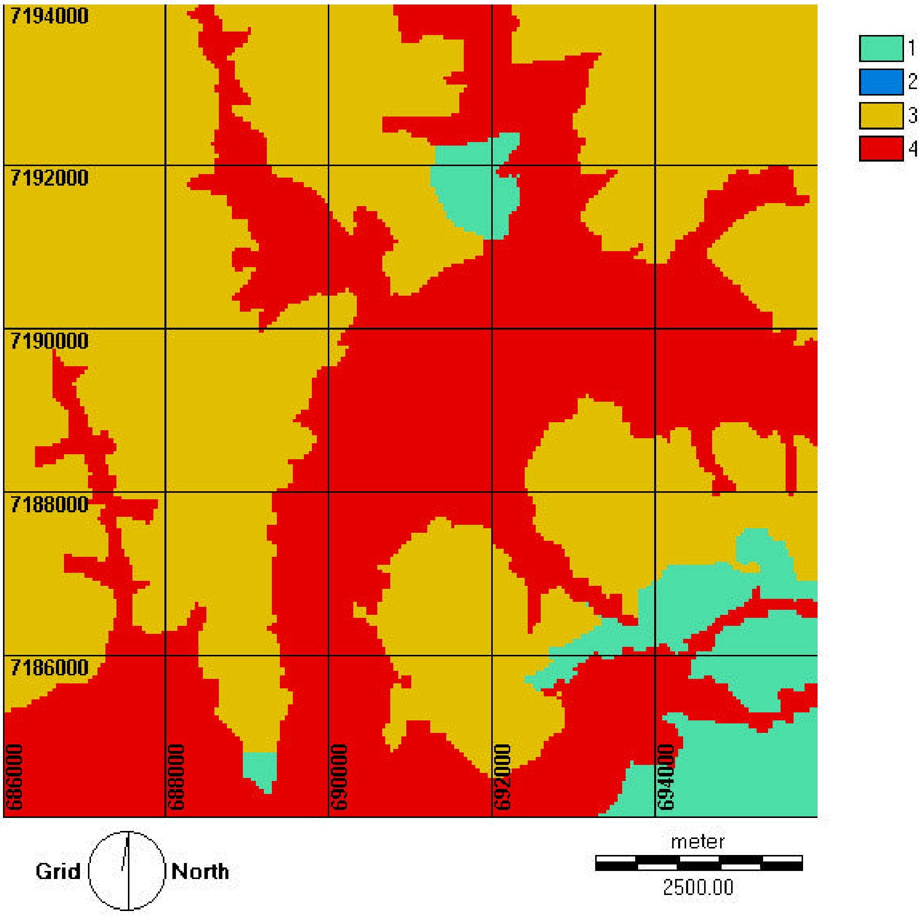


Figure 28: soil physical units; 1. very low permeability soils on migmatite or clays 3. Latosols/Cambisols having a moderate permeability 4. Organic soils/hydromorphic gleyic soils with a high permeability (EMBRAPA, 1984).

The next step is that the evaporation VPOT takes water (of the root-zone) from the soil storage. The size of the real evaporation VAKT depends from the saturation of the soil. The calculation takes place in 10 steps per day.
For this calculation the following simple relationship may be used:
$VAKT=VPOT*VFAKT$

where $VFAKT=PS/100$
The water content DS of the soil, that stands for the next time-step to disposal, is

DS=DS-VAKT

The quantity of water that has infiltrated in the root zone, which did not flow out as interflow or evaporated, infiltrates in the soil below the root zone. The base for further calculations is the water content/permeability relationship in the unsaturated zone [è-$K_{\O}$]. Therefore that the water contents at saturation of most relevant soils are well determinable and the pF 4.2 is available as well in tables (Bodenkundliche Kartieranleitung, 1994), also the water content/permeability relationship can be described as a x/y-function for the groundwater flux.
Since the main fluxes appear between water content at saturation (THETAMAX in % tot. Vol.) and field capacity (THETHAFK in % tot. Vol.) the percolation velocity can be written as:

KFNEU = KF*(THETAMAX-THETAKF) with KF is k_f at saturation

Field capacities are respectively 380 mm for very low permeability soils on migmatite or clays, for Latosols/Cambisols having a moderate permeability of 200 mm and for organic soils/hydromorphic gleyic soils with a high permeability of 100 mm. These field capacities are in the range of the mentioned soils according to the “Bodenkundliche Kartieranleitung” but the values used are a rough estimation.
If the water content is lower than the value of field capacity the following function that reduces the k_f at saturation is valid:

LKFN =10-0.2783*PTHETA+0.00446*PTHETA^2-0.0000266* PTHETA^3

With log($K_{\O}$): LKPSI=-LKFN+LKF with LKF=lOG(KFNEU)

And in accordance with KPSI=10^LKPSI is KPSI the percolation velocity for this time step in m/s. The new water content in each layer is now:

CONTENT=THETA*MAB-(KPSI(n)-KPSI(n-1)*86400/ZEIT*100 [mm]

Where MAB is the thickness of the soil layer.
The results consist of the water content and the velocity of percolation which are valid for the soil below the root zone, not for fluxes in bedrock.
In the MBB-version of MODBIL the groundwater hydrograph and groundwater runoff by using the Maillet-formula is computed.

4.4 Results

For the output of the MODBIL-version (MBC) the spatial distribution of the precipitation is calculated (fig. 29). The measured precipitation at the meteorological station at Iapar is corrected with a precipitation factor for the height (NFAKT) by
N =N * (1 + [height(m) – height of the station(m)] * NFAKT/10000)

Where NFAKT is 4.4 [%/100 m] is used and the height is derived from the DEM.

The potential evapotranspiration is derived from the meteorological data and corrected with the barometric height formula and Haude-factors (fig. 30). A correlation between the potential evapotranspiration and land use is visible. It is at its lowest where the forests are and at its highest were the settled surfaces are. In the agricultural areas the potential evapotranspiration is also high in comparison to the forests. In the agricultural areas a negative correlation is visible between the evapotranspiration and the height. At the grasslands it is slightly lower as at the farmlands.

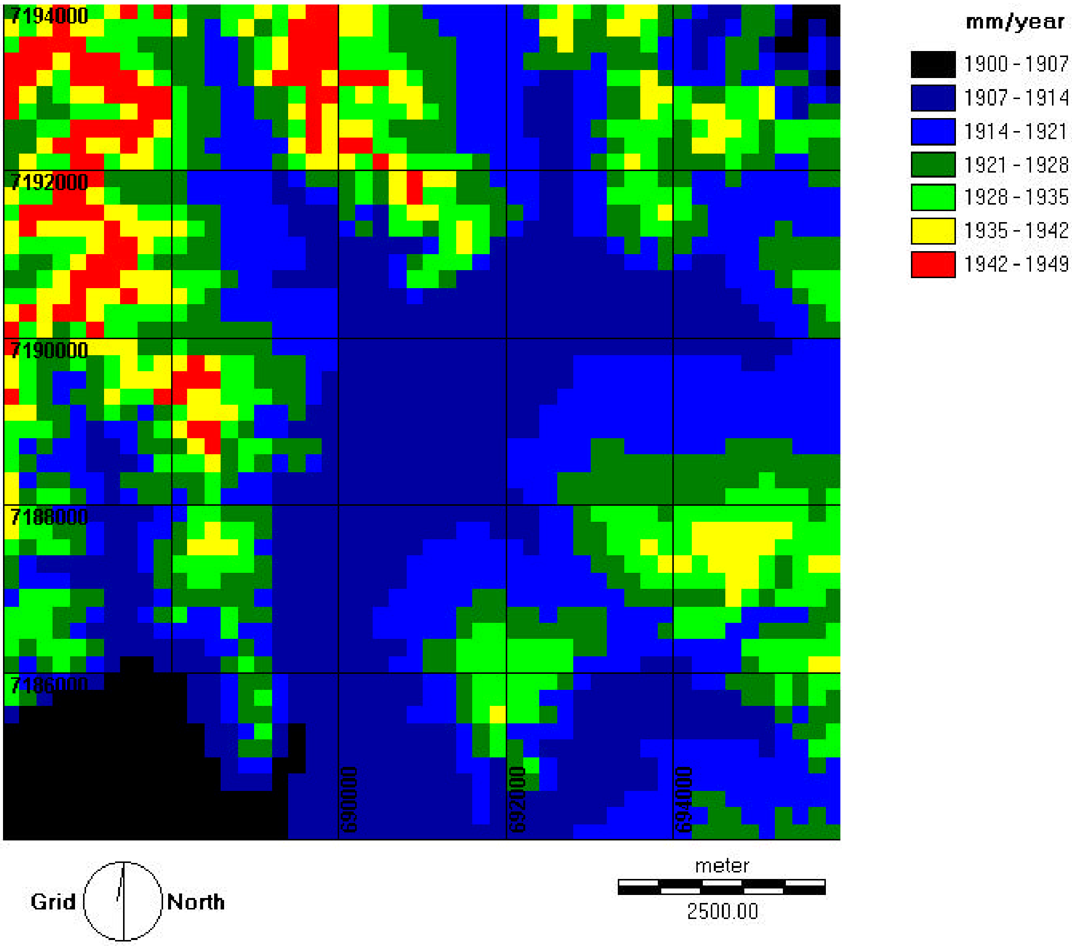


Figure 29: Precipitation [mm/year]

Effective evapotranspiration is dependent on the velocity that the precipitation may percolate through the soil or is retarded on the surface or in the soil so that it may evapotranspirate. This is also dependent on the relief because the water flows more rapidly off when the surface inclination is high and also the interflow is higher then when the land surface inclination is lower. The effective (real) evapotranspiration depends on the water saturation of the soil (the potential evapotranspiration takes water from the soil storage). The effective

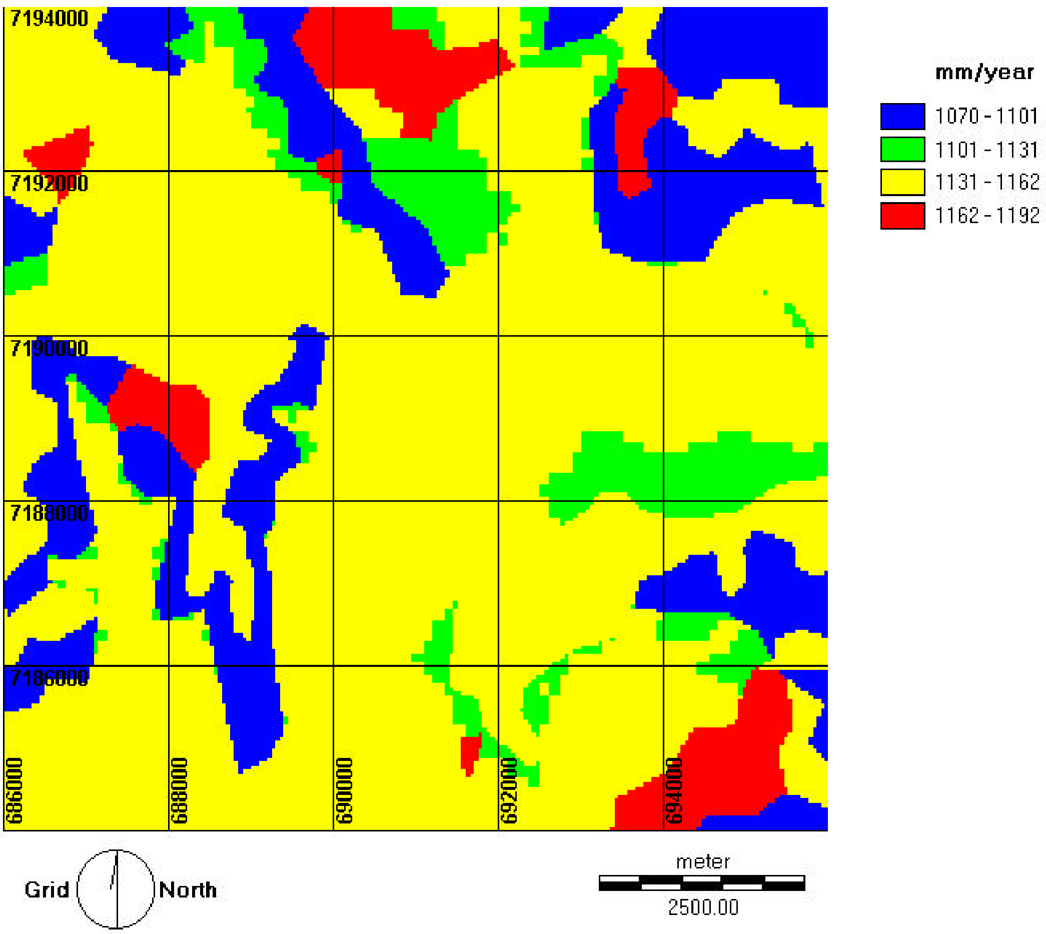


Figure 30: Potential evapotranspiration [mm/year]

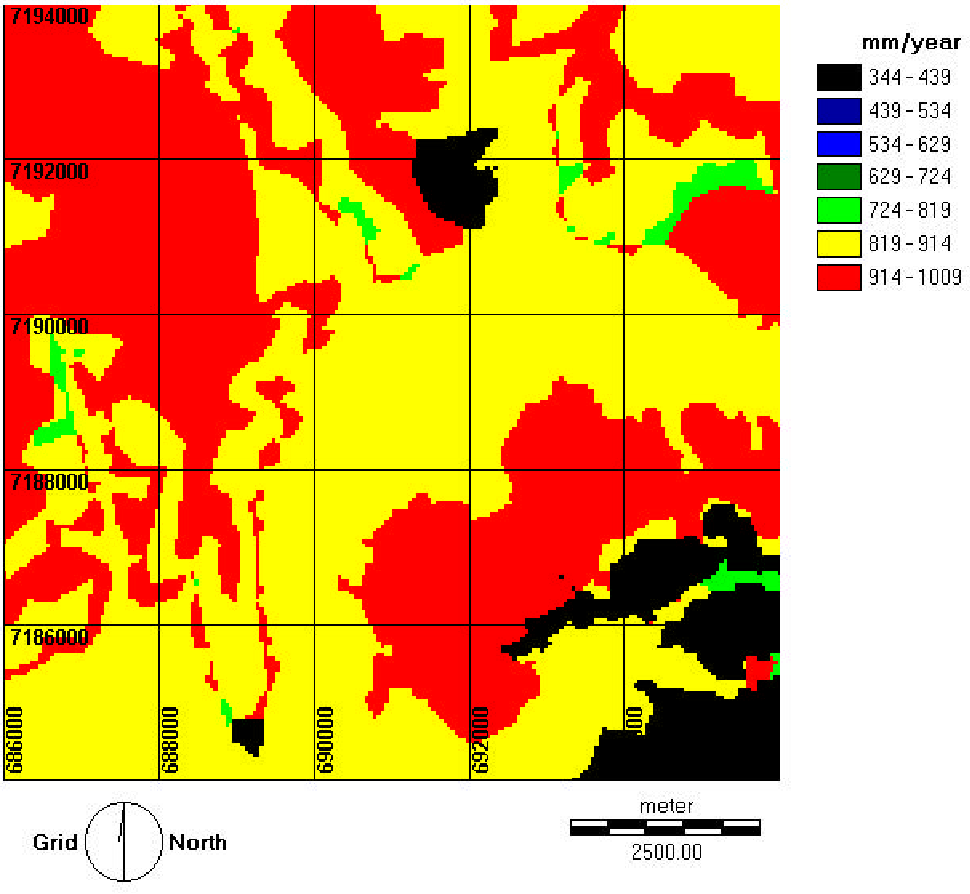


Figure 31: Effective evapotranspiration [mm/year]

evapotranspiration is illustrated in figure 31. In figure 31 the effective evapotranspiration is at its lowest where the soil (or subsoil) has a very low permeability (fig. 28).
because the interflow and the surface runoff (fig. 32) reach higher values. Where the soils have a moderate permeability the effective evapotranspiration is at its highest. Probably due
to a lower interflow and surface runoff in combination with a higher water quantity stored. This in contrast to units with a high permeability and a lower storativity.
In the forests the evapotranspiration is lower as in the agricultural areas in the same soil physical units. The forest have a relatively high infiltrating potential so that for the water to evaporate no time is left. In the settled areas that lie on soils with moderate permeability the evapotranspiration has about the same magnitude as the areas that have high permeability soils. This is not because of the same reason, namely that the water is more quickly drained, but because of higher overland flow and interflow (fig 32).
The same negative correlation between height and evapotranspiration as in the case of potential evapotranspiration is visible at the farmlands.
Interflow originates due to decreased permeability below the root zone. Interflow is highly
dependent on the slope, landuse (Fig. 27) and permeability together with the C/C_v-permeability.
In figure 32 the highest interflow/surface runoff values appear at the low permeability units, then the settled areas, followed by the higher lying areas with a moderate permeability. The interflow is at its lowest in the lower flat lying areas and which have on the same time a high permeability.
The forests though they are often in areas with a higher slope have lower interflow values.

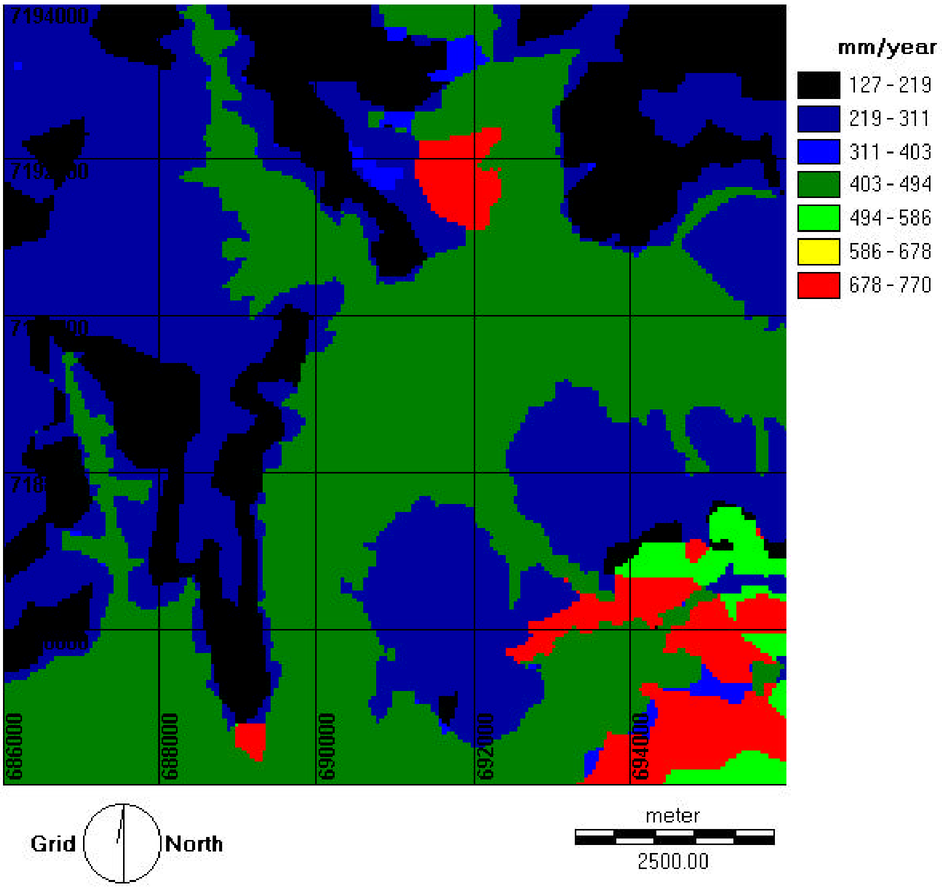


Figure 32: Interflow and surface runoff [mm/year].

The groundwater recharge is illustrated in figure 33. The recharge is at its highest in the lower flat areas with the higher permeabilities. In contrast, the areas with very low permeabilities have even a 0 recharge. The forests have lower recharge values, because of the high values relative to effective precipitation for the effective evapotranspiration and interflow values. The higher areas with a moderate permeability without forests or settlements have a moderately high recharge. In top of figure 33 in one of the settlements the dependence of the slope inclination is clearly illustrated. In the flat area with a low slope the recharge is higher then on the sloping area. As the area around this settlement in the flat area is higher. Where the groundwater recharge is high the vulnerability to pollution of the aquifer is higher in comparison to zones with lower groundwater recharge. Methods of vulnerability and the concept are described in chapter 6.
One drawback of modelling the recharge with MODBIL is that the groundwater level is not taken into account. When the groundwater level is very close to the surface the recharge will be very low and more of the runoff will be surface runoff.

