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OpenGeoSys Tutorial
Computational Hydrology II

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Foreword

This tutorial presents the application of the open-source software *OpenGeoSys* (OGS) (Kolditz et al., 2012) for hydrological simulations concerning conservative and reactive transport modelling. The material is based on unpublished manuals (Bauer, 2009) and results of a scientific project cooperation between China and Germany (SUSTAIN H_2O). This tutorial has already applied at several international training courses on the subject held in China (2014, 2015). This tutorial is the result of a close cooperation within the OGS community (www.opengeosys.org). These voluntary contributions are highly acknowledged.

The book contains general information regarding the hydrological modelling of a real case study and the step-by-step set-up of a model with OGS and related components such as the OGS Data Explorer. Benchmark examples are presented in detail.

This book is intended primarily for graduate students and applied scientists who deal with hydrological modelling. It is also a valuable source of information for professional geoscientists wishing to advance their knowledge in numerical modelling of hydrological processes including reactive nitrate transport modelling. As such, this book will be a valuable help in training of computational hydrological systems.

There are various commercial software tools available to solve complex scientific questions in hydrology. This book will introduce the user to an open-source numerical software code for hydrological modelling which can be adapted and extended based on the needs of the researcher.

This tutorial is the second in a series that will represent further applications of computational modelling in hydrological sciences. Within this series, one tutorial has already been published:

- Computational Hydrology I: Groundwater flow modeling, Sachse et al. (2015), DOI 10.1007/978-3-319-13335-5, http://www.springer.com/de/book/9783319133348
- Computational Hydrology II, Sachse et al. (2016), this volume

These contributions are related to a similar publication series in the field of environmental and energy sciences, namely:

- Geoenergy Modeling I: Geothermal Processes in Fractured Porous Media, Böttcher et al. (2016), DOI 10.1007/978-3-319-31335-1, http://www.springer.com/de/book/9783319313337
- Geoenergy Modeling II: Shallow Geothermal Systems, Shao et al. (2016, in press),
- Geoenergy Modeling III: Enhanced Geothermal Systems, Watanabe et al. (2016, in press),
- Geoenergy Modeling IV: Computational Geotechnics: Storage of Energy Carriers, Nagel et al. (2017*),
- Geoenergy Modeling V: Models of Thermochemical Heat Storage, Lehmann et al. (2017*)
- OGS Data Explorer, Rink et al. (2017*),

(*publication time is approximated).

Leipzig, Germany, August 2016

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Contents

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Chapter 1
Introduction

The tutorial explains the step by step development of a steady state groundwater model and a conservative and reactive transport model with the help of open source software, first of all the numerical modelling tool *OpenGeoSys*. The groundwater model was developed in the context of the SUSTAIN H_2O project which aims to develop and demonstrate management tools and practices for pollution reduction in the Songhuajiang-Liaohe River Basin (SLRB) in order to support the realization of the "12th Five Year Plan" of the Peoples Republic of China. Details on the project are available at www.craes.cn/cn/SUSTIANH2O. This case study focusses on the impact of urban development as well as potential groundwater pollution threats on the drinking water safety in the area. The best possible implementation of the groundwater system in the area was implemented as an *OpenGeoSys* simulation model.

1.1 Catchment Description

1.1.1 Topography and climate

The about 265 km^2 large study area is located within the Northeastern Chinese province Heilongjiang about 20-50 km south of the provincial capital Harbin upstream of the city Acheng. The Ashi River is bordering the area on the east whereas the remaining topographical boundaries are set by the catchment extension of smaller creeks draining to Ashi River. The landscape can be described as subdivided into two parts. A plateau with elevations from 168 to 192 m covers the western and southern parts of the catchment which to the east is sloping down in terraces to the 2.5 to 5 km wide flat Ashi River floodplain having an altitude between 138 to 145 m.