The disadvantage of MODBIL is that it computes the water balance for each separate cell, but that there is no interaction between adjacent cells. Which is important because interflow and surface runoff flow to adjacent topographically lower cells. This flow may infiltrate, evaporate etc. in the adjacent cells. The fact is that surface runoff is rarely observed and then when observed on barren soils, almost impermeable soils and then under extreme weather circumstances. This is inconsistent with the results of MODBIL, because it does not take into account the interaction between the different cells (or the interflow/surface runoff should be much more interflow than surface runoff). Probably when the cells are taken infinitesimally

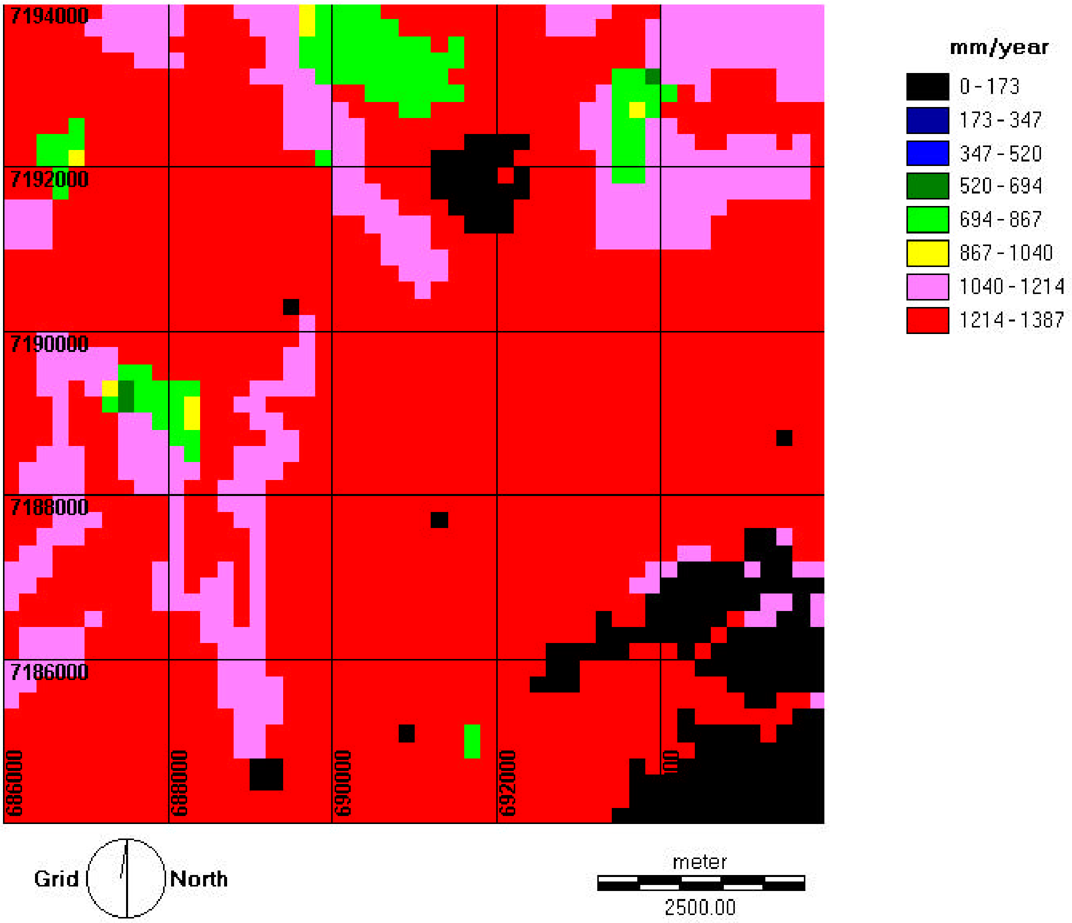


Figure 33: Groundwater recharge [mm/year]

small almost no surface runoff will be generated when an interaction between cells would exist. Except when the permeability of the units is extremely low and in the case of a shallow groundwater table.

Also is the result of the water balance a mean of the results which are probably different in time under the various weather circumstances. A year for example may be dry or wet. The parameter time is also very important for flow. Because to let a surface runoff be generated in a cell, flow into another adjacent cell and infiltrate or flow to the next cell, one has to go forward in time. Also the scale of these time-steps is very important, it is ridiculous to take one year as a time step to model the interflow/surface runoff. To model more or less the real situation these time-steps should be taken sufficiently small.

4.5 Conclusions

The distribution of the groundwater recharge magnitude is in the first instance independent on the precipitation which has a positive correlation with the height. In the areas with very low permeabilities and high field capacities the effective evaporation (E) is low, the interflow $R_{interfl}$ is high and probably a very high surface runoff R_o (fig 32) appears ($P_{eff} - E = R_{interfl} + R_o$).

Where the settled areas are the potential evapotranspiration is relatively high, with high effective evapotranspiration as surrounding areas having the same soil physical parameters. So that they have a relatively low groundwater recharge.

No real differences between areas with grasslands and farmlands are visible between effective precipitation, effective evapotranspiration, interflow/surface runoff and groundwater recharge. The influence of the soil physical parameters, together with evapotranspiration and the interflow/surface runoff determine that in the higher agricultural areas groundwater recharge is moderately high as in the basin (grasslands in more or less swampy areas) the groundwater recharge is at its highest. A drawback of the MODBIL hydrological model is that the depth of the groundwater table is not accounted for and because of that much of the computed recharge in the basin may be surface runoff while the soil is already saturated.

Summarising despite the former described limitation that no interaction between cells exist, in the overall MODBIL is a powerful tool to estimate the magnitude of components of the water balance. Because of the non-existence of the interaction between cells the groundwater recharge may be seen as the quantity that will at least infiltrate.

In zones of higher recharge the aquifer is at the same time more vulnerable to possible pollutants. The resulting recharge distribution will be discussed in chapter 6 as one of the methods used to estimate the vulnerability of the aquifer to pollution from the surface.

5 The construction and the calibration of the groundwater flow model

5.1 Introduction

From the data which were described in chapter 2 and observations in the field a hydrogeological model is constructed, which acts at the same time as a concept for the groundwater flow model. A hydrogeological model is an abstraction respectively a schematised description of the influences and their connections on the hydrogeology. (Arbeitskreis “Hydrogeologische Modelle”, 1999).

Because of the lack of data and the incomplete picture of the geology the resulting hydrogeological model only approaches the real situation. When the hydrogeological model is incorporated in the conceptual groundwater flow model and a simulation is executed, it does not immediately gets the same results for the hydraulic heads as the isohypses in the isoline map (fig. 17). Another point is that the isoline map is an interpolated map of unequally divided points. While some wells are constructed on a hill and others are constructed in the alluvium so that the interpolation may neglect the influence of the topography on the hydraulic heads.
This lack has partially been solved by taking stream water level points from the topographic map where a contact with the aquifer is expected. The water levels of the streams where chosen very carefully because it was obvious that some streams originated from perched aquifer(s) (also see fig. 34).
Depuit-assumptions are made for the model, because all the wells were filtered where suitable permeable layers were encountered, so that no differences in hydraulic head could be found between depths:

$$\left(\frac{\partial h}{\partial z} = 0\right) \qquad \text{(Eq. 5.1).}$$

The isoline map of the hydraulic head is the starting condition for the MODFLOW model (starting heads).
From the grid data interpolated in SURFER, containing the elevations and hydraulic heads, and the layers constructed in the Map Module of the Groundwater Modelling System (GMS) containing the hydraulic properties and boundary conditions, were assigned to the 3D-grid of the MODFLOW model so that a simulation may be executed.
For the groundwater flow model stationary conditions were assumed because there are to much data lacking to make a responsible transient model. In the future a transient model may be constructed because a monitoring program with the piezometers has been started.

Having the conceptual model constructed there are still many unknowns so that after its execution the fitting of the simulated and the measured hydraulic heads still may be improved. Unknown parameters may be derived from such a testrun by looking at the isoline map of the simulated hydraulic heads. For example improvements of the groundwater flow model may be by a different setting of the boundary conditions (e.g. the level of the drains is to high at some places), another configuration of hydraulic units or addition from unknown hydraulic units (e.g. the testrun gives a different curving of the isolines then from the starting heads) or other permeabilities for hydraulic units (e.g. when the gradient falls to rapidly in the groundwater flow direction a higher permeability has to be introduced). The purpose of those test runs and

consequent adjustments are to make the fitting of the simulated and the measured hydraulic heads as good as possible and with this the calibration of the model is meant.
The results of the successful calibration and the consequent uses of the calibrated model will be discussed in section 5.4.

5.2 Construction of the model

In GMS a hydraulic model was constructed by constructing layers (coverages) in the Map Module and by assigning them together with starting heads and the elevation model (interpolated in the 2D Scatter Point Module) to the grid in the 3D Grid Module (MODFLOW model). As is pointed out in section 3.3.2 GMS is subdivided into ten separate modules that may all handle specific data types that are necessary to build and/or execute and visualise a model.

For the hydraulic properties in the Map Module the coverages are assigned the following layer attributes for the MODFLOW model assuming stationary conditions: hydraulic conductivity, transmisivity, top elevation, bottom elevation, leakance, wet/dry flags. Additionally for the MODPATH model the aquifer porosity and the layer thickness are assigned as attributes. For the hydraulic properties 3 layers with the parameters (k_f only in the first layer, in the second and third layer T) are used.
The 2 upper layers for the hydraulic parameters represent spatial variability in lithology, as the third layer only represents bedrock. This was done to introduce some flexibility in the model, for the case a third layer was necessary. While this third bedrock layer is more or less impermeable this layer has more or less the status of inactive cells.
In the conceptual model the parameters of the aquifer are discretised in zones with hydraulic parameters having the same magnitude. This discretisation is often subjective, only approximated and may be poorly constrained by the data and the solution of the simulation and depends to a large extent to the chosen zonation.
A first zoning of hydraulic parameters was made according to the geological map (fig. 5) and observations in the field, which now apart from some changes made by schematisation and during calibration correspond to the first layer (fig. 37).
Important parameters like depth to bedrock and heterogeneities can not be deduced from the geological map. Where it was known that the depth of bedrock was limited (deduced from geoelectrical pseudo-sections, a geotechnical section for the Iraí-dam project or drill holes but also taking the faulting and distribution of the surface geology into account, illustrated in figure 5), the zones of bedrock were put into the second layer (fig. 38). This zonation of the bedrock is important because the rocks in the study area have very low permeabilities and correspond to practically inactive units. This is because of the hydraulic properties the bedrock units are assigned which in contrast to the properties of the loose sediments represent very sharp contrasts. Bedrock units on the same time are assigned specified heads (constant heads) or form the boundary with the groundwater flow model having specified heads.
From the well construction logs and pumping tests various permeabilities were deduced for the wells normally ranging from 10^{-5}-10^{-3} m/s (deduced from transmissivities).
According to drillhole log at the locality where the three geoelectrical pseudosections are in fig. 6, a very low permeability has to be expected. Another tool to estimate the permeability are the gradients between the isolines (fig. 17). All these observations where considered in the discretisation of the hydraulic units and for the units of higher permeability a k_f in the range of 10^{-5}-10^{-3} m/s was taken.

Taking the known of the hydraulic units in mind and by calibration, heterogeneities may be deduced (minimise the number of uncertain parameters and deduce the distribution of heterogeneities by inverse modelling to make the model fit to the real live situation, the isoline map of hydraulic heads).

But before the calibration is carried out heterogeneities have to be introduced, by discretising units resembling more or less the natural situation when possible. Not only is the discretisation often subjective, also the boundaries between the hydraulic zones are often schematic not resembling a natural situation because these boundaries were drawn with many assumptions. Although the hydraulic zones are schematic they are meant to represent the real configuration of hydraulic units having the real hydraulic properties of the materials. The hydraulic units are covered by the hydraulic zones (Fig. 39 and fig. 40) which are the resulting zones of layer 1 and 2 after calibration.
It is a fact that although the zones are schematic, the calibrated result of the groundwater flow simulation should be satisfactory.

For the boundary conditions the attributes drains (constant heads), recharge and for the 3 layers specified heads are assigned in the Map Module to MODFLOW.
The boundary condition drain with constant heads is assigned to the streams from which the assumption is made that that they are in contact with the aquifer.
Coverages representing streams and specified heads represent boundary conditions which are artificial and are often based on assumptions, which have to be proven during the groundwater flow simulation (calibration). Especially assigning a specified head to a rising area like the Serra do Mar with a low permeability is not so simple. The right magnitude may only be assessed during the calibration.
The specified heads represent the bedrock units and the South-eastern boundary of the hydrographic basin (constant head, Dirichlet-boundary condition; Kinzelbach, 1995, Balke et al, 2000).
The model grid is inactive past the South-eastern boundary which is formed by the Serra do Mar, because no water flows across this boundary.
Taking the isoline map of hydraulic heads into account the units across the Western boundary of the hydrographic area are not made inactive because groundwater flow across this boundary may be expected.

A coverage for the boundary condition recharge has been constructed by differentiating zones of varying permeability. This was done on the one hand taking in mind the data basis of the Iapar-climate station and the extrapolation of those data on the higher lying area of the Serra do Mar that forms the Eastern boundary with the hydrographic basin, and on the other hand considering the result of the water balance modelling with MODBIL (chapter 4).
It is assumed that the precipitation in the Serra do Mar is higher than at the climate station Iapar that is situated on a hilly ridge but in the valley. It is of course difficult to estimate the exact quantity that forms the recharge in the higher areas in the Serra do Mar which has on the other hand bedrock on shallow depths. The precipitation for the Serra do Mar computed with MODBIL also gave higher sums. The precipitation minus the evapotranspiration and soil field capacity flows as interflow through the regolith and overland flow towards the loose sediments in the valley, as the deep percolation can be neglected.
For the future hydraulic conditions when the reservoir of the Iraí-dam is filled, an additional layer has been constructed that contains the area of the reservoir as a polygon of general head

boundary condition. This layer is added so that a new model is generated with the original hydraulic conditions as the base.

Because of their importance and their high potential as calibration tools a further discussion about the boundary conditions as well as their presentation follows in the next section.

5.3 The boundary conditions

Boundary conditions are illustrated in figures 34 and 35, illustrated are specified heads and drains (streams). The units in figures 34 and 35 represent grid cells that are assigned these boundary conditions and represent bedrock units, the Eastern boundary of the hydrographic basin and streams.

Boundary conditions for units consisting of bedrock inside the hydrographic basin are represented by polygons with a specified head. The height of the hydraulic heads for these bedrock units were more derived by extrapolation then by observations.

For the area of the Serra do Mar that belongs to the hydrographic basin, the recharge and a flux that flows into the basin are taken in mind by the construction of the specified head boundary conditions for bedrock units. In the second layer the number of units of specified head has increased, taking in mind the shallow bedrock units. The bedrock units having a specific head are one of the tools to calibrate the groundwater flow model.

At the Eastern boundary a specified head boundary is constructed so that this can be used as a tool for calibration (because near this boundary no wells were available almost nothing was known about the hydraulic heads, but on the same time these heads have a large influence on the hydraulics of the model). At the same time some part of the specified head boundary forms the boundary between bedrock and loose sediments.

During calibration the specified heads can be changed to get the most favourable result. East of the hydrographic boundary the cells are made inactive.

Streams and rivers function as drains. Some smaller streams are derived from perched water tables and appear as sources but have no contact with the aquifer. This is clear by comparing the isohypses of the hydraulic head in the isoline map with the topographic map. Only streams having contact to the modelled aquifer are put in the groundwater flow model. The fact that streams have contact to the groundwater was not only deduced from the isoline map, but it was also found during calibration. The streams are assigned drains in GMS and consist of constant heads (Dirichlet-boundary condition). The cells active as drain are green in figures 34 and 35, in figure 36 active drains are blue as the streams not having contact with the groundwater table are black.

For the future hydraulic conditions when the reservoir of the Iraí-dam is filled, an additional layer has been constructed that contains the area of the reservoir as a polygon of general head boundary condition. This layer is added so that a new model is generated with the original hydraulic conditions as the base.

An additional kind of boundary conditions forms the recharge which varies with permeability of the soil and the height. This is why polygons are constructed which, more or less take these parameters into account. For the recharge zones simply the layer 1 of hydraulic zones was copied (fig. 37) to which recharges were assigned so that both the soil permeability and height influences on recharge are considered. With the model it is possible to see which situations are possible taking into account some known parameters.

In the model the volume of the surface flow and the groundwater recharge will be the same

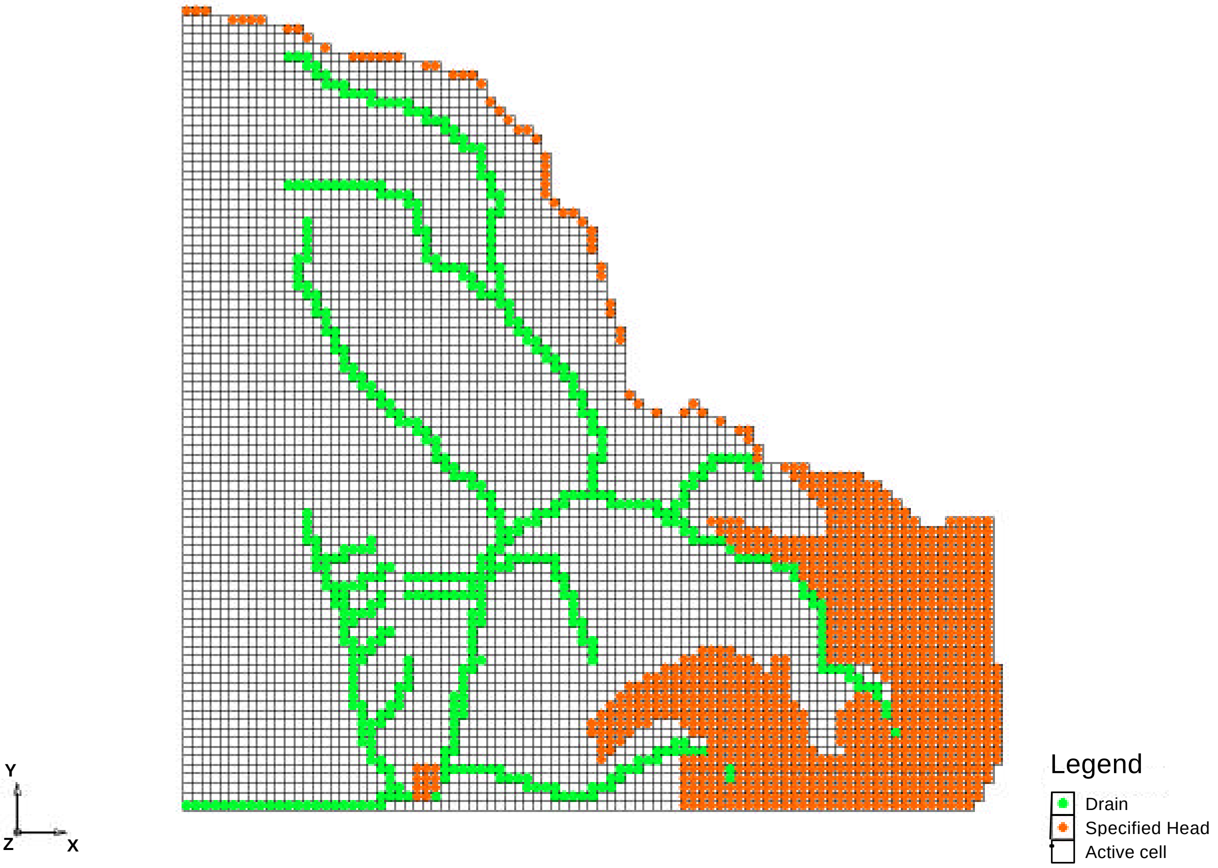


Figure 34: Boundary conditions of the groundwater model in layer 1.

quantity as the yearly total effective precipitation (in this case precipitation minus potential evaporation) which corresponds to 1.95 mm/(m^2*d).

For the drainage area and the Iraizinho-drainage area of 163 km^2, the surface flow is equal to 2.29 m^3/s as the mean discharge.

1.6 m^3/s as the mean discharge for the drainage area of the Iraí-reservoir is taken, this is 1.21 mm/(m^2*d) so that the surplus that may infiltrate is 0.74 mm/(m^2*d) which is taken as the mean groundwater recharge of the Iraí-basin according to the water balance described in section 2.6.1. This mean recharge is used in the basin where the permeability is thought moderate and consequently higher or lower than the mean for respectively permeable units and less permeable units.

A comparison with the water balance model MODBIL shows that the values used have more or less the same magnitude as the modelling result.

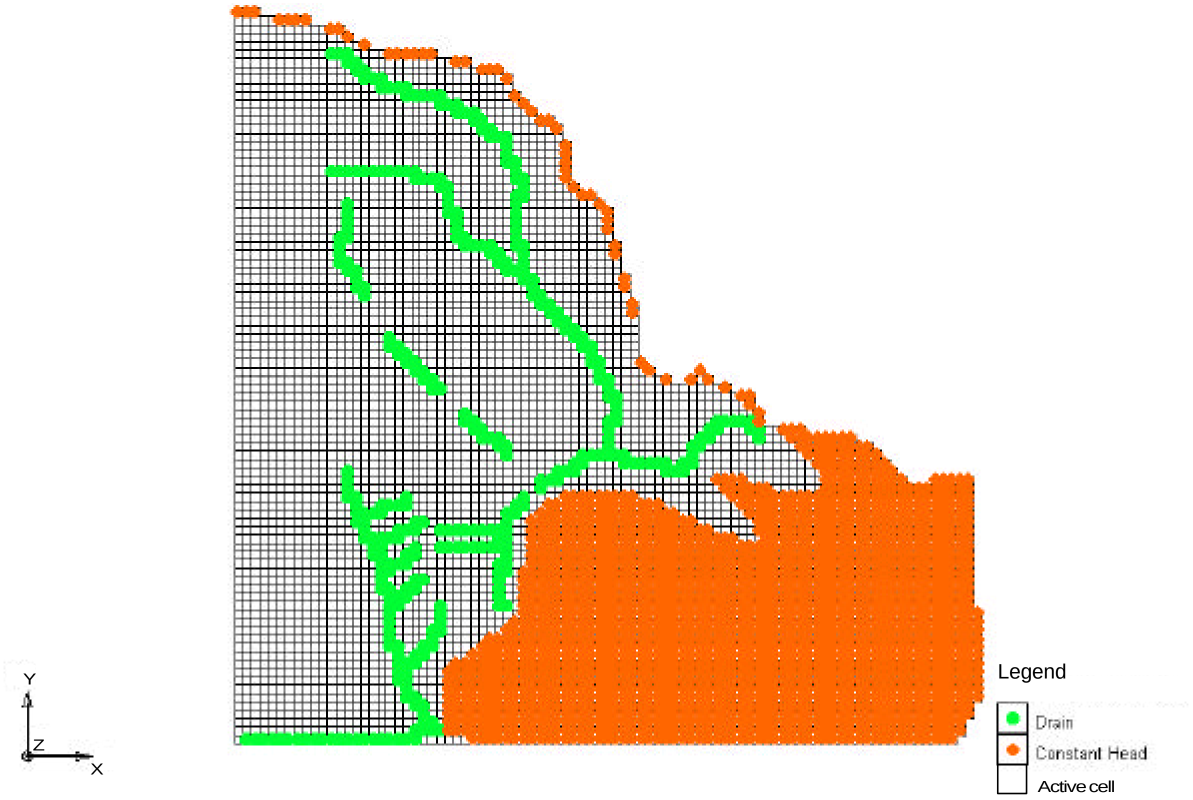


Figure 35: Boundary conditions of the groundwater model in layer 2.

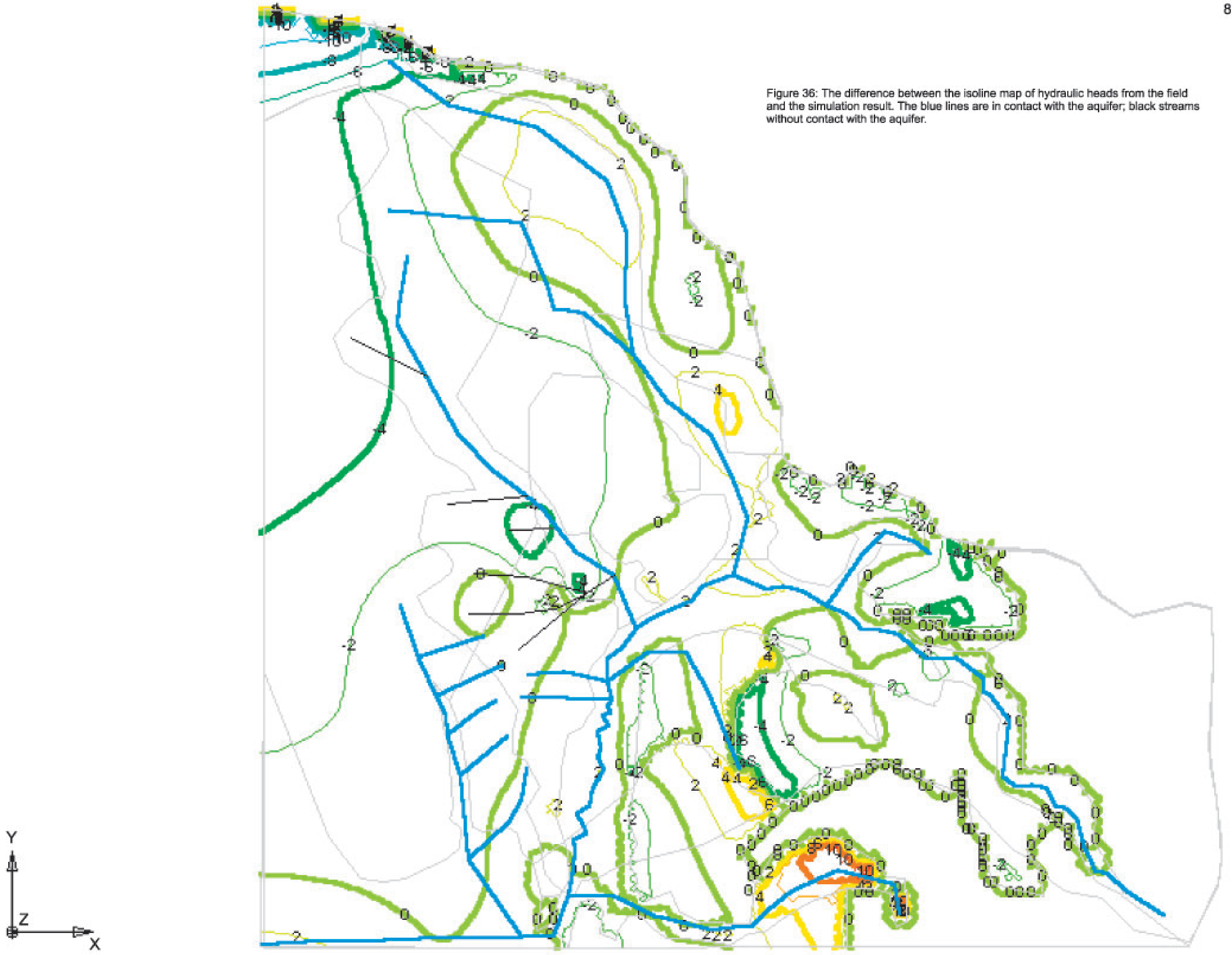


Figure 36: The difference between the isoline map of hydraulic heads from the field and the simulation result. The blue lines are in contact with the aquifer; black streams without contact with the aquifer.

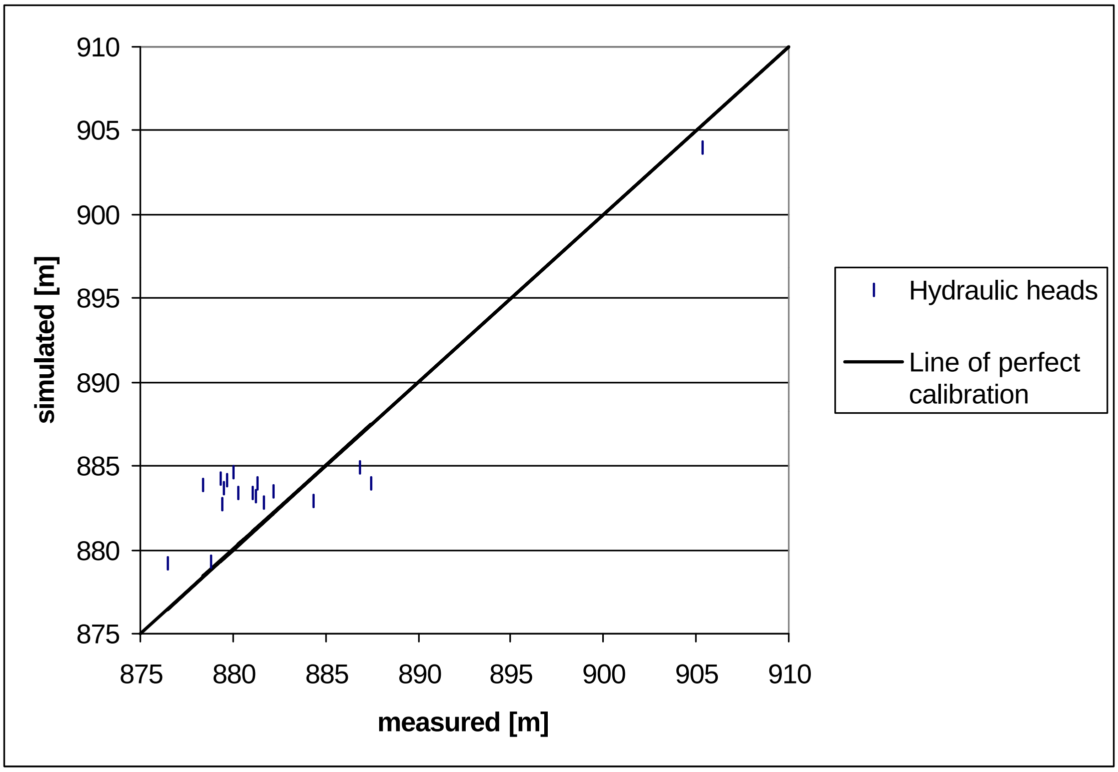


Figure 37: Indication of the quality of the model calibration by plotting measured hydraulic heads versus simulated hydraulic heads.

5.4 Results

The resulting isoline map is a result from an iterative computation of the input namely starting heads (fig. 17), zones with hydraulic properties, recharge and the boundary conditions (specified heads, drains, recharge, etc.). Figures 36 and 37 give an idea of the quality of the calibration. Figure 36 is a map of the difference between the isoline map of hydraulic heads from the field (fig. 17) and the isoline map of hydraulic heads from the simulation result (fig. 38). As figure 37 is a graphical representation of the measured values of wells versus the values of the groundwater flow simulation at the same localities.

The simulation result is a consensus with data of hydraulic heads that had a rather poor quality for the purpose of modelling, the model concept and model stability. Further the physical concept: action gives reaction is also valid for modelling results (making a situation better for a specific zone in the model, makes the situation worse in other zones). Nevertheless, the simulation result is satisfactory because despite the large differences in some parts, it explains the geohydrological system.

Considering the isoline map (fig. 38) it may be expected that the general groundwater flow is towards the West in the lower reach of the Iraí-basin (the isohypse strikes N-S). This is a flow across the Western hydrographic boundary and not through the trunk of the basin that runs North. This was explained in chapter 2 by the shallow bedrock (small through-flow section) and the larger through-flow section through the sediments in the west. Because in the lower reach of the Iraí-basin the groundwater is unconfined this hydraulic regime may have future influences on the geomorphology (possibly the Iraí will flow more to the West).

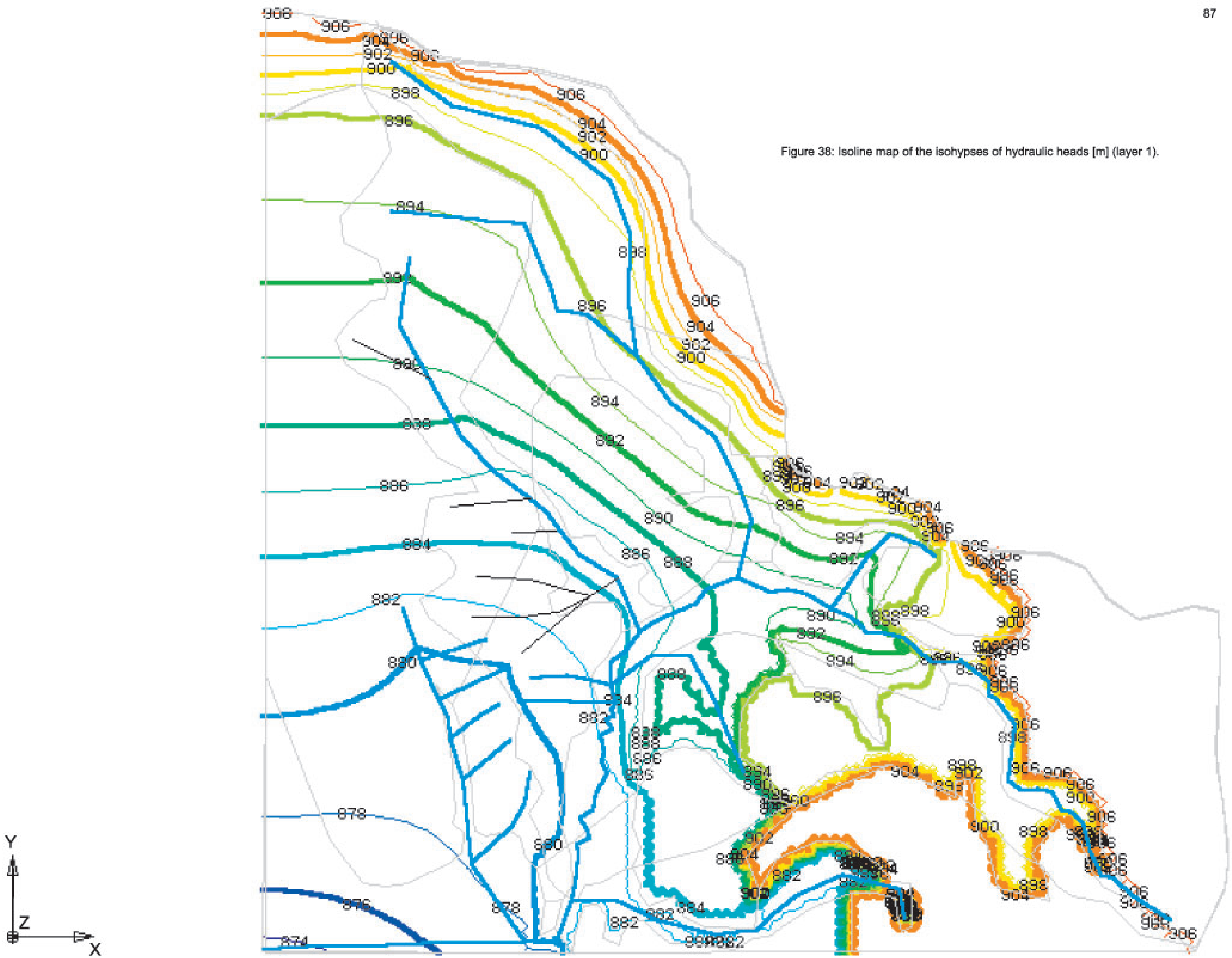


Figure 38: Isoline map of the isohypses of hydraulic heads [m] (layer 1).

Higher up the Iraí-basin at the area of Castelo Branco the flow lines are in a South-western direction (strike isohypses is SE-NW), as higher up at the Western boundary the isohypses strike E-W so that the flow lines are in the Southern direction.

Near the North-eastern boundary the permeabilities/transmissivities are low and the isohypses for hydraulic heads show a large gradient. In the area where the three geophysical sections are, these low k_f/T-data are because of the lithology (borehole 83 m depth to bedrock, soil material mainly consisting of silts/clays with rare gravel bands), as for the more Northern boundary this is probably because of shallow bedrock (low T).

At the boundary of the Eastern bedrock unit inside the hydrographic area the difference of the hydraulic heads between the specified head (bedrock) unit and the variable head (sediment) units is very large. It jumps at a magnitude of about 10 – 15 meters at once (e.g. 905 m to 890 m) so that at this boundary bedrock/sediments the hydraulic gradient is locally very large. This kind of sharp contrast also exists between the Eastern bedrock unit and the protruding bedrock units in the second layer and subsequently between the protruding bedrock layer (fig. 40, unit 14) and the sediments (unit 5).

In the adjacent zones the k_f /T are moderately high for the second layer as well for the upper layer apart from a zone (unit 3, fig. 39) where thick clays were found at the surface.

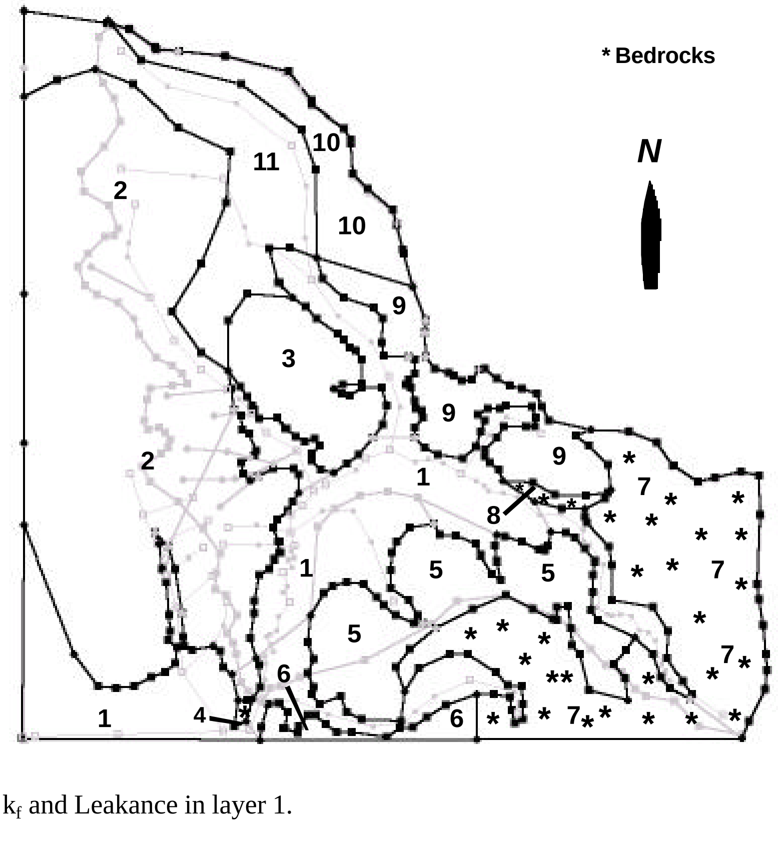


Figure 39: Hydraulic zones of k_f and Leakance in layer 1.

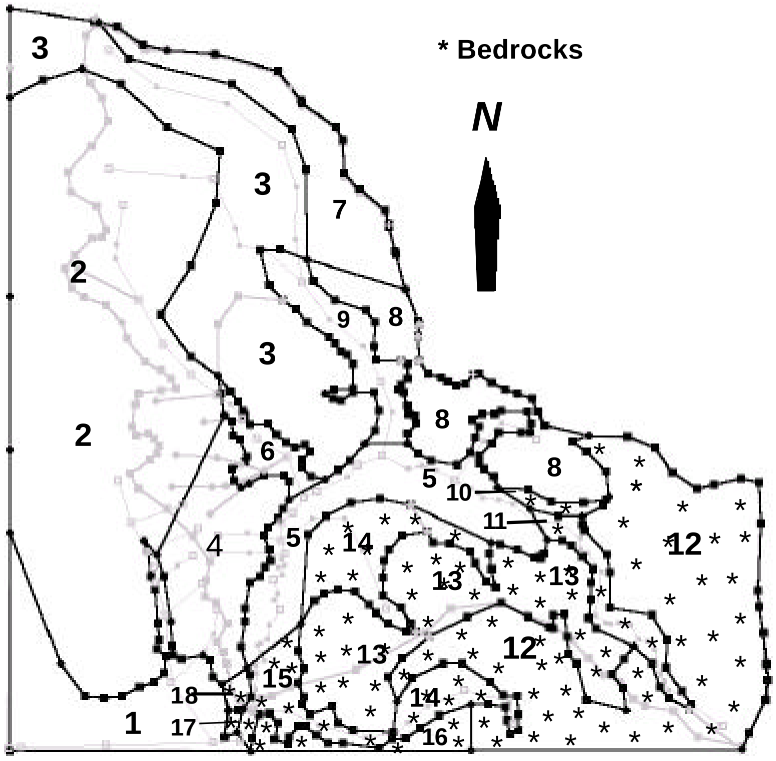


Figure 40: Hydraulic zones of k_f and Leakance in layer 2.