The investigation area has a cold temperate continental monsoon climate. Winters are long cold and dry with an average temperature of -18.8 °C - 18.8 °C and summers are short and warm to very warm with an average of 24.2 °C in June. Although the yearly averaged temperature is 3-4 °C measured temperatures could be in the range up to between -34.2 °C and 38.4 °C. The annual average rainfall is 515 mm, concentrated heavily in summer.

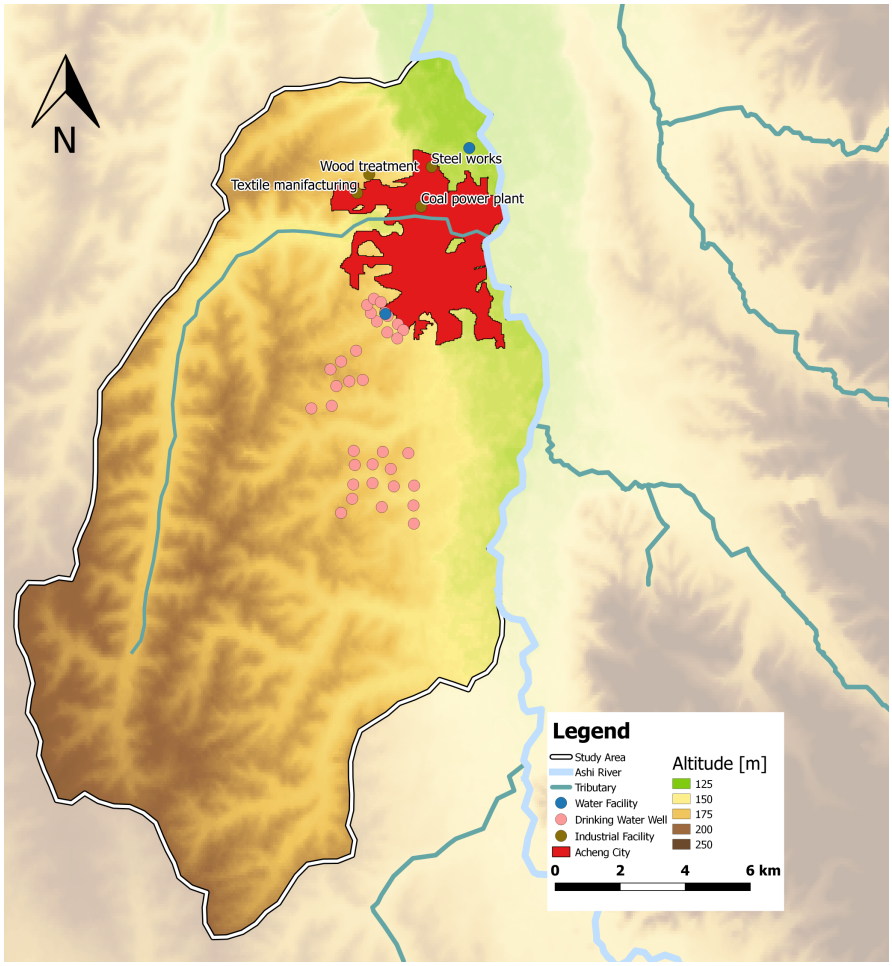

Fig. 1.1: Topography of the study area and facilities

1.1.2 Socio-economy and land cover

The entire Acheng district, which is ten times larger than the study area, had a population of 597,000 in 2014 which consists of 342,000 rural and 255,000 urban inhabitants. It can be assumed that the entire urban population lives within the study area which covers Acheng city almost entirely. Additionally, at least one-third of the total rural population lives in the study area as it belongs to the more densely populated areas in the district. Hence, the total population of the study area is roughly about 350,000.

Acheng district is an important commodity grain base in Harbin, with a total grain output in 2012 reaching 601 million kg. Particularly the area is important for the production of wheat, rice and maize.

Acheng city is an important industrial town in Heilongjiang, with 68 above-scale enterprises and more than 5000 small and medium-sized enterprises, preliminarily forming an industrial development pattern supported by such industries as mines, steel factories, building material cement, food and medicine, equipment manufacturing, new energy materials and intensive timber processing. There are 17 enterprises in Acheng District with sales income of more than ¥100 million.