In the upper reach of the "Alluvium" zone (unit 1 in layer 1 of hydraulic zones; fig. 39) the influence of the bedrock specified head units bordering the alluvium and the shallow (boundary unit 14/5 in the 2nd layer of hydraulic zones; fig. 40) rock constant head units are visible in the hydraulic head solution of the model. Large contrasts exist between the constant head of two rock units and between rock zones bordered by a unit with a much higher k_f /T so that the isohypses come together. This is visible for two zones of constant head representing bedrock units that protrude below the alluvium (represented by unit 14, layer 2) and are bordered by zone 5 layer 2 of the hydraulic head zones and the rock zone (unit 8, layer 1) at the surface that protrudes from Serra do Mar towards the West .
Towards the Southwest a clear decrease in the gradient of the hydraulic heads is visible so that a large increase of k_f /T may be expected.
Because of the arrangement of zones with various k_f /T the resulting isohypses show a change of strike at the boundaries of hydraulic zones, which at the same time indicate a change in groundwater flow direction. This phenomenon is attributable to a so called stream line refraction, which principle already has been pointed out in section 3.5.

The streams also have an influence on how the isohypses are curved. The streams (boundary condition drain) have a function as receiving water course (effluent streams). The isohypses are curved towards the streams. Only at the Iraí downstream were it streams near the Western boundary an influent stream regime at the Western stream bank is visible. This is because of the Western hydraulic gradient of the groundwater. As at the Eastern stream bank the regime is effluent. This also assumes a groundwater flow below the stream. When the Iraí-dam is ready an even higher gradient to the West is expected when the reservoir is filled: The water level in the

lake will have a minimum level of 882 m, a medium level of 888 m and a maximum level of 889.60 m. This will result in a higher influent regime for the reservoir at the lower reach of the basin as higher up the basin an effluent regime for the reservoir is expected. The influent regime in the lower reach has on the one hand a positive side that may have a negative side on the other hand. Because of the influent regime a higher recharge in the area of Castelo Branco appears, so that more water could be pumped from the wells. Because this water from the basin is filtered and needs some time to reach the wells a purification of the water appears. This will be necessary because the tributaries Canguiri and Rio Timbo flow through settled areas and raised faecal coliforms and total coliforms were found in the water (also of BOD_5, total nitrogen and phosphorus). This could be a negative point because before the wells are reached by the recharged water bacteria may die (residence time) and the BOD_5, total nitrogen and phosphorus may be mineralised or filtered. On the other hand other unknown species that were not analysed (together with the former mentioned species) may reach the wells. That is why the groundwater regime with the reservoir is tested and also the scenario of possible pollutant transport is carried out by a particle tracking simulation with MODPATH. This will also clear the question if there is a danger of bacterialogical contamination (according to the German Water Quality Protection Standards the particles are not allowed to reach a well within 50 days by advective transport).
The results of the simulation of the groundwater regime after construction of the Iraí-dam are illustrated in figure 41.

In the hydraulic flow model that represents the situation after the construction of the Iraí-dam the natural hydraulic regime has clearly changed to a hydraulic regime influenced by the water level of the reservoir. In the hydraulic model this water level has been put on 888 m, corresponding to the medium level.
At the boundary of the reservoir very sharp gradients exist at the most part of the Eastern side and the lower reach of the reservoir including the dam section.
Above the diagonal running NW-SE from the Canguiri (C in figure 41) the hydraulic regime of the reservoir is effluent and below this diagonal it is influent.
The gradient SW of the Canguiri is higher as before the construction of the Iraí-dam but moderate in comparison to the lower reach of the reservoir.

5.5 Conclusions

The simulation result is satisfactory because despite the large differences in some parts of the area between the simulated and measured heads as visible in the graph giving an indication of the quality of the model calibration and the map illustrating the differences the groundwater flow model explains the geohydrological and hydraulical system.
Summarised the zones with various k_f/T, the streams and the specified head boundary conditions are the main influences on the distribution of the isohypses in the isoline map.
Additionally the influence on recharge/discharge of the aquifer is dependent on the gradient between streams (the reservoir in the future) and the groundwater and the k_f of the lithology.

Considering the isoline map of the calibrated model it may be expected that the general groundwater flow is towards the West in the lower reach of the Iraí-basin.
The streams (boundary condition drain) have a function as receiving water course, except near the Western boundary an influent stream regime at the Western stream bank is visible. As at

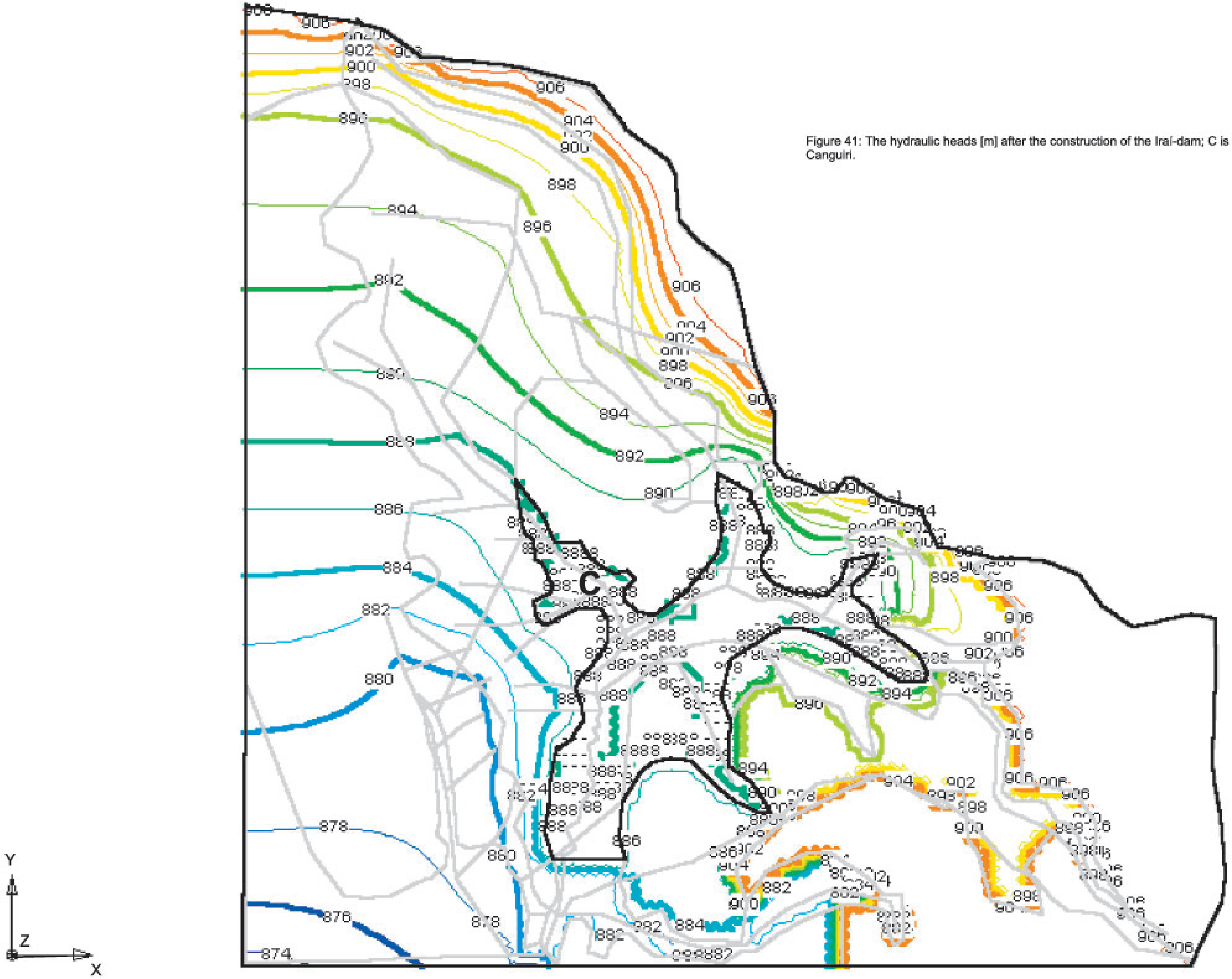


Figure 41: The hydraulic heads [m] after the construction of the Iraí-dam; C is for Canguiri.

the Eastern stream bank the regime is effluent. This also assumes a groundwater flow below the stream.

When the Iraí-dam is ready an even higher hydraulic gradient to the West is expected when the reservoir is filled. This will result in a groundwater recharge West of the above mentioned diagonal.

If the water of the reservoir has been heavily imposed by pollutants this may be negative.

Because this water from the basin is filtered and needs some time to reach the wells a purification of the water appears so that when the surface water has not been to heavily imposed by pollutants this should not be a problem, if the residence time is long enough that the water will be safe for pathogenic bacteria when it reaches the wells. Because raised numbers of faecal coliforms and total coliforms were found in the surface waters.

To test the microbiological safety a MODPATH particle tracking simulation is carried out and is described in chapter 7. To make a general estimation of the vulnerability of the aquifer to pollution, a vulnerability assessment is made which results are described in chapter 6.

The effectiveness of the elimination of other possible pollutants is difficult to follow. Because no advective-dispersive, diffusive, adsorptive modelling and on the same time modelling degradation of matter are carried out.

6 Pollution vulnerability assessment of the Iraí-basin, a comparison of several methods

6.1 Introduction, which methods have been used

With almost 6 million inhabitants is the urban region of the state capital Curitiba, one of the most expanding metropoles of Brazil. With the substantial demographic growth and not always controlled expansion of the urban areas the environment is threatened. Especially the natural resources like drinking water are threatened, from which mainly the surface waters are exploited. With a drinking water deficit it is necessary to quickly develop of the natural resources and protect them like the groundwater.

Protection areas have to be assigned for both surface water as groundwater. The advantage of groundwater is, that there exist barriers that protect the groundwater for most part. As surface waters are directly influenced by their environment. Bacteria may not die before they reach the surface water, organic material may reach the water before it is filtered out and has degraded, heavy metals, phosphates, ammonium, etc. are readily available and not adsorbed by clay, etc.

For outlining protection strategies for groundwater against pollution which are not to be unnecessary restrictive, aquifer pollution vulnerability or the ability of the cover above an aquifer to protect the groundwater (which can be considered an intrinsic characteristic) needs to be mapped and ranked.

Preferably groundwater resources should be used because the subsurface resources are better protected and their potential is not fully used. It may be considered to cover a part of the demand with these resources with groundwater. On the other hand while it could be that the groundwater resources are not sufficiently available in the area of Curitiba that is surrounded and underlain by crystalline rocks there may be no other way then to exploit the surface water as well. But because of the water quality aspects it is preferable where possible that the groundwater resources are exploited.

Because of the urgency and considerations of cost the method to asses the aquifer vulnerability should be simple and readily available for simple data. Although it is more consistent to evaluate vulnerability to pollution by each class of contaminants individually or by each group of polluting activities less refined and more generalised systems of aquifer vulnerability mapping have to be used because of insufficient resources and inadequate data to achieve this ideal. But less refined and more generalised systems of aquifer vulnerability mapping can still be technically valid and of practical use at reconnaissance level (Foster, 1987). In this study 3 often used methods are compared. These methods are the BGR protection ability assessment of the cover of the uppermost aquifer (Eckl, Hahn & Koldehoff (1995), the DRASTIC-vulnerability index (Aller et al, 1987), G.O.D pollution risk assessment (Foster, 1987). All the above mentioned methods generalised aquifer pollution vulnerability systems have to be simplified once more because of the lack of data. Some of these simplifications are always necessary because of some factors there is never enough information (e.g. the dimensions of the aquifer) or because of a complete lack of data (soil map 1 : 600,000, one climate station in the area). In these methods it has also been counted for such simplifications. All these methods were used in a GIS, which was worked out by my college Dipl. Geol. Günter Kus who worked with ArcView.

Another method was used that was designed by Kus (Kus, Wijnen and Udluft, 2000; Kus 2001) and should be seen as an additive method. This method considers the accumulation of debris and contaminant matter by surface runoff in depressions of the land surface. The derivation of so called accumulation zones is done by modelling the drainage system and precipitation catchment areas from which ranked zones of accumulation are derived.

This method is valid everywhere where an important part of the runoff is in the form of surface runoff.
Another method that can be used is with a hydrological model like MODBIL or similar hydrological model that models the (soil) water balance. The zones with a higher groundwater recharge may be seen as the more vulnerable zones.

6.2 The discussion of various methods used

6.2.1 The BGR protection ability assessment of the cover of the uppermost aquifer

This classification is developed by the BGR (Bundesanstalt für Geowissenschaften und Rohstoffen) in the Federal Republic of Germany and estimates the protection ability of the cover of the uppermost aquifer.
The estimation of the protection ability of the cover is subdivided in the soil zone and the subsoil overburden.
At the same time the retention period in the cover may be estimated by this method.

For soil the specific retention (nFK) is the measure for the storability of the water available for the plants in the soil, which has a large influence on the retention period of the water in the soil and because of that also on the evaporation and recharge. The nFK is mainly affected by the grain size, consolidation and humus content of a soil. Under the soil the root zone is understood. Also the infiltration quantity is taken into account.
The retention period in the groundwater overburden below the soil zone depends together with the infiltration rate on the hydraulic characteristics of the rock (loose sediments or solid rock).
The hydraulic characteristics depend on the distribution of voids.
Because of their different hydraulic characteristics loose sediments and solid rocks are assessed according to different criteria.
In this case the overburden of the aquifer only consist of more or less loose sediments or regolith.
The parameters for the protection ability of the soil zone are the specific retention and the infiltration water quantity. The parameter specific retention may be estimated when the soil material is known but not tested in the laboratory from the “Bodenkundliche Kartieranleitung (KA3)” of the AG Bodenkunde (1982), which is a soil mapping guide for the German soil classification.
The rating for the specific retention for the protection ability (factor B) may be taken from table 4. The infiltration quantity may be estimated when available from data of the annual recharge, otherwise from the precipitation minus the potential evaporation (which is equal to the effective precipitation).
The rating for the infiltration quantity (W) may be taken from table 5. In this case the effective precipitation is 712.1 mm/y.

Table 4: The rating for the specific retention

nFk [mm] to 1 m depth	Rating B
> 250	750
> 200 – 250	500
> 140 – 200	250
> 90 – 140	125
> 50 - 90	50
50	10

Table 5: The rating for the infiltration quantity (* instead of groundwater recharge the effective precipitation N-ETPpot may be taken).

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Groundwater recharge [mm/a*]	N-ETPpot [mm/a*]	Faktor W
100		1.75
> 100 – 200	100	1.5
> 200 – 300	> 100 -200	1.25
> 300 – 400	> 200 - 300	1
> 400	> 300 - 400	0.75
	> 400	0.5

The multiplication of the factors B and W give the protection function value of the soil S_1.
The parameters for the protection ability of the subsoil may be subdivided into lithology, thickness of the overburden, infiltration quantity and in two special cases when a perched water table and/or artesian conditions exist. The latter case is non-existent in the survey area and perched water tables are existent but because of lack of data not much is known, so that these parameters are not taken into account. Values for the rating of the lithology may be taken from a table (Eckl, Hahn & Koldehoff , 1995). In this case only one lithology is taken for the overburden for the simple reason that the spatial distribution of the different lithologies (in the loose sediments) not much is known, so that this simplification is necessary. The lithology is simply multiplied with the overburden thickness (depth to groundwater) which is again multiplied by the infiltration quantity (factor W) to get the protection ability of the subsoil groundwater cover.
The thickness of the groundwater overburden has been extracted from the difference of heights between the digital elevation model and the isoline map of hydraulic heads.

The protection ability of the cover over the groundwater S_g is estimated by adding the protection ability of the soil zone S_1 and the protection ability of the subsoil S_2. The grading of the protection ability of the cover S_g and the retention period may be taken from table 6.

Table 6: Classes of the overall protection ability

Overall protection ability	Value of the overall protection ability Sg	Magnitude of the residence time of the infiltrating waters in the overburden
Very high	> 4000	> 25 years
High	> 2000 – 4000	10 - 25 years
Moderate	> 1000 – 2000	3 - 10 years
Low	> 500 – 1000	Several months to ca. 3 years
very low	500	Some days to about 1 year, in karst often less

Because of simplifications the only variables that are used are the nFK and depth to groundwater (which is equal to overburden thickness). The other factors are all constants or

which is the case with the factor perched water table were not taken into account because no data were available. The aquifer was not artesian, so that no additional points were added to the protection ability of the cover.

6.2.2 The DRASTIC-vulnerability index

The Drastic system is a superposition of a relative ranking system on mappable units. Hydrogeologic settings incorporate the major hydrogeologic factors which are used to infer the potential for contaminants to enter groundwater. These factors form the acronym DRASTIC and include depth to groundwater, net recharge, aquifer media, soil media, topography, impact of the vadose zone (i.e. the material in the unsaturated zone, below the soil) and hydraulic conductivity of the aquifer. The relative ranking system uses a combination of weights and ratings to produce a numerical value the DRASTIC Index which helps to prioritise areas with respect to pollution potential.

The weights of the factors taken into account which were developed to express the relative importance of each factor are shown in Table 7. The rating for each factor is to express the impact on pollution potential (Tables 8 and 9 and Aller et al, 1987). For Net recharge a general rating of 9 is taken which is the highest rating for a net recharge > 254 mm, a rating of 8 for the aquifer media

Two different ratings for the Soil Media are taken namely Organic soils with 8 and loam with a factor value of 5. The aquifer medium has become a rating of 8. The values given in the tables vary because their value distribution is computed in a GIS as the other values are assigned directly to the maps that function as a base for the computation of the DRASTIC index.

Table 7: Assigned weights to DRASTIC Features.

Feature	Weight
Depth to Water	5
Net Recharge	4
Aquifer Media	3
Soil Media	2
Topography	1
Impact of Vadose Zone	5
Hydraulic Conductivity of the Aquifer	3

Table 8: Depth to water.

Depth	Rating
0- 1,5 m	10
1,5 – 4,5 m	9
4,5 -9,1 m	7
9,1 – 15,2 m	5
15,2 – 22,9 m	3
22,9 – 30,5 m	2
> 30,5 m	1
* original classification was for depth in feet	

Table 9: Ranges and ratings for topography (percent slope).

Range	Rating
0 - 2	10
2 - 6	9
6 –12	5
12 – 18	3
> 18	1

This system allows the user to determine a numerical value for any hydrogeologic setting by using an additive model. The equation to determine the DRASTIC Index is:

$$D_RD_W + R_RR_W + A_RA_W + S_RS_W + T_RT_W + I_RI_W + C_RC_W = \text{Pollution Potential}$$

Once a DRASTIC Index has been computed, it is possible to identify areas which are more likely to be susceptible to groundwater contamination relative to one another. The higher the DRASTIC-Index, the greater the groundwater pollution potential.

6.2.3 The G.O.D pollution risk assessment

The GOD-system relates primarily to vulnerability of ingress of pollutants to the saturated zone and not to lateral transport within that zone and is based on the identification of:

a. groundwater occurrence (G)
b. overall aquifer class in terms of grade of consolidation and lithological character (O)
c. depth to groundwater table or strike (D)

Table 10: Groundwater occurence.

Aquifer type	Rating
None	0
Artesian confined	0.1
Confined	0.2
semi-confined	0.3
semi-unconfined (covered)	0.5
Unconfined	1

Table 11: Overall aquifer class for loose sediments.

Sediment type	Rating
Residual soils	0.4
Alluvial silts/loess	0.5
Aeolian sands	0.6
Alluvial and fluvio-glacial sands + gravels	0.7
Colluvial gravels	0.8

Table 12: Groundwater depths indexes.

Groundwater depth	Index
> 100 m	0.4
50 – 100 m	0.5
20 –50 m	0.6
10 – 20 m	0.7
5 - 10 m	0.8
2 - 5 m	0.9
< 2 m	1

Table 13: Output aquifer pollution vulnerability.

Vulnerability	Product of the ratings
None	0
Neglectible	0.1
Low	0.1 - 0.3
Moderate	0.3 - 0.5
High	0.5 -0.7
Extreme	0.7 – 1

Each step leads to a ranking on a scale up to unity, the product of which is the final score for aquifer vulnerability in relative, qualitative terms (Table 13).

6.3 The results

The methods of the BGR and the DRASTIC-index both take into account the unsaturated zone (vadose zone), the relief (slope), and the soil media. The difference between the method of the BGR and DRASTIC-index is the description of the impact of the soil medium. The method of the BGR explains better how the rating is obtained namely over the nFK. As the DRASTIC-index gives simply a soil medium a rating. The advantage of the method of the BGR is that when data are available of the nFK that they may be used and otherwise may be estimated with the soil medium in the “Bodenkundliche Kartieranleitung (KA3)” of the AG Bodenkunde (1982). In the flood plain the protection ability as computed by the BGR-method is low as the higher areas have a high protection ability. It is not known exactly if the lower specific retention in the floodplain is has the higher impact, or that the depth to groundwater is decisive. Probably both parameters combined are responsible for the low protection ability of the aquifer. Outside the floodplain the value of the protection ability are according to the contour lines so that the depth to groundwater is here decisive for the distribution of the protection ability.

As a result of this study was the observation that the mathematical linking of the factors of the GOD indexes gave a to low pollution vulnerability. Because the lowest index determines the magnitude of the GOD vulnerability rating, because the indexes are simply multiplied.

According to this index with one aquifer class (sediment type), one class for groundwater occurrence (confined aquifer), the decisive factor was simply the depth to groundwater. So that the values for the pollution vulnerability is simply according to the contour lines.

The method that derives so called accumulation zones by surface runoff (Kus, 2001) is another method that has validity, though this method could be improved when the protection ability of the overburden is also taken into account. This accumulation can take place during heavy rainstorms.

The accumulation takes preferably place in the lower areas on low inclined surfaces.

The higher areas have a very low pollution vulnerability (fig. 45). Actually the severity of the pollution vulnerability increases the further down the relative position in the drainage system is generally.

The hydrological modelling method that is carried out with the MODBIL Water Balance Model is a very reliable method to estimate the pollution vulnerability when the recharge is used as quantification for the pollution vulnerability (fig. 46). Because the result is the outcome of the modelling of physical processes taking into account the quantity of water available due to atmospherical processes, taking into account the retention and interflow/surface runoff of water due to soil physical characteristics of the soil, the unsaturated zone and the slope. But not taking into account depth to groundwater.

Actually in the case of the result of the MODBIL hydrological modelling, the result is much different comparing to all other results. As described in chapter 4 MODBIL may be seen as a detailed meteorological-soil physical modelling system. Because the depth to groundwater is not taken into account the result is so different, but again the flood plain has the highest possible values for recharge (and so the highest pollution vulnerability). But this time also some of the highest areas have the highest values for recharge, probably due to slope, land use and/or because the measured precipitation at the meteorological station at Iapar is corrected with a precipitation factor for the height according to the digital elevation model. The distribution of the pollution vulnerability is for the MODBIL-model actually much more differentiated because this is a real physical model and not a GIS that combines various map layers to a result.

In figure 46 the zones with a high recharge are equivalent to zones with a high pollution vulnerability.

The results are presented in the maps (figs. 42 - 46).

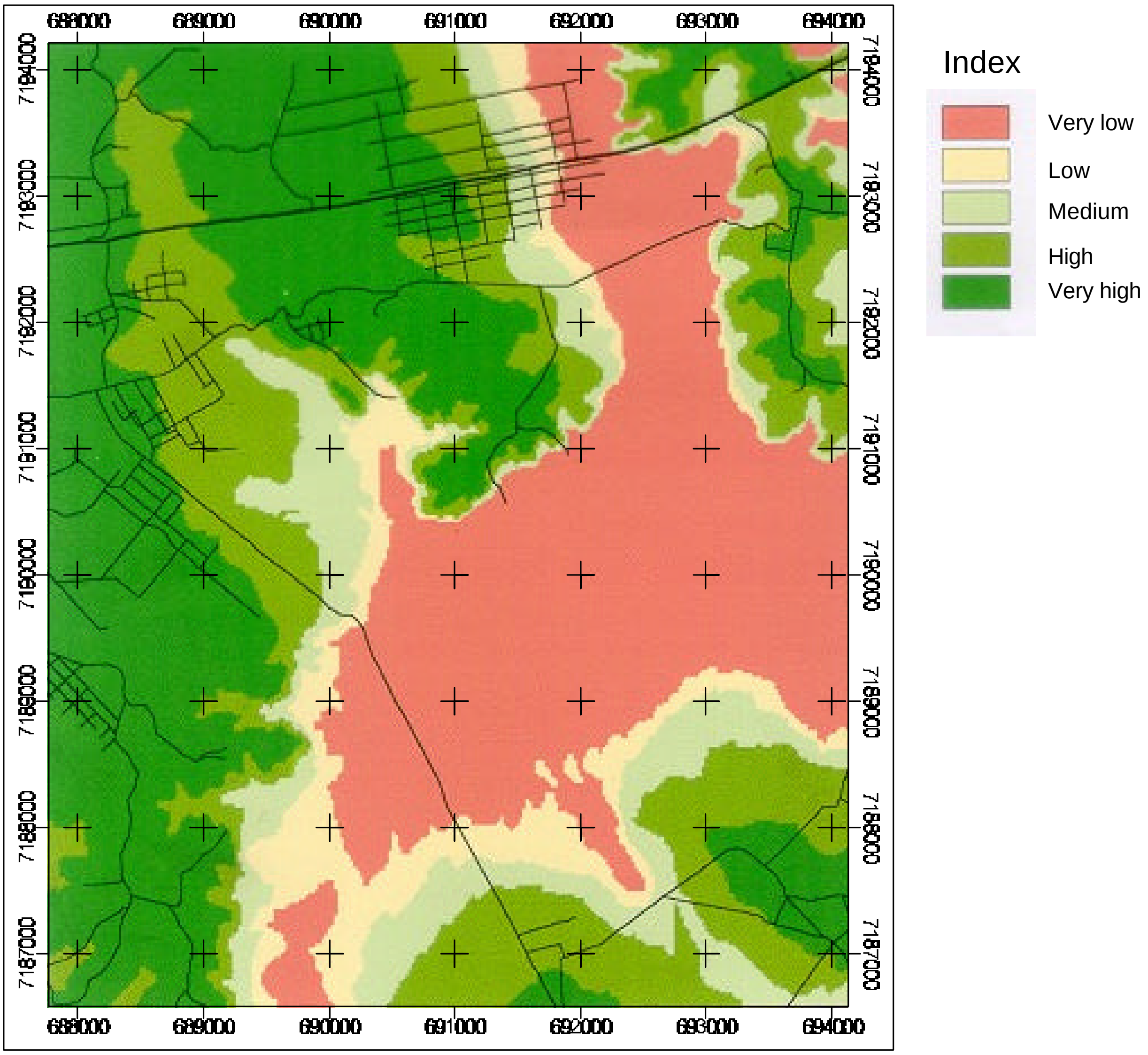

Figure 42: The protection ability of the overburden according to the BGR

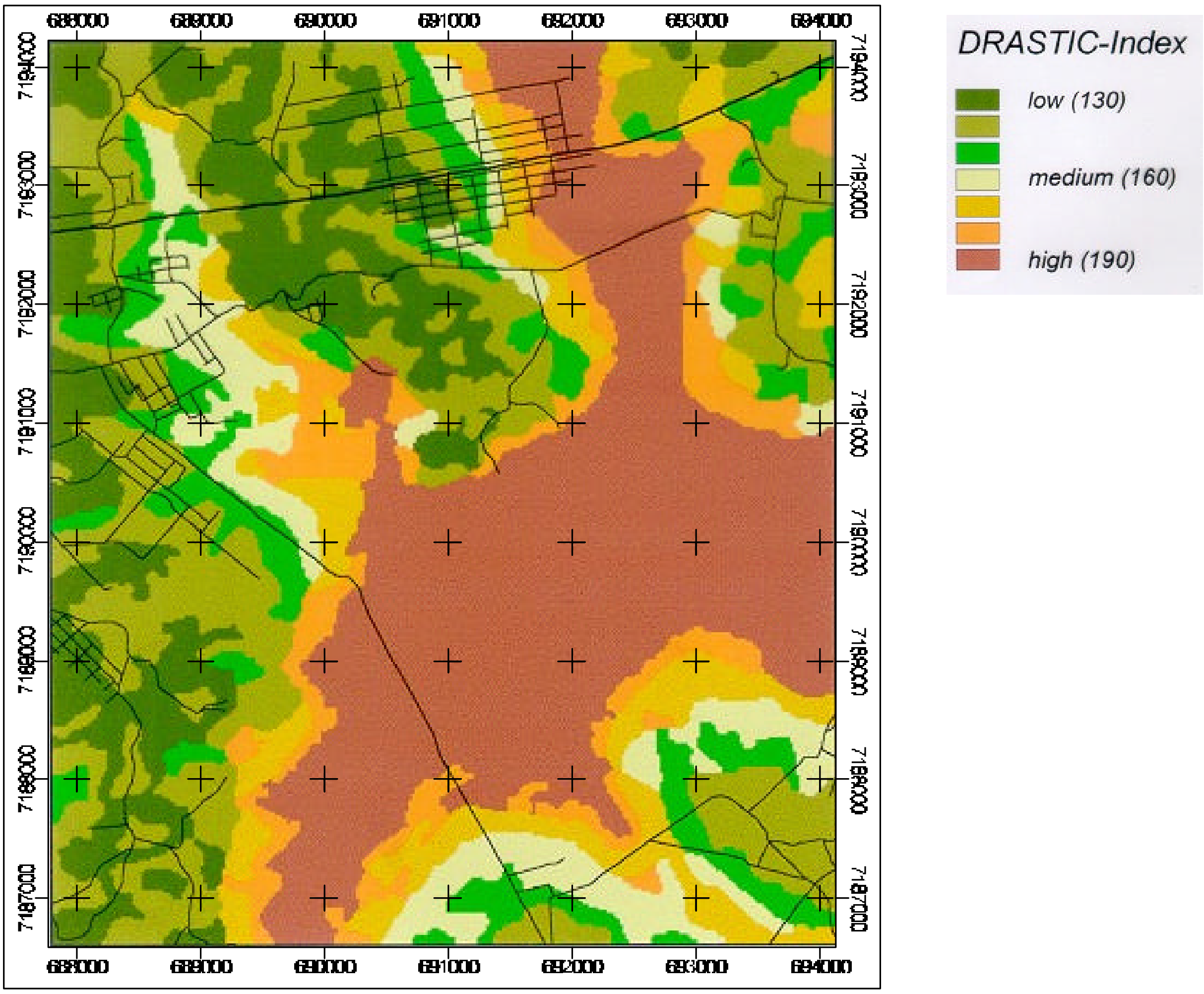

Figure 43: The pollution vulnerability according to the DRASTIC-index

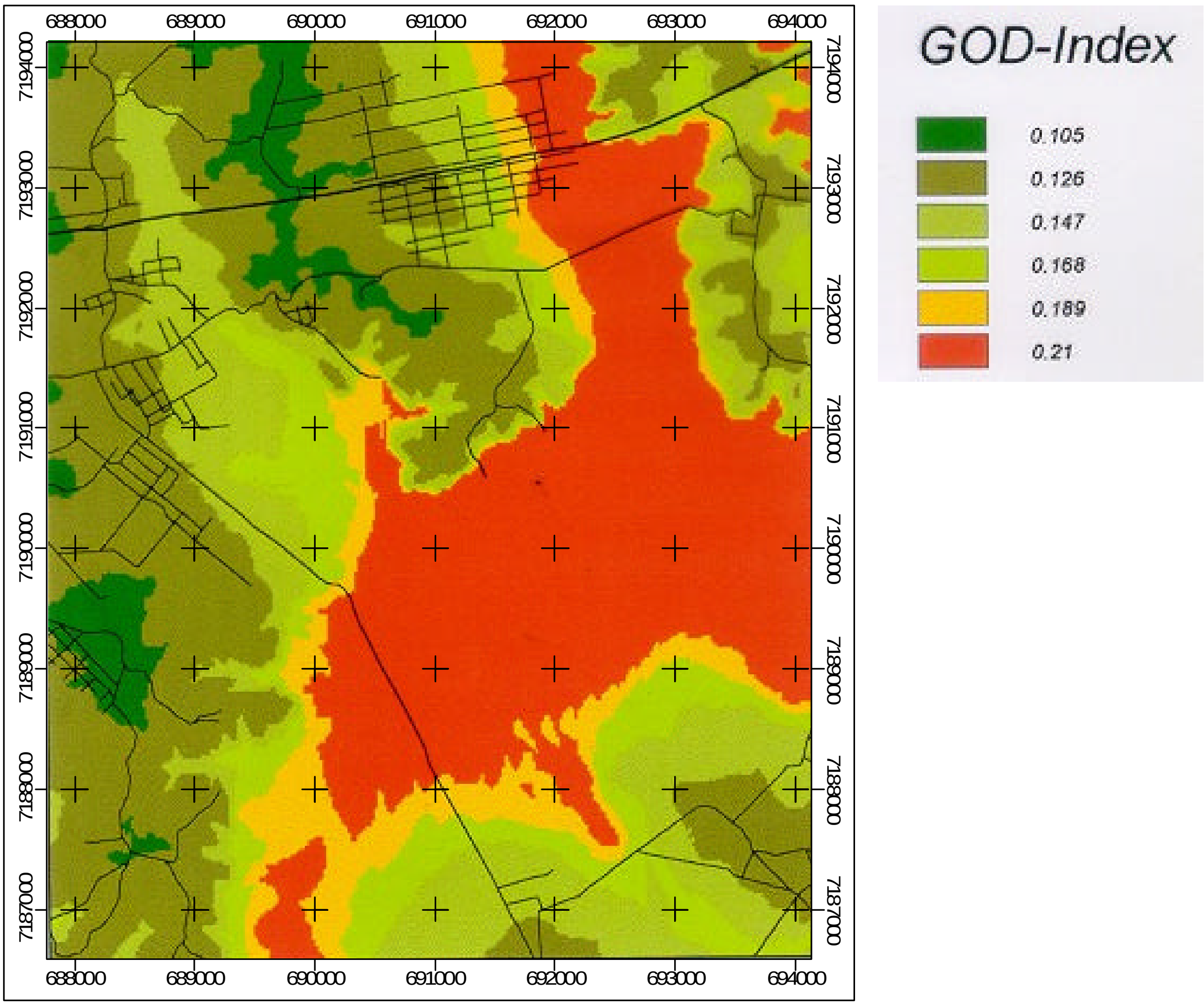

Figure 44: The pollution vulnerability according to the GOD.

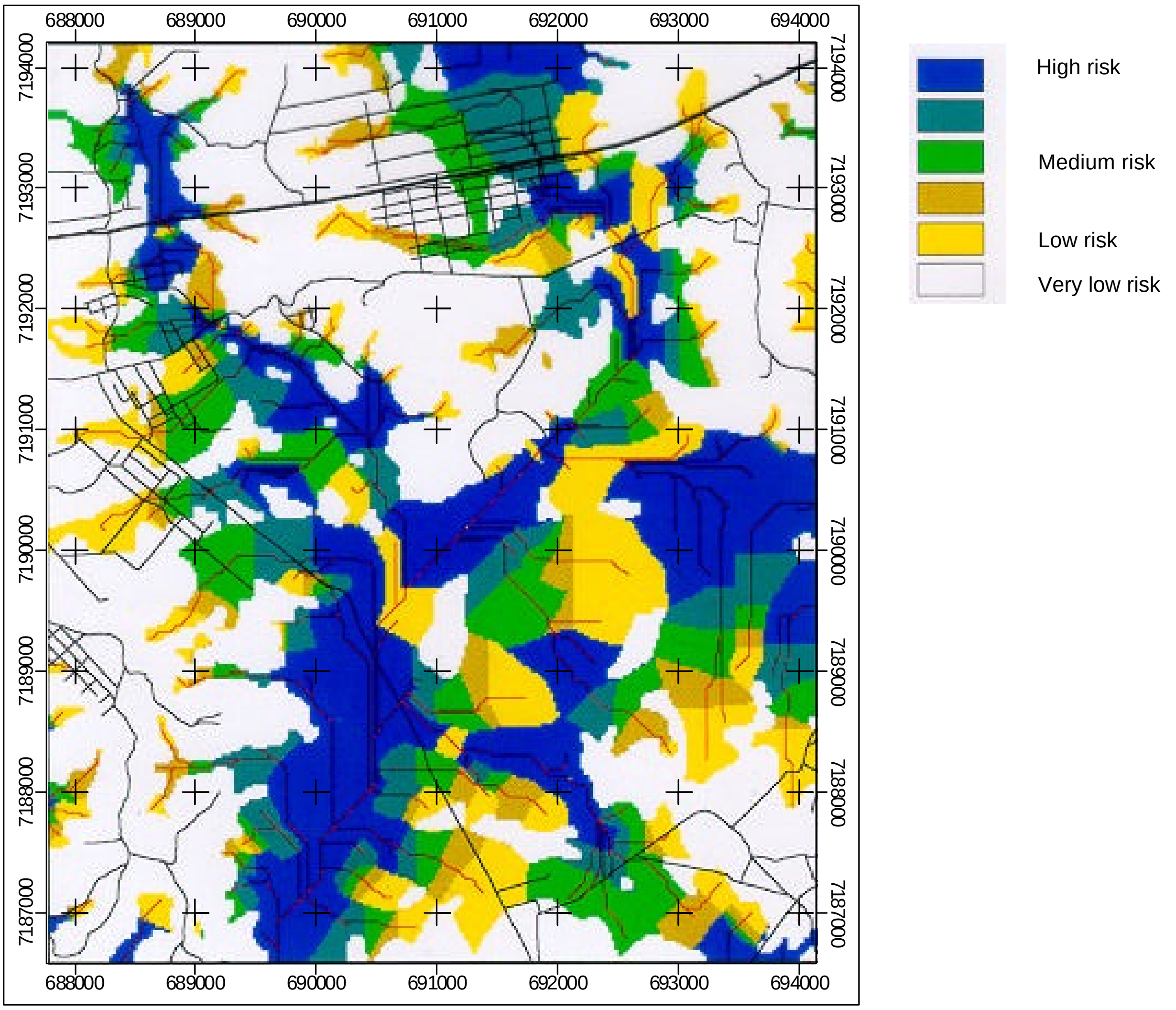

Figure 45: The method to modelling the accumulation zones by Kus (2001).

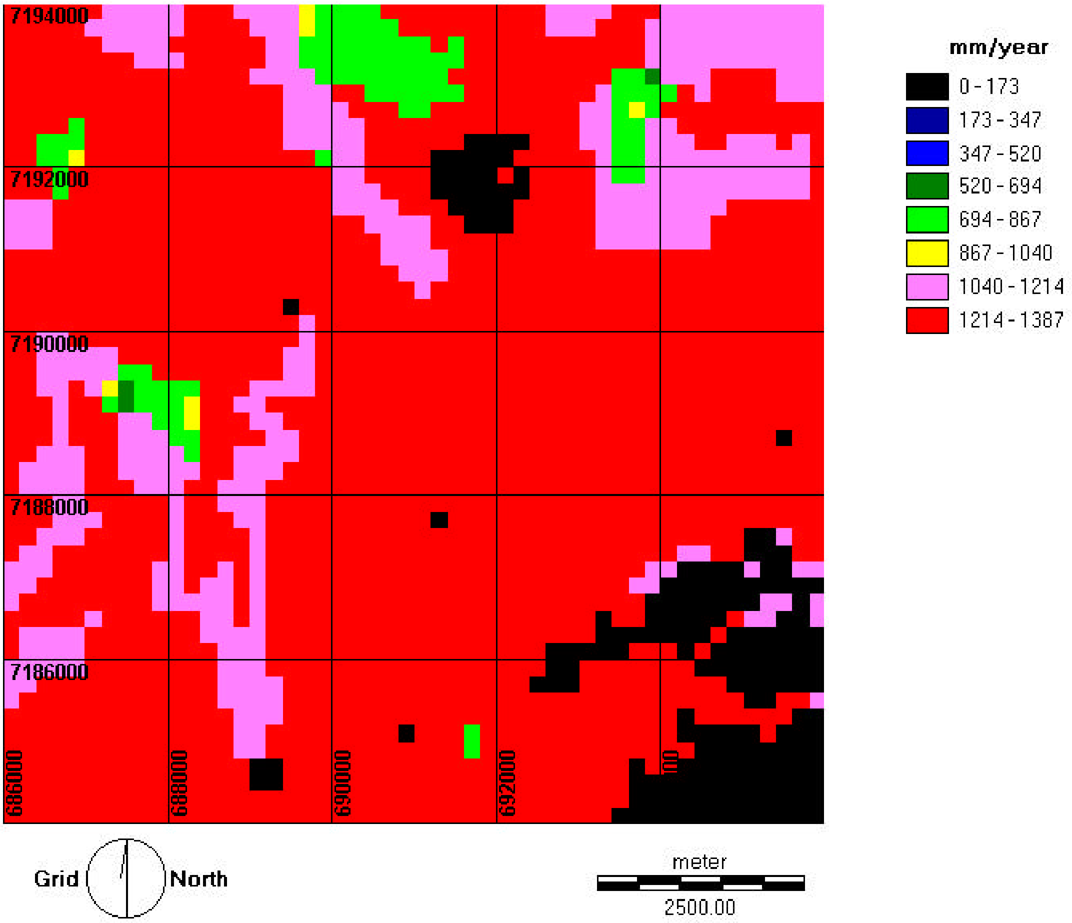

Figure 46: The groundwater recharge computed with MODBIL.