This socio-economic pattern of Acheng district is reflected in the land-cover of the study area. The large majority (85.32 %) of the study area is covered by 226 km^2 of farmland followed by 30.5 km^2 (11.47 %) of settlements, 5.6 km^2 of forests (2.11 %), 2.5 km^2 of grassland (0.95 %) and 0.4 km^2 of water bodies (0.15 %).

1.1.3 Hydrology

Ashi River (Fig. 1.4) is one of the primary tributaries on the right bank of Songhua River, which flows through Harbin city. The Ashi River originates from Maoer mountain town in Shangzhi city, flowing through the study area close to Acheng city before entering Songhua River in the area around Harbin Yatai Cement Company at river kilometer 213. The study area accounts for about 8 % of total catchment area which is about 3534 km^2.

Although, the Ashi river system had 79 tributaries, the only larger one flowing through the study area is Fanjia River, which drains into Ashi River in Acheng city.

Ashi River is a representative of mountainous rivers in northern China. The river runoff supply primarily reflects the rainfall distribution in the headwaters and to a minor extent by groundwater. The average measured discharge at Acheng city hydrological station is about 80 m^3/s but can increase up to 824 m^3/s in the wet period in summer. On the other hand, water flow may decrease to almost zero during the dry period in winter prior to completion of upstream Xiquanyan Reservoir in 1992. Weirs on the Ashi River downstream

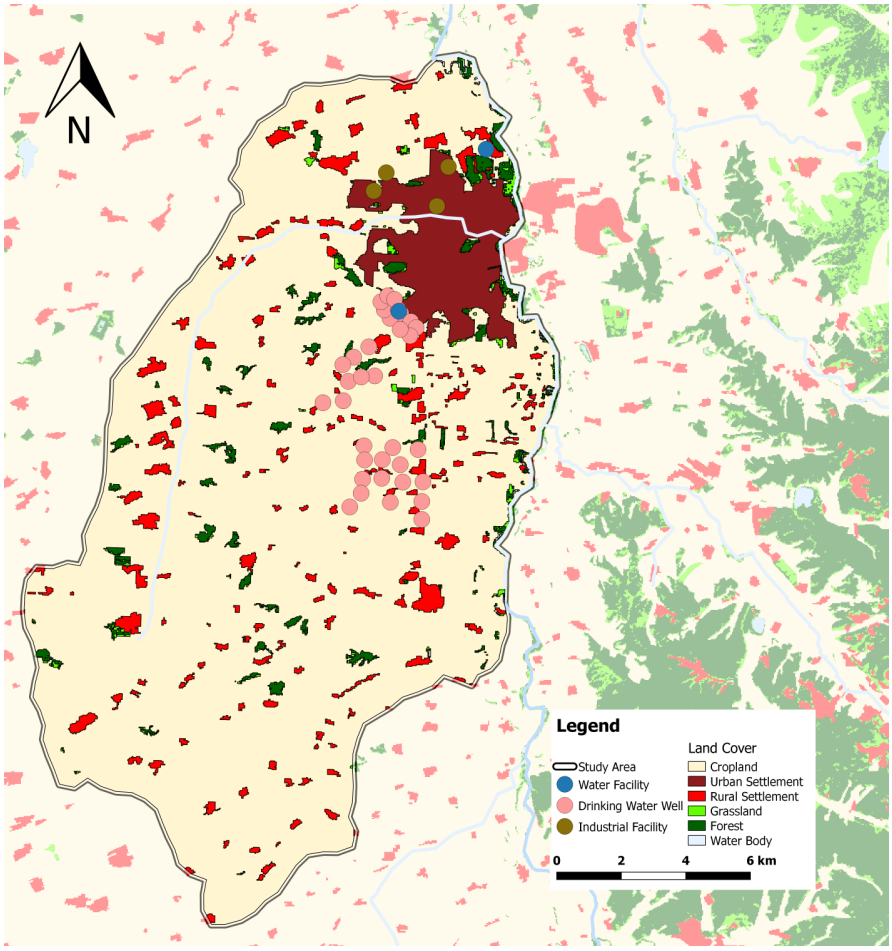

Fig. 1.2: Land use at the study site

of Acheng City keep river levels high above this point partly to provide irrigation water for the local area.