6.4 Conclusions

With all the methods in the area were the reservoir is, a higher vulnerability to pollutants was found. Because it is the area were preferentially accumulation may occur because of low slopes and because of the lower topography, together with the higher permeability of the soils.
None of the methods used, does take all aspects into account.
The G.O.D. uses the less parameters, from which overall aquifer class (O) and groundwater occurrence (confined aquifer) (G) are simply constants, the decisive factor is simply the depth to groundwater (D).
The G.O.D has on the same time a limited suitability because of the mathematical linking of the factors, the drawback of the DRASTIC is that the soil rating is not based on quantitative properties and though it takes the slope inclination into account it does not take into account if the unit lies low or high.
As the method of the BGR needs quantitative properties for the soil, but for the topography it does not take into account were the unit is positioned. The method that derives accumulation

zones is very limited because it only takes the topography into account. The main advantage of the BGR-method is that the residence time in the unsaturated zone until the water reaches the groundwater may be estimated.

Determining the recharge with a hydrological model like MODBIL has the advantage that vulnerability (in the form of the recharge magnitude) physical and quantitative parameters are used. MODBIL also takes into account the slope. The distribution of the pollution vulnerability is for the MODBIL-model actually much more differentiated than for the GIS-based methods because this is a real physical model and does not combine various map layers to a result like a GIS.

The drawbacks of MODBIL are that it does not take into account were the modelled units are topographically positioned and no depth to groundwater is taken into account.

7 The Particle Tracking Model

7.1 Introduction

The tributaries Canguiri and Rio Timbo to the Iraí-reservoir flow through settled areas and raised numbers of faecal coliforms and total coliforms were found in the water (also of BOD_5, total nitrogen and phosphorus). On the same time the hydrological modelling with MODBIL and all other groundwater pollution vulnerability methods used, showed that the groundwater below the floodplain that will be flooded by the reservoir has a high vulnerability to pollution.

That is why a scenario of possible pollutant transport is carried out by a particle tracking simulation with MODPATH for the flow regime that resulted from the calibrated groundwater flow model and that together with the reservoir (Chapter 5).

After the groundwater flow simulation is executed with the calibrated MODFLOW model and the additional reservoir layer, the MODPATH particle tracking simulation is carried out.

The particle tracking modelling is carried out for the period before the existence of the reservoir and after its construction, to make a comparison. This is also done to get an idea how the change of hydraulic gradient accelerates the advective transport of the modelled particles.

Particle tracking is used to trace out flow paths, or pathlines, by tracking the movement of infinitely small imaginary particles placed in the flow field.

Particle tracking is used in two ways: to help to visualise the flow field and to track contaminant particles. In this study its purpose is mainly to track the movement of possible contaminant particles from the Iraí-reservoir and then especially how much time is needed to reach the wells at Iapar.

This residence time is interesting to evaluate if the wells are microbiologically safe. For this residence time a travelling of at least 50 days is needed, according to the German Water Quality Protection Standards.

When this is satisfied and the pathlines cross the well area, it is still necessary to monitor the water quality of the wells additionally to the normally analysed quality parameters on contaminants.

The particle tracking simulation has been carried out for the situation before and after the construction of the dam to compare the different routings and residence times of the particles.

Because of the higher hydraulic gradients the movement of the particles will probably be faster and because the distance of the Iraí-river to the wells is generally larger than the distance of the lake to the wells, the particles have an additional advantage in the situation after the construction of the Iraí-dam.

Though the water of the reservoir is clearly anthropogenetically influenced (periodic high number of faecal coli cells in the tributaries of the Iraí-reservoir), the pessimistic scenario that high concentrations of contaminant matter will reach the wells will probably not occur because of dilution, mineralisation in the reservoir and purifying efficacy of the soils and aquifer. With the available data it is only possible to construct scenarios in this matter and hoping that nature purifies the water from possible contaminants. Further with the groundwater flow model only the advective term of the transport formula is known. The dispersive, diffusive, retardation and decay terms of the transport formula are not known.

Because in the aquifer retardation probably has a neglectable impact (assuming a perfect tracer) on the transport velocity of the matter in water, the velocity in the aquifer is higher than modelled with MODPATH. On the other hand the resistance to infiltration of the

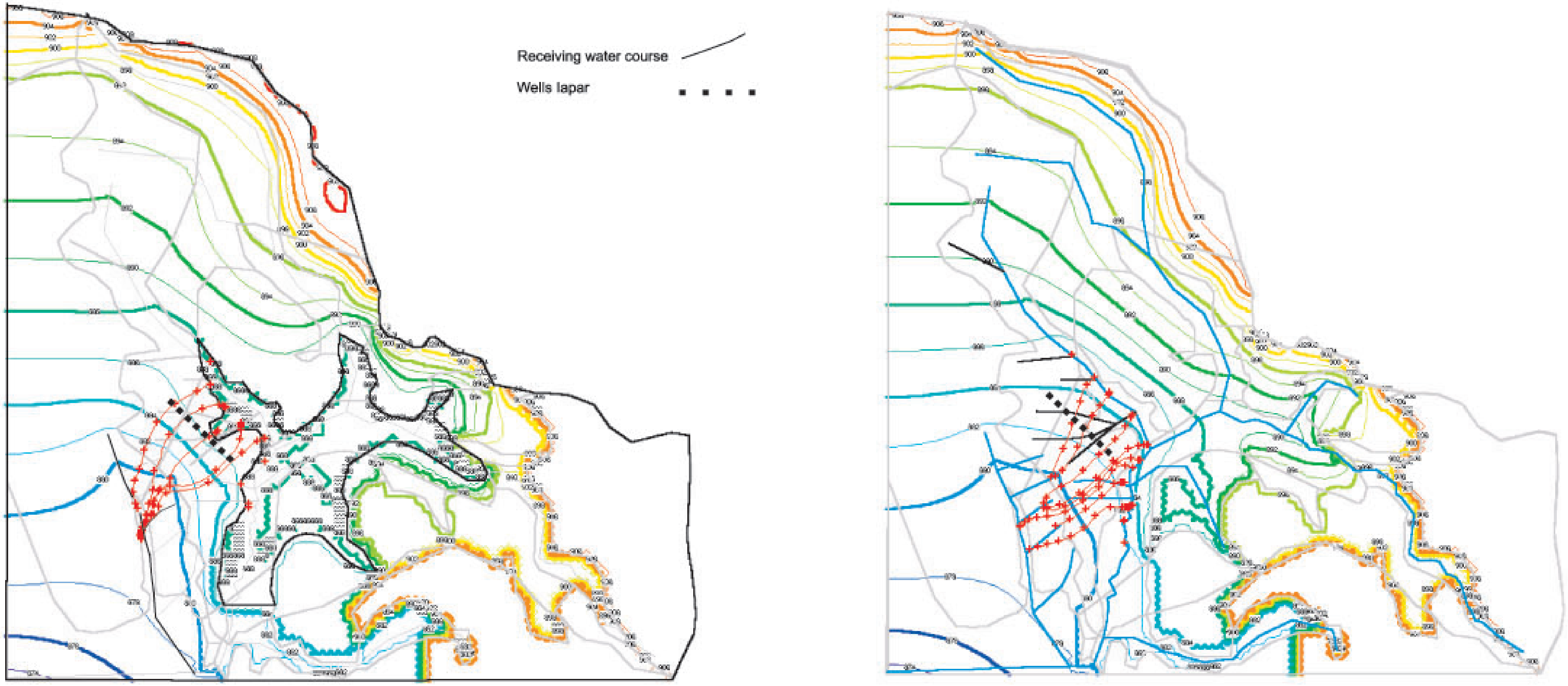

Figure 47: Particle tracking models from the Iraí-basin before (right) and after (left) the construction of the Iraí-reservoir, the red points illustrate the 200 days interval of the particle positions.

reservoir water may compensate the lacking dispersivity term in the advective transport formula. If the water is suitable for the replenishment of the water in the aquifer due to bank storage the water quality of the reservoir water is decisive. If the wells are affected in a negative way or not also depends on the purifying efficacy of the soils and the aquifers.

7.2 Results and conclusions

Generally the tracked particles move to the west over the boundary of the hydrographic basin, which was to be expected taking the hydraulic gradient into account. Both in the situation before and after the construction of the Iraí-dam the particles were unable to cross a stream that clearly acted like a receiving water course (fig. 47) in the adjacent Western catchment area. Actually most particles are already caught by the tributaries of this stream in the adjacent catchment area. In the situation after the construction of the dam only one tributary of the receiving water course is involved as in the situation before the construction three tributaries of the receiving water course are involved.

This is actually because of the changed hydraulic gradient and is mere chance. Because of the higher gradients in the situation after the dam construction the particles meet with the receiving water more upstream as the particles would have reached the receiving water course before the construction. Also the streamlines are closer to each other and are more concentrated after the construction of the reservoir, because of the higher gradient towards the trough of hydraulic gradient following the stream in the next catchment area (only reach a single tributary of the receiving water course). The closer spacing of the stream lines actually means that more water is flowing through the aquifer after the construction of the reservoir.

The particles need much more time to move from the reservoir towards the wells as the prescribed 50 days, this is also valid for the situation before the construction of the dam. The time needed to reach the wells before the reservoir existed was about 600 days and afterwards about 400 days which is in both situations at least 8 times the prescribed 50 days.

This means that the risk of contamination by pathogene bacteria is neglectable.

As was expected the particles move faster in the situation after the dam construction, as was to be expected because of the higher hydraulic gradient.

The hydraulic gradient both in the situation before and after the existence of the reservoir makes that the tracked particles move to the west over the boundary of the hydrographic basin. Both in the situation before and after the construction of the Iraí-dam the particles were unable to cross a stream that clearly acted like a receiving water course.

Because of the higher gradients in the situation after the dam construction the particles meet with the receiving water more upstream as the particles would have reached the receiving water course before the construction. Also the streamlines are closer to each other and are more concentrated, because of the higher gradient towards the trough of hydraulic gradient following the stream in the next catchment area. The streamlines that are lying closer to each other also mean that the quantity of water flowing through the aquifer has increased. Because the particles in both situations reach the wells after much more than 50 days, the risk of contamination by pathogene bacteria is neglectable.

As was expected the particles move faster in the situation after the dam construction because of the higher hydraulic gradients. Because the distance of the Iraí-river to the wells is generally larger than the distance of the lake to the wells the particles have an additional advantage in the situation after the construction of the Iraí-dam.

Because of the higher hydraulic gradient the particles move not only faster but move closer next to each other and are more concentrated towards one point (the trough of hydraulic heads positioned were the receiving water course is).

Though it is certain that the 50 days prescription of the minimum residence time is satisfied the pathlines cross the area of the wells. It would therefore be wise to monitor the water of the wells additionally to the normally analysed quality parameters on contaminants for at least some period of time that the reservoir is in function. This period of time should at least be 2 years because the tracked particles reach the wells starting from the reservoir in about 400 days.

This monitoring could on the same time have the purpose to test the influences of the agricultural land use at Iapar (e.g. higher values of herbicides, pesticides etc.).

To get an idea of contaminants that are contained by the reservoir water it should be sampled and analysed. Because when the nature of the pollutant matter in the reservoir is known it is known for what kind of pollutants should be monitored at the wells. On the same time an improved transport model could be constructed when species are found with known retardation, dispersive etc. properties.

The water of the reservoir is clearly anthropogenetically influenced, the pessimistic scenario that high concentrations of contaminant matter will reach the wells will probably not occur because of the dilution. The water quality of the reservoir water is decisive on the impact on the aquifer together with the purifying efficacy of the soils and the aquifers.

The transport of matter may be much faster in the aquifer than modelled by the particle tracking model when the dispersive term (assuming a perfect tracer) of the transport formula is also taken into account. On the other side the resistance to infiltration of the reservoir water may compensate for this lack.

8 Summery and Conclusions

In 1500 as Pedro Alvares Cabral was on the search for India across the Atlantic but discovered Brazil. At this time he could not have foreseen the tremendous social problems Brazil is coping nowadays.
The tremendous social problems that are in the first place because of the very unequal division of the natural wealth of the country. The very unequal division of the natural wealth of the country has its direct impact throughout the society of Brazil.
The development of the larger cities is one of tremendous uncontrolled growth because people fleeing unemployment, from whom most of them came from the country hoping to find employment.
The city of Curitiba and its direct vicinity (Metropolitan Region of Curitiba) with about 5.2 million inhabitants experiences the same kind of developments like most other larger cities in Brazil.
The study area is actually in the direct vicinity of the urban region around Curitiba and is the Iraí-basin Northeast of Curitiba. The Iraí-basin is a sub-basin of the structural Curitiba-basin that again belongs to the Iguaçu river basin.

The explosive expansion of the population raised a high increase in the demand for water resources and the uncontrolled settlement poses a large problem for the environment.
The possible founding of illegal settlements in the direct vicinity of Iraí-reservoir which is constructed in this catchment area to meet the demand for drinking water endangers the water quality of the reservoir. Additionally it will most probably be polluted by the tributaries of the Iraí-reservoir which flow through populated areas. The possibly polluted surface water from the reservoir may possibly pollute the groundwater which is exploited in the near vicinity of the reservoir (at Iapar). On the other hand the water level of the reservoir is higher than the Iraí-river so that a positive impact may be an extra replenishment by bank storage provided the contamination of the reservoir is not to serious so that the purifying efficacy of the cover of the aquifer and the surface water will suffice.
From this background a modelling study was carried out to estimate the possible impact of the surface water on the groundwater quality near the wells.

The particular problem that was used for the modelling problem consisted of various aspects from various disciplines.
In the first place the geology/geomorphology was needed to dimension the modelled volume, climatology/meteorology together with soil physical parameter to study and model the water balance. Soil sciences were also needed to understand some of the water quality aspects, that was important for the positioning of wells as well for their technical construction details.
For the reservoir that acts as a source for replenishment by bank storage for nearby wells the possible stresses on the quality of the reservoir water has to be studied. This introduces several other aspects like the possible causes of surface water quality like sanitation and several other considerations that have to be made on the water quality because of the lack of data. Considerations about the use of the water resources and the fact that the water provision of the city of Curitiba lags behind the demand, the necessity to exploit new water resources in the form of surface water or ground water, what for benefits have surface water and which benefits have groundwater resources or what disadvantages.
The advantage for the use of groundwater resources is the better natural protection against pollution. But a disadvantage may be the possible scarcity of these resources because the region

of Curitiba is dominated by cristalline rocks as for surface waters this scarcity is definitely not existent.
The analyses of the waters of the tributaries of the at that moment future reservoir, showed major anthropogenic influences, but the parameters tested were very limited.

From the water balance the term recharge is important to estimate the maximal responsible extraction by wells from the groundwater resources in the catchment area and is at the same time an important boundary condition for the groundwater flow model. The mean of the recharge water balance is computed with precipitation, evaporation and river discharge data. As a comparison the water balance was computed with MODBIL. MODBIL is a detailed meteorological-soil physical modelling system that computes the precipitation, Haude (potential) –and effective evapotranspiration, interflow and groundwater recharge.
The distribution of the groundwater recharge magnitude is in the first instance independent of the precipitation which has a positive correlation with the height. In the areas with very low permeabilities and high field capacities the effective evaporation is low, the interflow is high and probably a very high surface runoff appears.
Where the settled areas are the potential evapotranspiration is relatively high, with high effective evapotranspiration as surrounding areas having the same soil physical parameters. So that they have a relatively low groundwater recharge.
No real differences between areas with grasslands and farmlands are visible between effective precipitation, effective evapotranspiration, interflow/surface runoff and groundwater recharge. The influence of the soil physical parameters, together with evapotranspiration and the interflow/surface runoff determine that in the higher agricultural areas groundwater recharge is moderately high as in the basin (grasslands in more or less swampy areas) the groundwater recharge is at its highest. A drawback of the MODBIL hydrological model is that the depth of the groundwater table is not accounted for and because of that much of the computed recharge in the basin may be surface runoff while the soil is already saturated. As an additional drawback of MODBIL is that no interaction between cells in the model exist. The surface runoff could be much less when this would be allowed to stream to adjacent cells.
Despite the limitations that no interaction between cells exist and the depth of the groundwater table is not accounted for, in the overall MODBIL is a powerful tool to estimate the magnitude of components of the water balance. Because of the non-existence of the interaction between cells the groundwater recharge may be seen as the quantity that will at least infiltrate.

For the modelling hydraulical data are needed. How are these parameters tested, what is the quantity of water that is available in a period of time (e.g. a year), what is known about the groundwater quality or what is possibly threatened by human ?
All those aspects connected are needed for a modelling study in the first place. Another aspect is has a groundwater modelling study an added value and what goal(s) does one want to achieve with such a study ?
The result of this modelling study is a hydraulic model and based on that a particle tracking model.

From the grid data interpolated in SURFER and layers constructed in the Map Module of GMS containing the hydraulic properties and boundary conditions were assigned to the 3D-grid of the MODFLOW model so that a simulation may be executed.
After constructing the simulation model, MODFLOW has been ran to see how the model input behaves. Is it stable in other words does the model converse ? Does it correspond more or less to the real live situation ?

To approximate the real live situation as close as possible constructing the conceptual model all available information was used. For the shaping of the hydrogeological model the following information was used the geologic map and observations in the field, well and geotechnical data and information from geoelectrical lines for the water exploration. To construct the isoline map of hydraulic heads the static levels of the wells were used. The isoline map again was used to discriminate between zones of higher and lower conductivity using the varying distances between the isolines.

To approximate the change of permeability the principle of refraction of stream lines is used, which are assumed perpendicular to the isolines of hydraulic heads. Together with the boundary conditions recharge, specific heads for the South-eastern boundary, bedrock units and streams this information was used to construct the conceptual model. Some of the information especially the boundary condition specific heads are for some part based on assumptions.

The following step is the calibration step that consists of making the simulated hydraulic heads fit to the real live situation as good as possible (inverse modelling) and so to get information on uncertain parameters at the same time. Another preliminary is that the model should always be stable. Without a stable model it is impossible to tell if it represents the real situation in the first place !

Having the calibration done as good as possible the groundwater model has the following characteristics that are valid for the situation before the existence of the reservoir as after its construction:

The zones with various k_f /T, the streams (after the dam construction the reservoir) and the specified head boundary conditions have the main influence on the hydraulic regime.

Sharp contrasts exist between specified head units and variable head units and between adjacent specified head units with different fixed heads normally representing bedrock units.

The general hydraulic gradient indicates that the groundwater flow is towards the West in the lower reach of the Iraí-basin.

The streams (boundary condition drain) have a function as receiving water course, except near the Western boundary an influent stream regime at the Western stream bank is visible. As at the Eastern stream bank the regime is effluent. This also assumes a groundwater flow below the stream.

After the construction of the Iraí-dam the hydraulic gradient has increased, because the water level in the reservoir is higher than the hydraulic gradient that existed before its construction. The reservoir introduces at the same time a very sharp contrast between the hydraulic heads and the level of the lake, at its Western side so that immediately at the bank of the reservoir a very high gradient exists.

The next step in the groundwater modelling is to construct a particle tracking model with MODPATH, but first an approximation is made of the pollution vulnerability of the aquifer by various methods.

With a drinking water deficit for the water provision of the city of Curitiba it is necessary to quickly develop more (and eventually other resources, like the groundwater) of the natural resources and protect them. For outlining protection strategies for groundwater against pollution which are not to be unnecessary restrictive, aquifer pollution vulnerability or the ability of the cover above an aquifer to protect the groundwater (which can be considered an intrinsic characteristic) has been mapped and ranked. Also the necessity to make a particle tracking model may be tested. Is the aquifer below area covered by the reservoir vulnerable to pollution ?

The method of the BGR explains better how the rating is obtained namely over the nFK, as the DRASTIC-index gives simply a soil medium a rating. The advantage of the method of the BGR is that when data are available of the nFK that they may be used and otherwise may be estimated with the soil medium in the "Bodenkundliche Kartieranleitung".

For the water balance raster maps of the various components of this balance were made with MODBIL, for which the zoning of the recharge could be used to estimate the vulnerability of the aquifer.

With all the methods to estimate the vulnerability, in the area were the reservoir is a higher vulnerability to pollutants was found. Because it is the area were preferentially accumulation may occur because of low slopes and because of the lower topography, together with the higher permeability of the soils.

The groundwater flow field computed by simulation of the hydraulic flow model is used by the particle tracking algorithm of MODPATH. A MODPATH simulation is carried out because two tributary streams of the Iraí-reservoir are polluted by flowing through populated areas and the hydraulic gradient towards the aquifer in which the wells at Iapar have been constructed increased. So that probably the transport velocity of the groundwater increased and possibly the direction of the streamlines has changed. The time that the reservoir water can reach the wells should be taken into account because of a possible bacteriological contamination and a change of flow direction will influence other parts of the aquifer.

The hydraulic gradient both in the situation before and after the existence of the reservoir makes that the particles move to the west over the boundary of the hydrographic basin with the particle tracking simulation. Both in the situation before and after the construction of the Iraí-dam the particles were unable to cross a stream that clearly acted like a receiving water course.

Because of the higher gradients in the situation after the dam construction the particles meet with the receiving water more upstream as the particles would have reached the receiving water course before the construction. The higher hydraulic gradient is the cause that the flow lines are lying closer to each other indicating that more water flows through the aquifer after the construction of the Iraí-dam. Because the particles in both situations reach the wells after much more than 50 days, the risk of contamination by pathogene bacteria is neglectable.

As was expected the particles move faster in the situation after the dam construction because of the higher hydraulic gradients.

Because the pathlines cross the area of the wells, it would be wise to monitor the water of the wells additionally to the normally analysed quality parameters on contaminants for at least some period of time that the reservoir is in function. This period of time should be at least 2 years because the tracked particles reach the wells starting from the reservoir in about 400 days.

This monitoring could on the same time have the purpose to test the influences of the agricultural land use at Iapar (e.g. higher values of herbicides, pesticides etc.).

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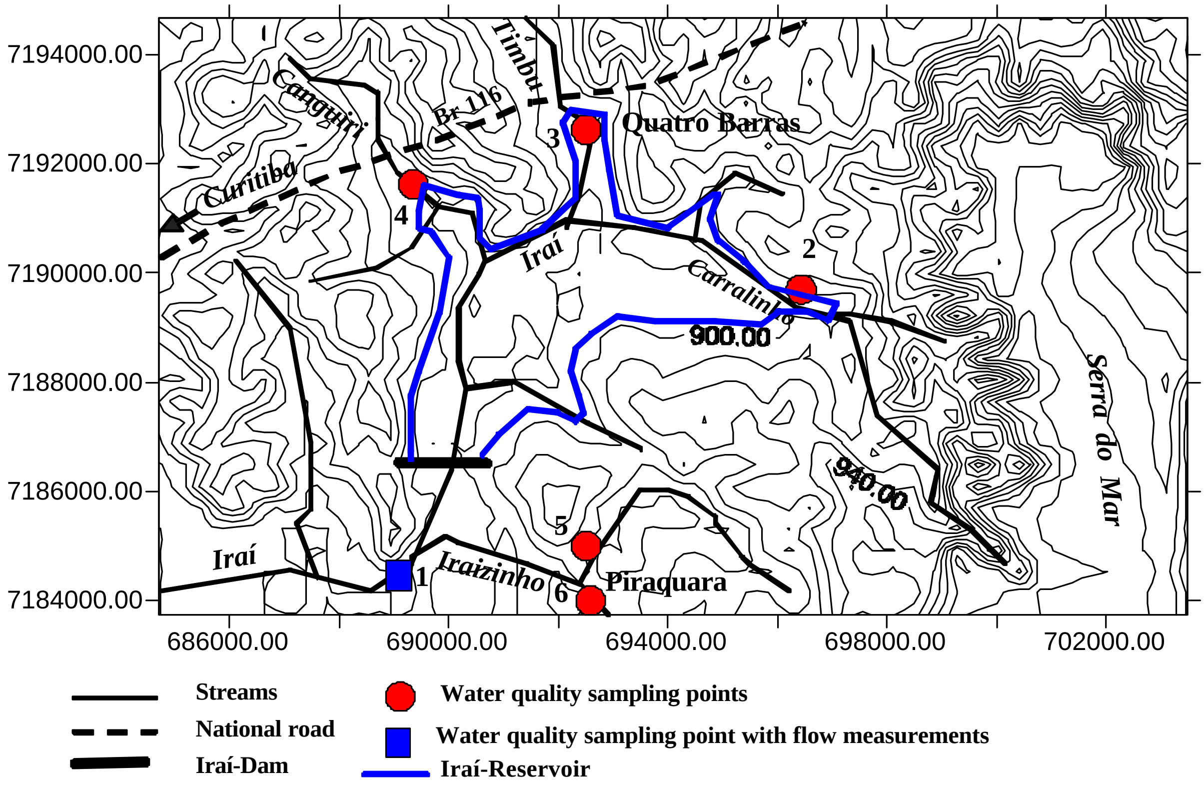
Appendix A: Flow and analysis data of Surface Waters



Water quality sampling point: : 1. Rio Iraí, Olaria do Estado; 2. Rio Carralinho; 3. Rio Timbo; 4. Rio Canguiri; 5. Rio Iraizinho; 6. Rio do Meio (after Suderhza, 1997).

1. Analysis of Surface Waters: Rio Iraí, Olaria do Estado

Date	Dissolved O2 (mgl)	Faecal Coli (N/100 ml)	pH	BOD (mg/l)	Tot. N (mg/l)	Tot. P (mg/l)	Turbidity (NTU)	TDS (mg/l)	Temp. (°C)	Tot. Coli (N/100 ml)	COD (mg/l)	Cond. (µs/cm)	Kjehl N (mg/l)	Air Temp. (°C)	Weather
09.04.87	6,74	500	7,3	1	1,03	0,004	5,6	126	22						
19.05.87	5,3	800	6	1	1,62	0,03	18	60	17						
11.08.87	7,82	30	8,1	1	0,65	0,032	7,6	75	25						
19.11.87	7,1	170	7,3	4	1,15	0,063	96	77	23						
14.03.88	6,74	500	6,5	1	1,02	0,064	9,4	88	21						
03.05.88	5,88	3000	6,6	1	0,95	0,077	35	101	19						
23.06.88	7,38	8000	6,6	1	3,5	0,06	7,6	83	17						
23.09.88	6,38	800	6,9	2	0,82	0,076	15	123	19						
22.02.89	6,14	8000	6	1	0,91	0,05	14	182	24						
20.04.89	8,2	5000	6,9	2	0,68	0,129	17	70	21						
22.08.89	8,2	300	6,7	5	0,7	0,023	8	56	17						
02.07.90	7,28	500	6,8	2	0,58	0,036	6,8	77	16						
10.09.90	7,2	2300	6,7	1	0,68	0,04	10	100	15						
28.02.91	6,24	300	6,9	2	1,05	0,051	12	75	24	1400	10	58	0,73	31	good
11.06.91	7,78	700	7	2	0,75	0,04	11	35	14		9	71	0,51	15	good
03.10.91	6,4	13000	6,9	3	3,22	0,138	8,2	56	16	50000	8	79	2,45	16	rain
04.02.92	3,4	1700	6,5	7	1,44	0,121	16	75	22	5000	29	33	1,38	24	good
14.09.93	7,3	3000	6,5	1	0,78	0,044	9,9	78	14	8000	8	45	0,45	14	good
19.10.93	5,3	6000	6,9	17	0,8	0,067	33	208	20	300000	52		0,6	20	rain
24.11.93	6,12	1300	6,8	2	0,63	0,042	12	91	24	5000	13	45		28	good
13.01.94	5,8	1300	7,1	3	1,37	0,077	14	152	20	5600	19	64	0,77	24	good
04.04.94	7,7	1100	7,4	2	0,6	0,03	8,1	79	20	8000	10	42	0,22	22	good

05.05.94	6,9	700	7	2	1,12	0,062	5	67	18	2900	10	44	0,77	26	good
10.08.94	7,1	5000	6,9	2	1,52	0,092	8,4	108	15	23000	10	68	0,67	18	good
06.10.94	6,9	1700	7,1	2	1,31	0,071	10	143	20	3400	5	64	0,78	18	rain
30.11.94	6,4	800	6,9	2	0,82	0,049	12	42	20	800	10	48	0,47	26	good
06.03.95	5,4	15600	6,7	1	0,98	0,083	20	89	22	21600	9	48	0,71	23	good
27.06.95	5,8	11000	7,2	3	1,35	0,082	31	121	14	110000	20	66	0,92	16	good
31.07.95	7,3	2000	7,1	3	0,99	0,048	6,7	54	17	8000	13	48	0,62	27	good
16.10.95	6,6	5000	6,8	4	1,12	0,071	14	272	17	23000	16	48	0,89	18	good
Mean	6,63	3337	6,9	2,7	1,14	0,062	16,0	98,8	19,1	38287	14,76	53,1818	0,68	21,5	

2. Analysis of Surface Waters: Rio Carralinho

Date	Dissolved O2 (mgI)	Faecal Coli (N/100 ml)	pH	BOD (mg/l)	Tot. N (mg/l)	Tot. P (mg/l)	Turbidity (NTU)	TDS (mg/l)	Temp. (°C)	Tot. Coli (N/100 ml)	COD (mg/l)	Cond. (µs/cm)	Kjehl N (mg/l)	Air Temp. (°C)	Weather
04.12.91	7,4	1.300	7,3	2	2,4	0,142	7,8	90	23	7000	7	32	1,4	30	good
03.02.92	6,1	8.000	5,9	5	1,7	0,075	0,9	151	22	23000	14	29	0,82	27	bad
30.03.92	8,7	2200	6,3	2	0,71	0,053	14	54	21	8000	9	32	0,45	25	bad
13.04.92	7,2	130	6,5	1	0,42	0,044	7,5	74	20	210	6	33	0,22	28	bad
05.05.92	7,8	1300	5,7	2	0,36	0,048	12	54	17	3000	11	31	0,37	22	bad
22.06.92	8,9	110	6,4	3	0,72	0,04	7,5	75	16	2200	6	31	0,37	22	good
06.07.92	8,5	5000	5,9	4	1,59	0,169	44	133	15	24000	14	35	0,89	14	bad
03.08.92	9,3	500	5,9	3	0,84	0,031	14	53	11	3000	8	27	0,45	11	bad
14.09.92	8,8	130	6,2	1	0,33	0,044	9,8	36	15	3000	4	28	0,07	20	good
06.10.92	8,7	300	6,4	1	0,47	0,098	10	46	18	5000	6	34	0,17	27	good
03.11.92	8,3	300	7	2	0,48	0,053	15	60	20	1100	7	33	0,26	28	good
02.12.92	8	5000	5,9	2	0,6	0,089	40	94	18	8000	4	30		20	bad
13.01.93	7,7	700	6,6	2	0,71	0,038	19	74	21	50000	13	33	0,44	25	bad
02.03.93	7,6	500	6,4	4	0,41	0,032	14	65	20	5000	16	31	0,21	27	good
31.03.93	7,4	300	6,7	2	0,36	0,02	9,5	73	20	2300	6	34	0,11	27	bad
31.05.93	8,8	2300	6,5	2	0,53	0,109	46	110	16	13000	10	32	0,19	23	bad
14.06.93	9,5	350	6,7	3	0,49	0,094	17	86	15	2200	12	30	0,19	20	good
05.07.93	9	80	7,3	1	0,34	0,03	8	64	17	700	6	32	0,1	27	good
11.08.93	79,1	130	6,5	2	0,42	0,017	5,7	108	10	800	10	34	0,05	17	good
01.09.93	8,5	800	6,6	2	0,99	0,062	24	102	19	2300	8	40	0,34	26	good
14.10.93	8,2	230	6,7	1	0,54	0,066	7,2	67	19	3000	4	31	0,33	24	good
25.01.94	7,8	230	7	2	0,63	0,031	14	54	21	2200	6	36	0,42	27	good
05.04.94	8,7	300	8	3	0,37	0,015	12	46	19	800	16	33	0,17	25	good
04.05.94	8,2	80	7,1	1	0,64	0,014	7	25	18	1700	9	36	0,36	24	good
08.08.94	9,1	130	6,8	2	0,53	0,032	6,1	46	15	3000	8	35	0,22	20	good
04.10.94	8,3	2	7,1	2	0,67	0,029	29	90	17	1100	8	41	0,37	16	bad
29.11.94	7,8	27	6,9	1	0,51	0,03	12	67	19	22000	10	37	0,39	21	bad
20.02.95	7,5	2800	6,6	1	0,33	0,022	16	117	19	7600	10	29	0,15	22	good
27.06.95	8,6	300	6,6	1	0,82	0,026	16	76	16	7000	8	40	0,53	19	good
01.08.95	8,9	2	7,1	3	0,7	0,014	4,9	59	15	1700	7	37	0,48	19	good
Mean	8,28	1.118	6,6	2,1	0,687	0,052	15,00	74,97	17,7	7130	8,8	33,2	0,28	22,8	

3. Analysis of Surface Waters: Rio Timbo

Date	Dissolved O2 (mgl)	Faecal Coli (N/100 ml)	pH	BOD (mg/l)	Tot. N (mg/l)	Tot. P (mg/l)	Turbidity (NTU)	TDS (mg/l)	Temp. (°C)	Tot. Coli (N/100 ml)	COD (mg/l)	Cond. (µs/cm)	Kjehl N (mg/l)	Air Temp. (°C)	Weather
04.12.91	5,7	3000	7,2	2	0,81	0,102	44	164	29	160000	17	104	0,35	30	good
03.02.92	7,3	140000	6,8	9	1,3	0,1	3	230	25	900000	38	64	0,78	27	bad
03.03.92	7,1	130000	7	2	0,66	0,125	22	111	21						
31.03.92	7,1	50000	6,7	6	0,79	0,057	30	83	21						
13,04,92	6,8	30000	7	11	1,2	0,115	18	115	23	500000	32	90	0,68	28	bad
06.05.92	7,3	17000	6,4	4	6,82	0,08	15	88	17	800000	17	75	6,76	19	bad
23.06.92	7,8	50000	7	3	1,4	0,075	10	100	19	999999	22	87	0,64	26	good
06.07.92	7,5	140000	6,4	1	2,37	0,133	160	280	15	999999	22	87	1,5	15	bad
04.08.92	8,5	17000	6,3	3	1,61	0,053	19	34	12	999999	14	56	0,56	13	bad
09.09.92	7,2	400	6,7	16	1,05	0,066	18	123	18	999999	35	80	0,43	20	good
06.10.92	5	50000	6,7	14	1,86	0,183	36	195	20	999999	54	142	1,64	25	good
03.11.92	3,1	280000	7,2	28	2,22	0,16	28	153	25	999999	69	181	2,16	28	bad
12.01.93	7,1	20000	6,4	2	1,17	0,113	53	100	23	80	24	52	0,83	28	bad
03.03.93	7,1	130000	7	2	0,66	0,057	22	111	21	999999	18	65	0,29	25	bad
31.03.93	7,1	50000	6,7	6	0,69	0,1	30	83	21	999999	22	83	0,33	24	bad
31.05.93	8,3	80000	6,8	2	0,98	0,1	45	126	17	300000	10	32	0,33	23	good
14.06.93	8,8	7000	7	3	2,76	0,168	12	20	16	140000	12	66	0,28	21	good
05.07.93	7,9	5000	7,4	4	0,77	1,26	15	96	16	500000	22	88	0,41	27	good
10.08.93	8,1	7000	6,9	5	2,21	0,084	14	108	19	220000	22	116	1,05	12	good
01.09.93	5,8	130000	7	34	2,81	0,072	64	317	13	999999	167	197	2,21	26	good
14.10.93	8	6000	7,2	3	1,31	0,301	18	117	23	80000	9	63	0,54	24	good
25.01.94	6,2	23000	7	4	2,39	0,054	22	295	20	70000	28	120	2,18	26	good
21.03.94	7,2	8000	7,2	5	1,59	0,037	11,4	110	22	23000	19	90	1,1	23	good
05.04.94	6,8	1700	7,3	8	1,97	0,091	68	81	23	4000	24	111	1,57	21	good
29.06.94	9,6	3300	6,5	14	1,82	0,052	34	188	9	17000	84	91	0,97	11	good
08.08.94	9,3	7000	6,9	3	2,11	0,062	7,5	113	16	80000	15	100	1,37	20	good
11.10.94	5,2	17000	7,1	56	1,55	0,087	35	155	21	50000	94	528	1,5	15	good
30.11.94	6,1	12800	7,2	7	1,56	0,049	11	475	23	96000	23	135	1,3	26	good
20.02.95	7,5	7600	7	2	0,97	0,013	20	140	20	22800	11	65	0,33	22	good
28.06.95	8,1	1700	7	4	2,76	0,083	22	94	17	28000	18	98	2	24	good
01.08.95	7,6	200	7,3	7	2,61	0,095	17	138	17	30000	28	115	2,12	19	good
04.10.95	8	5000	6,9	3	1,84	0,094	11	114	17	30000	10	86	1,16	17	good
Mean	7,2	44678	6,9	8,5	1,77	0,132	29,2	145,5	19,3	428245	33,0	111	1,29	21,7	

4. Analysis of Surface Waters: Rio Canguiri

Date	Dissolved O2 (mgl)	Faecal Coli (N/100 ml)	pH	BOD (mg/l)	Tot. N (mg/l)	Tot. P (mg/l)	Turbidity (NTU)	TDS (mg/l)	Temp. (°C)	Tot. Coli (N/100 ml)	COD (mg/l)	Cond. (µs/cm)	Kjehl N (mg/l)	Air Temp. (°C)	Weather
13.04.92	5,3	70000	6,6	2	1,41	0,08	7	82	21	170000	11	152	0,73	28	bad
06.05.92	5,7	80000	6,7	3	0,67	0,093	12	70	18	300000	5	134	0,43	19	bad
22.06.92	7,4	700000	7	5	1,97	0,209	8	84	17		22	149	0,78	22	good
06.07.92	7,4	130000	6,7	20	0,86	0,236	46	128	15	170000	110	133	0,52	15	bad
04.08.92	8,3	22000	6,6	2	2,11	0,035	10	44	13	80000	8	83	0,61	13	bad
09.09.92	7,9	280000	6,9	10	1,54	0,084	8	106	17	999999	21	125	0,47	20	good
06.10.92	5,5	140000	6,8	8	2,54	0,156	11	144	18	999999	13	186	1,31	24	good
03.11.92	3,7	300000	7,1	9	1,69	0,174	8,6	130	21	999999	17	215	1,17	28	good
01.12.92	7,7	23000	6,8	2	1,9	0,132	37	103	20	230000	14	98		25	bad
12.01.93	7,4	110000	7,2	3	2,02	0,081	17	150	21	30000	15	92	0,57	21	bad
02.03.93	7	500000	7,1	15	1,02	0,033	150	424	23	999999	43	88	0,55	27	bad
31.03.93	6,9	30000	7	1	1,14	0,081	9	84	20	80000	3	126	0,29	24	bad
31.05.93	8,5	30000	7,2	2	1,44	0,094	26	117	17	220000	13	101	0,23	23	bad