The water depth in the municipality of Acheng is between 0.35 m and 4.25 m, depending on the discharge. During the dry season, the observed runoff in river lowlands consists to considerable parts of urban sewage.

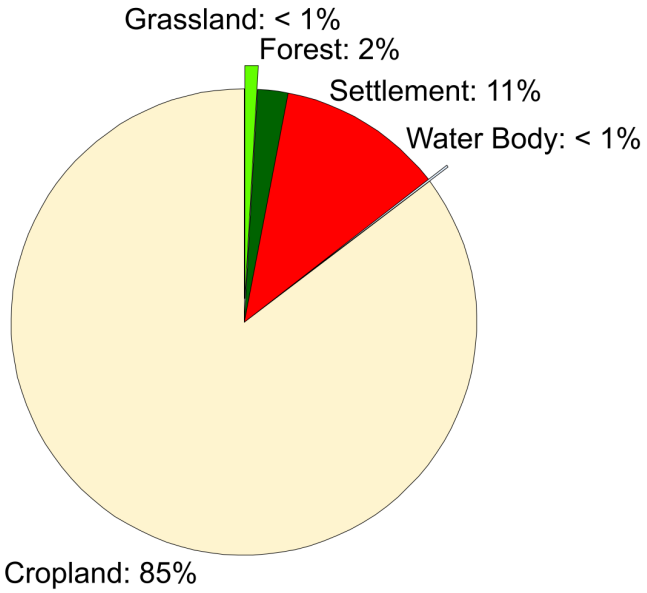

Fig. 1.3: Land cover distribution

1.1.4 Hydrogeology

The aquifer conditions of the area are complex (Feng et al., 2014). Based on borehole data, the hydrogeology of the area can be generally described as a three-layered system. One Quaternary aquifer, which is mainly confined in the study area serves as a potential water resource (Wang et al., 2014). The upper layer consists of Aeolian loess material which is frequently cut through by gullies and ravines leading to the outcropping of deeper geological layers in the river beds and flood plains of the study area (Fig. 1.2). The upper layer is, for most parts of the area, above the stable groundwater level and therefore has a poor water quantity.

The lower quaternary aquifer, which has a multilayer structure is the main aquifer of the study area. It consists of middle-Pleistocene sand, pebbly sand and gravel. It is rich in water and has a thickness between 5-30 m (Wang et al., 2014). The lower aquifer can be considered as confined in most parts of the study area but outcrops to the surface in the Ashi river flood plain which leads to interaction between ground and surface water. The aquifer is separated by an overlying aquitard consisting of clay with low permeability and an underlying bed rock (aquiclude) made of argillaceous sandstone.

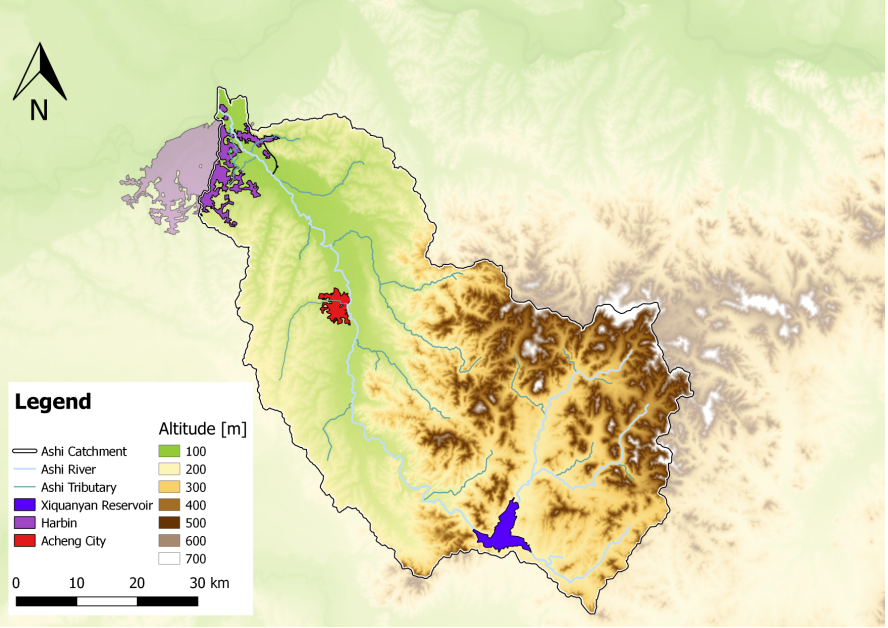

Fig. 1.4: Course of Ashi River and its tributaries

The groundwater in this study area is mainly recharged by precipitation. The drain off consists of discharges to the river and from artificial exploitation as well as evaporation.

1.1.5 Water Quality

The surface water quality in Ashi River deteriorates with the travel time. Upstream of Xiquanyan Reservoir the water quality can be considered as good. Hence, water from Xiquanyan Reservoir has become increasingly important to supply Harbin, especially since pollution of the Songhua River, has become serious with frequent incidents. For instance, a notorious case of contamination occured in 2005 with dimethyl benzene and nitration-grade benzene released from the explosion of a local petrochemical plant discharged into Songhua River.

Ashi River currently meets Grade III standards in the middle part of the river upstream of the city of Acheng. In contrast most of water quality monitoring sections in the parts downstream of Acheng city is worse than Grade V according to the Chinese water quality standard (Fig. 1.5). The main pollution source upstream of Acheng is the agricultural non-point source pollu-

Fig. 1.5: Water Quality in Heilongjiang Catchment, modified from (Ministry for environmental Protection of the People's Republic of China, 2013). On average, Ashi River meets the worst river quality level

tion (herbicides, insecticides, and nutrients) which is complemented by point source pollution from domestic sewage (COD/BOD, Ammonia) and industrial wastewater (heavy metals and toxic organic pollutants) from Harbin and Acheng District further downstream. There are numerous outfalls of industrial wastewater and domestic wastewater and sufficient wastewater gathering and treatment services are lacking. The water pollution influences living conditions and crop production greatly as well as the public health of people at the river side. Another obstacle in reaching better surface water quality is the large ratio of wastewater to natural runoff during dry season when additional surface water is abstracted for local irrigation.

The groundwater in the study area has a quality which makes it usable for both drinking water supply and as raw water for agriculture and industry. The major cations are calcium (23.9-282.4 mg/l Ca^{2+}) and magnesium (3.9-42.8 mg/l Mg^{2+}). Iron (1.7-1.8 mg/l Fe) and manganese (1.4-1.6 mg/l, Mn) concentrations are above the threshold, which is very common for groundwater in this area and geochemically induced. The dominating anion is bicarbonate (51.7-406.8 mg/l HCO_3^-) followed by chloride and sulfate concentrations which are one magnitude less (Wang et al., 2014). The pH of the water can be considered as almost neutral. Data from the early 1990s showed that both organic pesticides (DDT and HCH) and heavy metals (arsenic, cadmium, chromium, etc.) were detectable but significantly below the thresholds. Additionally Nitrate concentrations were very low with 0.76-0.81 mg/l $NO_3^- - N$, although the area was used for agricultural purposes already. Newer studies measured groundwater nitrate concentrations between 0-13.9 mg/l with a

mean of 2.4 mg/l $NO_3^- - N$ (Wang et al., 2014) which inversely correspond with the depth of the aquifer below surface.