14.06.93	8,7	130000	7,3	3	1,34	0,117	8	109	16	130000	9	111	0,14	21	good
05.07.93	6,8	110000	7,4	3	1,23	0,146	9	144	18	220000	9	165	0,46	27	good
10.08.93	7,3	50000	7,1	3	3,17	0,092	8	96	13	130000	13	157	0,86	12	good
01.09.93	4,6	80000	7,2	5	4,32	0,25	7,1	215	20	80000	27	259	2,14	25	good
25.01.94	5	80000	7,2	3	2,3	0,112	13	122	21	240000	9	168	1,4	26	good
05.04.94	4,7	170000	7,8	5	2,1	0,112	7,7	144	20	500000	22	203	1,35	20	good
04.05.94	3,1	50000	7,3	4	3,23	0,161	7,3	112	18	130000	24	241	2,53	24	good
03.08.94	7,9	170000	7,2	1	2,13	0,068	4,6	83	14	170000	7	108	0,99	14	good
10.10.94	3,6	999999	7,2	6	5,49	0,439	4,3	198	21	999999	20	258	5,4	28	good
29.11.94	4,9	80000	7,3	3	2,6	0,127	15	41	20	80000	14	148	1,35	22	good
20.02.95	7,5	80000	7,3	1	1,28	0,048	10	171	20	80000	9	91	0,37	22	bad
28.06.95	6,1	220000	7	5	3,5	0,178	7,8	94	17	640000	12	162	2,3	23	good
31.07.95	6,5	200	7,5	2	2,99	0,17	6,5	123	17	800000	11	140	2,32	23	good
03.10.95	6,9	70000	7,2	2	1,94	0,11	8,4	149	17	900000	6	100	0,97	19	good
Mean	6,4	174267	7,1	4,7	2,15	0,134	17,3	128,4	18,3	412916	18,0	148	1,35	22,0	

5. Analysis of Surface Waters: Rio Iraizinho

Date	**Dissolved O2 (mgl)**	**Faecal Coli (N/100 ml)**	**pH**	**BOD (mg/l)**	**Tot. N (mg/l)**	**Tot. P (mg/l)**	**Turbidity (NTU)**	**TDS (mg/l)**	**Temp. (°C)**	**Tot. Coli (N/100 ml)**	**COD (mg/l)**	**Cond. (μs/cm)**	**Kjehl N (mg/l)**	**Air Temp. (°C)**	**Weather**
11.10.91	8,3	70	6,9	1	0,52	0,048	2,1	40	16	1300	5	58	0,41	24	good
24.02.92	4,8	2200	6,6	2	0,4	0,063	1,2	207	24	8000	15	51	0,39	29	bad
04.10.93	7,6	14000	6,7	7	0,86	0,158	18	210	18	35000	33	38	0,72	18	bad
19.01.94	5,2	500	6,9	2	0,48	0,01	5	166	23	9000	4	48	0,43	25	good
08.08.94	9,8	28000	7,2	1	0,23	0,014	2	65	15	70000	5	150	0,15	20	good
10.04.95	6,6	5000	7	1	0,51	0,027	4,3	97	22	13000	4	52	0,4	25	good
Mean	7,1	8295	6,9	2,3	0,5	0,053	5,4	130,8	19,7	22717	11	66	0,42	23,5	

6. Analysis of Surface Waters: Rio do Meio

Date	**Dissolved O2 (mgl)**	**Faecal Coli (N/100 ml)**	**pH**	**BOD (mg/l)**	**Tot. N (mg/l)**	**Tot. P (mg/l)**	**Turbidity (NTU)**	**TDS (mg/l)**	**Temp. (°C)**	**Tot. Coli (N/100 ml)**	**COD (mg/l)**	**Cond. (μs/cm)**	**Kjehl N (mg/l)**	**Air Temp. (°C)**	**Weather**
04.10.93	8	14000	6,3	3	0,73	0,028	43	240	18	70000	19	21	0,6	18	bad
19.01.94	1,7	170	6,4	2	1,15	0,01	2,3	104	24	1200	8	42	1,1	25	good
08.08.94	7,4	2	6,4	1	0,33	0,008	2,3	50	18	280	6	28	0,28	20	good
21.02.95	7,8	80000	6,7	1	0,59	0,025	17	71	28	80000	11	30	0,54	27	good

Appendix B: Well and piezometer data

Topographic data on wells and piezometers						
Wells/piezometers	**Latitude**	**Longitude**	**Easting**	**Northing**	**Height**	**Static level**
Faz.Canguiri Exp.1	25° 25' 05"	49° 07' 38"	688358.33	7187438.67	903,831	878.831
Faz.Canguiri Exp. 2	25° 23' 30"	49° 07' 06"	689293.752	7190349.25	936,431	926.931
Faz.Canguiri, esc. 1	25° 23' 05"	49° 07' 51"	688046.743	7191136.16	h	h-23.78
Faz.Canguiri, esc. 2					h	h-24.17
Faz. Canguiri 3	25° 24' 26"	49° 07' 59"	687788.285	7188646.92	901.811	877.83
Iapar 1	25° 23' 01"	49° 07' 26"	688747.273	7191249.45	899	879.517
Iapar 2	25° 22' 58"	49° 07' 08"	689251.716	7191338.68	910	881.332
Iapar 3	25° 23' 05"	49° 07' 21"	688885.305	7191124.4	898	880.301
Iapar 4	25° 23' 16"	49° 07' 08"	689243.917	7190780.82	893	881.245
Iapar 5	25° 23' 08"	49° 07' 17"	688995.816	7191030.52	h	h-17.56
Iapar 6	25° 23' 06"	49° 07' 15"	689052.585	7191091.28	898	882.172
Iapar 7	25° 26' 07"	49° 03' 39"	688831.3	7190778	899	881.655
Iapar 8	25° 23' 20"	49° 07' 01"	689437.842	7190654.98	891	881.077
Iapar 9	25° 23' 35"	49° 06' 44"	689906.49	7190186.76	894	884.34
Colonia Penal	25° 24' 57"	49° 05' 55"	691240.123	7187644.13	h	h-9
Castelo Branco 1	25° 22' 38"	49° 07' 15"	689064.702	7191952.84	892	880
Castelo Branco 2	25° 23' 26"	49° 04' 54"	692985.018	7190419.85	h	h-12.80
Adalto Botehlo 1	25° 23' 44"	49° 06' 47"	689818.727	7189910.98	h	h-8.84
Aracatuba 1*	25° 22' 38"	49° 07' 15"	689064.702	7191952.84	h	h-3.04
Aracatuba 2	25° 22' 47"	49° 07' 26"	688765.3	7191672	891.421	879.311
Aracatuba 3	25° 22' 46"	49° 07' 34"	688538.7	7191716	895.162	879.692
Aracatuba 4	25° 22' 55"	49° 07' 43"	688268.8	7191454	906.241	
Aracatuba 5	25° 21' 26"	49° 04' 54"	693038.016	7194112.31		
Aracatuba 6*	25° 21' 23"	49° 05' 28"	692102	7194210		h-9.21
Penitencaria 2	25° 24' 40"	49° 04" 22"	693846.592	7188129.95		
Menino Deus	25° 21' 03"	49° 05' 40"	691761.993	7194838.41	h	h-14
Quatro Barras Sede1	25° 22' 41"	49° 04' 29"	693703.753	7191794.48		
Piezometer 1	25° 25' 12"	49° 05' 19"	692248.921	7187182.3	895.702	887.452
Piezometer 2	25° 24' 26"	49° 04' 12"	694122.963	7188540.14	901.642	
Piezometer 3	25° 23' 27"	49° 07' 16"	689006.328	7190454.18	894.764	
Piezometer 4	25° 23' 25"	49° 07' 12"	689121.989	7190505.33	894.563	879.433
Piezometer 5	25° 23' 14"	49° 07' 56"	689583.739	7190822.2	891.678	878.388
Piezometer 6	25° 23' 22"	49° 07' 06"	689282.478	7190603.02	891.678	888.858
Piezometer 7	25° 23' 10"	49° 06' 15"	690719.962	7190932.55	891.961	886.861
Piezometer 8	25° 23' 15"	49° 07' 46"	688168.864	7190836.29	910.352	895.222
Piezometer 9	25° 21' 23"	49° 04' 56"	692983.764	7194201.05	938.879	904.869

Table hydraulical and some technical data on wells and piezometers							
Location		**N.E (m)**	**T (m2/s)**	**kf (m/s)**	**Length filter(s) (m) #**	**Filter depth (m)**	**Cementation depth (m)**
Faz.Canguiri Exp.1		878.831	3.77E-03	0.001008	4	46.5-50.5	
Faz.Canguiri Exp. 2		926.931			12	58-62	
						70-78	
Faz.Canguiri, esc. 1		h-23.78	1.39E-03	0.000068	20.5		
Faz.Canguiri, esc. 2		h-24.17	1.09E-03	5.77E-05	5.7		
Faz. Canguiri 3		877.83	9.06E-04	1.01E-04	9	39.3-45.3	
						48.3-51.3	
Iapar 1		879.517	1.26E-03	7.88E-05	16	27.5-31.5	
						41.5-51.5	
						52.5-54.5	
Iapar 2		881.332	1.73E-04	1.44E-05	12	38.5 - 50.5	
Iapar 3		880.301	1.22E-03	6.09E-05	20	21.4- 25.4	
						33.4-49.4	
Iapar 4		881.245	0.07514	9.26E-05	16	35.55-51.55	
Iapar 5		h-17.56	2.37E-03	8.94E-05	16	39.6- 55.6	
Iapar 6		882.172	2.79E-03	9.13E-05	16	36.8-52.8	
Iapar 7		881.655	1.48E-03	9.27E-05	16	28.5-44.5	
Iapar 8		881.077	1.60E-03	0.0001	16	27.3-41.3	
						49.3-51.3 *	
Iapar 9		884.34	2.10E-03	0.000117	18	27.5-41.5	
						49.5-53.5	
Colonia Penal		h-9	1.96E-04	0.000014	14	19-33	19
Castelo Branco 1		880	7.65E-04				
Castelo Branco 2		h-12.80	3.76E-03	0.000235	16	20-37	
Adalto Botehlo 1		h-8.84	0.0031	6.15E-05	16	21-37	11
Aracatuba 1*		h-3.04	5.88E-03	0.000367	50.4	51.6 - 102	
Aracatuba 2		879.311	9.62E-04	6.01E-05	16	22.5 - 30.5	
						34.5 - 42.5	
Aracatuba 3		879.692	1.36E-04	9.71E-06	16	30.5 - 44.5	20
						48.5 - 50.5	
Aracatuba 4				0	14	51 - 63	16
						63 - 67	
Menino Deus		h-14			7	5 - 8 m	
						22-26	
Aracatuba 6*		h-9.21	2.36E-04				45.5
Piezometer 1		887.452	2.12E-06		12	10 - 20 m	10
						23 - 25 m	
Piezometer 2							
Piezometer 3					12		9
Piezometer 4		879.433	2.85E-04		11		8

Piezometer 5		878.338			10		11
Piezometer 6		888.858			8		8
Piezometer 7		886.861			5		8
Piezometer 8		895.222				30 - 35 m	
						42 - 46 m	
						49 - 55 m	
						60 - 72 m	
Piezometer 9		904.689	5.84E-06		15		8

* filter in basement rock

the filter length has been taken as the aquifer thickness

Groundwater Chemistry

in mg/l

Place	Name	pH	ec	Alka	Ca	Mg	Na	K	Fe	HCO_3	SO4	NO_3	CL	CO2	SiO2	NH4	PO4
			S/cm	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l
1	Aracatuba 1	7,00		118	22,66	7,97	21,80	1,16	0,12	118,00	4,50	5,00	11,00		35	0,00	
2	Aracatuba 2	6,60		70	13,10	5,90			2,70	70,00	5,10	4,00	14,00	35			
3	Escola 1	8,09		123	21,60	7,70	19,00	1,40	0,14	118,00	0,00	0,00	1,40		45	0,00	
4	Leiteria	6,70		56	11,37	2,31	7,20	1,10		56,00	6,70	3,00	0,14	28	23,8	0,00	
5	Faz. C. Micro	8,10		157	28,40	11,30	24,00	1,90	0,07	157,00	1,00	0,00	15,00	2,98	39,6	0,00	
6	Iapar 1	6,80		119	24,70	11,60				118,50	1,00	0,25	0,00	37,9			
7	Iapar 2	7,20		81,9	13,80	7,70			0,10	81,90	0,60	0,50	0,50	10,6		0,00	
8	Iapar 3	6,90		84,4	12,40	57,30			3,10	84,40	3,20	0,12	1,10	21,1		0,05	
9	Iapar 4	6,80		64,8	9,40	3,60			0,20	64,80	0,60	0,05	1,00	20,7		0,00	
10	Iapar 5	7,00		92,3	13,10	7,90			1,60	92,30	0,00	0,01	1,00	18,5		0,00	
11	Iapar 6	6,80		75,6	9,70	4,70			0,30	75,60	0,00	0,09	0,00	24,1			
12	Iapar 7	7,30		151	10,70	22,20				150,90	5,90	0,10	0,00	15,1			
14	Iapar 8	6,46	98,70	53	5,81	1,92	11,55	1,74	0,75	64,71	0,26	0,05	0,50	21,1	46,5	0,01	0,263
15	Iapar 9	6,28	81,70	38,8	3,83	1,16	12,17	1,45	0,68	47,29	0,14	0,08	2,75	20,2	47	0,00	0,145
13	Menino Deus	7,65	170,00	62	6,37	1,74	2,75	13,34	2,39	62,00	0,00	0,01	0,00	2,36	70	0,07	
16	Colonia Penal	8,67		165	40,70	11,60	14,00	3,50	0,10	154,00	0,00	26,00	9,00		31,7	0,00	
17	P. C. Branco 2	6,90		45	5,06	4,20	7,10	1,10		45,00	5,30	0,05	0,47	15	23,2	0,02	
18	P.Z-03	6,40	111,00	56,1	5,90	2,84	9,41	2,04	2,58	68,44	0,00	0,00	0,98	20,2	44	0,00	0,38
19	PZ-04	6,95	205,00	44,9	5,45	2,00	6,70	2,00	3,97	54,75	0,00	0,00	0,51	63,7	14	0,00	0,42
20	PZ-05	6,80	87,00	44,8	4,79	2,15	8,47	2,47	1,94	54,75	0,00	0,00	1,41	12,3	44,6	0,00	0,1
21	PZ-06	6,68	48,00	27,5	2,60	0,85	6,43	2,08	0,17	33,60	0,00	0,25	0,98	5,28	43,2	0,00	0,27
22	PZ-08	7,47	145,00	182	43,71	13,12	18,80	1,60	0,38	221,50	0,00	0,00	0,00	29,6	35,9	0,00	0,22
23	PZ-09	7,86	208,00	182	29,41	10,52	27,00	2,80	0,09	162,26	0,00	14,00	12,16	27,8	34	0,00	0,041

Appendix C: Small guide to construct a MODFLOW model in GMS

Small guide of GMS

Because the reference manual and tutorial of GMS do not excel pedagogically and was very difficult to learn, the author found it necessary to put his experiences and his knowledge that was gained with difficulty to paper. So that at least his colleagues do not encounter the same difficulties to construct a MODFLOW-model in GMS. Many times additional correspondence with the organisation of Environmental Modelling Systems Incorporated who sell the GMS product was necessary to come forward. Further information may be found on their homepage: http://www.ems-i.com and for questions or help e-mail tech2@ems-i.com
The author has made a small guide of the steps that were taken by the author to construct the MODFLOW model and hopefully might help others that are forced to use GMS as a software package. The steps taken in GMS to come from the raw data used here to a model that is suitable for simulation

Several steps are involved in setting up a conceptual model and converting the conceptual model to a numerical model. These steps are carried out in the **Map module** of GMS. In the **Map module** feature objects are used to provide GIS capabilities within GMS. Feature objects include points, arcs and polygons. Feature objects have to be grouped into layers or coverages similar to a layer in a CAD or Polyplot drawing.
Each coverage is assigned a coverage type which controls which set of attributes are associated with the coverage. The appropriate attribute set for a coverage depends on the intended use of the coverage.
In this case the attribute sets for MODFLOW/MT3D are used which consist of local sources, aerial attributes and layer attributes.
The MODFLOW/MT3D local sources/sinks is used to define rivers, wells, drains and other sources/sinks as a part of a conceptual model. MODFLOW/MT3D aerial attributes is used to define aerial attributes like recharge and evapotranspiration zones as part of a conceptual model. MODFLOW/MT3D/MODPATH layer attributes is used to define layer data such as leakance, transmissivity, and porosity as part of the definition of a conceptual model.
A set of coverages have to be constructed representing a conceptual model of a groundwater modelling problem. This representation can be used to generate MODFLOW and MT3D numerical models.

The best way to start is to have a digital image imported and displayed in the background in the form of a TIFF file representing a map or an aerial photograph of the site, and create the coverages.
After the coverages are created the MODFLOW data must be initialised as follows:

- Switch to the **3D Grid module**
- Select the **Basic Package** command from the **MODFLOW menu**
- Select the **New** button at the top of the dialog. This initialises the data structures used to store the MODFLOW arrays
- Select the packages that are used
- For a transient simulation, set up the stress periods necessary for the simulation. For a steady state simulation, go to the **BCF Packages dialog** and select the steady state option
- In the **BCF Package dialog**, select the appropriate layer type for each of the layers

To import necessary data for layers for the MODFLOW model (under the **map module** or **3D-grid module**)
The grid constructed of the surface elevations is imported in GMS in the **map module**. The following steps have to be taken:

- **import DXF**
- **DXF® TIN**
- **Triangulate**

Or when a Surfer file is available:

- **Import**
- tick **Surfer grid ® 2D grid** (the file grid has to be saved GS ASCII (*.grd) in SURFER)
- **grid® 2D Scatter Points**

Actually the latter is not necessarily the best way to handle the data because all handling and conversion of data may introduce errors and deviations from the original data.

For good display **Display options** under display may be used.

Because the simulation program MODFLOW that uses 3D, cell-centred, finite difference, saturated flow models for simulation several other steps have to be taken to build the land elevations into a MODFLOW-model.
The TIN's have consequently to be converted from TIN's to 2D-scatterpoints and consequently be interpolated to a 2D-grid that will be the first component of the MODFLOW-model. In the **3D-gridmodule**:

- **create grid**, for the origins the lowest values are taken !
- in the MODFLOW-menu select **new** under **Basic Package**
- select **grid® 2D-grid** (creates a 2D-grid that matches the 3D-grid exactly

In the **2D-scatter points module** under **interpolation**:

- in **Interp. Opts** (Interpolation options) chose the interpolation method and under
  some of the interpolation methods options may be chosen (e.g. which kind of
  function has to be used or a semivariogram has to be constructed)
  to 2D-Grid has to be chosen to interpolate the 2D-scatter points to a 2D-grid and
  also tick **map elevations**. This is the first layer in the MODFLOW-model
- **Save**

The next step is to import the next layers like the hydraulic heads and bedrock depths which have been constructed as Surfer grids in this case. Because GMS may have only one 2D-grid in memory at a time the grids that have to be imported, have to be imported separately from the existing simulation set-up (MODFLOW-model). That is why the MODFLOW-model has to be closed. Everything may be carried out under the **2D-scatter point module**

- **New** under **File**
- The question 'Are you sure you want to delete everything ?' and **OK** is clicked

to make it possible to import e.g. the grid of the hydraulic heads

- **Import** under **File**
- Tick **Surfer Grid ® 2D-grid**; **Select Grid® 2D-scatter points**
- **Save**

Now a scatter point file of the hydraulic heads is constructed. It is advisable to close the scatter point file at all times, because the MODFLOW-model may change the values of the scatter point file in an unexplainable way. Then the MODFLOW-model may be opened again and afterwards the scatter point file. The scatter points may be interpolated in the **2D-scatter point module** and in the **3D-grid module** in the **Basic Package** under **Starting heads** the **Use 2D data set® layer** is clicked.

- the **Data set to Layer** dialog appears
- click **Apply to variable cells only**, because only the interpolated values should be incorporated in the layer
- **Select Data Set**. 3 layers are visible in this case: **The Default**, **elevation_interp** and **z_interp (mapped and active)**. The latter active layer is selected by default so no changes have to be made. All the layers may be looked at by clicking **Info**
- **Save**
- If an additional layer has to be added, **New** and then execute the same procedures as the former hydraulic heads grid.

After the conceptual model is constructed and a grid has been created, the final step in converting a conceptual model to a MODFLOW numerical model is to select the **map ® MODLOW** command.
When the model is ready check the simulation to see if there are any obvious errors or potential problems. Save the simulation with the **Save simulation** command and **run MODFLOW**.
To look at the result tick **Read solution**.
With the result of the MODFLOW simulation it is possible to make a transport simulation.

When another grid has to be imported instead of an existing one in MODFLOW (e.g. starting heads) it is important to first construct a scatter point file of this grid and then close this before the MODFLOW-model is opened, the scatter-point file may be opened after the MODFLOW-model is opened, after that the scatter points may be interpolated and read into the starting heads file. This is important because if you open the MODFLOW-model when the scatter point file is open the values of this file are changed in an unexplainable way.

When a MODFLOW-model is opened, it is important to first open the simulation and then the files under File because otherwise GMS does not recognise the grid.