1.2 Potential pressures and impacts on Acheng water supply

In contrast to Harbin, the city of Acheng is supplied by groundwater. The water work opened in 1992 with 20 wells in a well field southeast of Acheng city which extract groundwater from the Quaternary aquifer. In 2003, a second well field with 15 wells was opened further south in 2003 in order to cover an increasing water demand (The location of both well fields can be obtained from Fig. 1.1). In 2014, the daily extraction rate of well field 1 was about $35,000\,m^3/d$ and of well field 2 about $10,000\,m^3/d$. The maximum single pumping rate per well is $500\,m^3/h$ and night pumping is preferred due to lower electricity prices.

Table 1.1: Investigated suspected sites within the study area and the corresponding possible pollutants

Suspected Site	Potential threats
Steel works	Hydrocarbons, Phenol, PAH, Cyanides, Heavy metals
Coal power plant	Heavy metals, PAH, Phenol
Wood treatment facility	Hydrocarbons, BTEX (e.g. Benzene), PAH, POP, PCE, Phenol, Heavy metals
Textile manufacturing facility	Hydrocarbons, COD, PCH, POP

1.2.1 Chemical pollutions by industrial point sources

As mentioned above, the city of Acheng is home for several enterprises which may potentially pollute the aquifer either during incidents or on a regular scale. At least four enterprises which deal with potential water harming substances are located within the study area (For specific location see Fig. 1.1). These are the steel work, the coal power plant, the wood treatment facility and the textile manufacturing facility of Acheng city (Tab. 1.1).

The potentially emitting types of pollutants highly depend on the used processes. A steel works may emit suspended solids in all productions steps, oil (< 50 mg/l) in the rolling mill as well as cyanides (up to 1g/l) and aromatic organic compounds such as Phenol (up to 1.5 g/l) in the water draining from

the coke oven plant and the blast furnace (Geny and Dohen, 1972). Furthermore, heavy metals and polycyclic aromatic hydrocarbons (PAHs) may seep from coal piles on the property of the steel works and the coal power plant into the soil and groundwater. Experiments could show that PAH leachate from coal piles may reach several 100 μg/l containing also the carcinogenic Benzo(a)pyrene with up to 30 μg/l (Stahl Jr et al., 1984).

The usage of wood preservatives and organic paints may lead to groundwater contamination in the surrounding of the local wood treatment facility. A study on groundwater samples at five different wood treatment facilities in the US could measure simple volatile aromatic hydrocarbons (BTEX) concentrations of, in sum, up to 600 μg/l. Furthermore, semi-volatile PAH concentrations in the groundwater were in sum up to about 40 mg/l, mainly composing of 4-methylphenol ($\sim$ 11 mg/l), naphthalene ($\sim$ 7 mg/l) and phenanthrene ($\sim$ 5 mg/l) (Rosenfeld and Plumb, 1991). Groundwater samples may also contain elevated concentrations for persistent organic pollutants (POPs) like Pentachlorophenol (Ake et al., 2003) or inorganic compounds such as arsenic, chromium, copper and zinc (Rosenfeld and Plumb, 1991).

Polyester and textile manufacturing facilities possibly pollute soil and groundwater with hydrocarbons, chlorinated organic compounds (PCH) and high loads of COD. Particularly, high Perchloroethylene concentrations in the groundwater up to 4 mg/l could be measured in the vicinity of polluted sites (Nelson et al., 1990). Additionally Pigments and dyes used for textiles could contain persistent organic pollutants like Pentachlorophenol, Dioxins and polychlorinated biphenyls (PCB). The more soluble ones like pentachlorophenol (PCP) which could reach the soil and groundwater by textile wastewater discharge (Krizanec and Marechal, 2006).

1.2.2 Nitrate pollution from diffusive sources

As shown above, more than 85 % of the study site (227 km^2) is used for agricultural purposes. The main cultivated crops are wheat and maize. In China, total N fertilizer consumption became the highest in the world in 1985 and increased continuously in the 1990 (Ju et al., 2004). In 2000 the mean application rate was 155 kg N $\cdot ha^{-}1$ which is also the assumed application in the study area today. In Northern China, excessive fertilization with ammonium-based N fertilizer combined with poor utilization rates caused extremely large amounts of nitrate to accumulate in soil profiles (Zhang et al., 1996). Heavy rainfalls in the summer month leach the nitrate into deeper zones of the upper Loess layer and finally into the groundwater. Artificial irrigation enhances this effect. Former studies estimated that between 5 % and 20 % of the applied N reach the groundwater whereas the trend is increasing due to saturation processes in the soil matrix (Gu et al., 2013). Although assuming that an raising awareness of the existing nitrogen surplus will cap N fertilizer

application rates on current values, the groundwater of the study area will receive a total input of up to 253.32 t NO_3 (111.6 kg/ha) annually.

1.2.3 Future water demand

China experienced a significant increase in water demand in the domestic, industrial and agricultural sectors in the recent past which was mainly driven by population and economic growth, urbanization and changing life styles. This has caused a potential scarcity of available water in several areas such as North-East-China. It was forecasted that the Harbin area will have a shortage in water supply capacity of 950000 m^3/d in 2020, which triggered the construction of new reservoirs (Mopanshan reservoir) and supply routes (Lu, 2007).

Hence, we will compare the water demand today with a twenty-year forecast in order to see how an increasing water demand affects water supply and the groundwater regime.

The annual central water supply V_S needed to cover the demand at the study site can be calculated by:

$$V_S = r_D \cdot V_D \cdot P + r_I \cdot V_I + r_A \cdot V_A \tag{1}$$

Where V_I and V_A are the annual water demand in the industrial and agricultural sector, V_D the domestic per capita water demand, P the population size and the factors r_D, r_I and r_A describe to which ratio the sector specific demand is satisfied by the central water supply system.

In 2015, 73 % of the total Chinese population had access to tap water whereas a large discrepancy exists between rural households (55 %) and urban households (87 %) (World Health Organization, 2015). Regarding the population distribution of the study site, this results a today average r_D value of 0.78 which may increase to a piped connection ratio of about 95 %, in future which is a typical value for industrialized western countries. The average water demand in China is about 85 l/(ca · d) which is assumed to be valid for the study area (Griffiths and Zabey, 2009). Furthermore, it is expected that the domestic water demand will at least double within 20 years reaching a level similar to western industrialized countries which need between 120 liter (Germany) and 260 liter (Spain) of water per person and day (European Environmental Agency, 2002). Nevertheless, this future demand will be still less than the current domestic water demand of Beijing which is approaching 225 l/(ca · d) (Zhang and Brown, 2005). The population of the study site is assumed to be constant.

In China, irrigation is applied on more than (70 %) of the total grain production area and is using more than (80 %) of the total water demand (Seckler et al., 1998). In 1990, annual agricultural water demand in the study

area was assumed to be 120 million m^3/a (Heilongjiang Research Institute for Environmental Sciences(HRIES), 1983). For China, different scenarios show that agricultural water demand could increase by 65 % until 2025 based on the values of 1990 (Seckler et al., 1998). Linearly extrapolating to 2015 and 2035, this would result in an upper limit for agricultural water demand in the study area of 175 million m^3/a and 235 million m^3/a, respectively. As mentioned above, most of the water for irrigation is currently taken from Ashi River upstream of the weirs and from private wells which make a r_A value of 0 reasonable for the year 2015. Particularly, the extraction of surface water from Ashi River during the dry season deteriorates water quality in the river significantly. Hence, it is assumed that irrigation water supply from central groundwater fed supply system may go up to 10 % in 2035.

In 1990, prior to the construction of the water work industrial water demand in Acheng was expected to be 15 million m^3/a provided by private pumps (Heilongjiang Research Institute for Environmental Sciences(HRIES), 1983). In Songhua-basin, industrial water demand increased by 84 % from 1993 until 2003 (Amarasinghe et al., 2004). Reflecting Chinas annual growth rates it is not unlikely that this growth will continue into the future, particularly also in the study area. This would mean that the industrial water demand in 2014 was about 51 million m^3/a and will increase to about 170 million m^3/a within 20 years. The existing domestic demand and the given supply values by the water works suggest that less than 20 % of the industrial water demand are currently satisfied by the central water supply system. It can be expected that this may increase up to 50 % within 20 years.

Finally, these assumptions lead to the calculation of a future water demand of up to more than 130 million m^3/a in 2035 which has to be supplied by the water work. This is about eight times of the current water supply.

Table 1.2: Estimation of water demand and supply today and in 20 years

Sector	Demand $[m^3/a]$	Connection ratio $[-]$	Required supply by WW $[m^3/a]$
2015			
Households	10,858,750	0.78	8,469,825
Industry	50,784,000	0.16	7,955,175
Agriculture	175,714,285	0	0
Total	237,357,035		16,425,000
2035			
Households	217,175,000	0.95	20,631,625
Industry	171,934,310	0.5	85,967,155
Agriculture	234,771,428	0.1	23,477,142
Total	428,423,238		130,075,922

Chapter 2
Modelling strategy

2.1 Work flow

The numerical model should represent the best characterization of the groundwater flow and solute transport process for the aquifer system of the study area in Ashi catchment. In order to simulate the processes, a large number of input data sets from different sources are required. By employing the *OpenGeoSys Data Explorer* we are able to integrate hydrological, geological and geographic input data from different sources to set-up the model. The framework of the *OGS Data Explorer* also supports the creation of finite element meshes and boundary and initial conditions to complex, unstructured geometries (Rink, 2013). Beside *OpenGeoSys* and *OpenGeoSys Data Explorer*, *Paraview*, *QGIS* and *Notepad++* are applied for visualization and further preprocessing/postprocessing steps.

For this case study, a step by step description of the complete model setup will be provided in the following, including remarks on the simulation and post processing of the three-dimensional flow-model. The model set-up covers several steps and three different models of the same study area will be created within the tutorial.

1. Stationary Groundwater flow model
    a. Model geometry (*OGS Data Explorer*)
    b. Surface and subsurface meshes (*OGS Data Explorer*)
    c. Boundary conditions (*OGS Data Explorer*, *Notepad++*)
    d. Process specification, material and numerical parameters, time steps (*Notepad++*)
    e. Simulation (*OGS*)
    f. Results and post processing (*ParaView*)
2. Reactive Nitrate transport model within a stationary flow field
    a. Kinetic biodegradation reaction definition (*Notepad++*)

   b. Boundary conditions (*QGIS*, *Notepad++*)
   c. Extension of existing files (*Notepad++*)
   d. Simulation (*OGS*)
   e. Results and post processing (*ParaView*)

3. Reactive point pollutants model within a transient flow field

   a. First-order decay reaction (*Notepad++*)
   b. Boundary conditions (*QGIS*, *Notepad++*)
   c. Results and post processing (*ParaView*)

2.1.1 Overview of available data-sets

All available topographical, geological and hydrological data of the Ashi River study area catchment were organised and digitalised in the geographic information system *QGIS*. The input data for the model setup contain:
Raster files:

- Digital elevation model of the Ashi catchment (Ashi_DEM.asc)
- Raster data of hydrogeological subsurface layers: unconfined loess layer (unc.asc), Aquitard (aqd.asc) and confined aquifer (conf.asc)
- Groundwater recharge (GWR.asc)

Shape files:

- Boundary of the study area (boundary_line.shp)
- Course of Ashi River (Ashi_River.shp)
- Location of drinking water wells and the water work (wellfield_bottom.shp; wellfield_top.shp)
- Location of Suspicious sites (suspicious_sites_3D.shp)

The digital elevation model with a resolution of three arcseconds, which is about 93 m at this latitude, was obtained from the freely available data set of the Shuttle Radar Topography Mission (`http://www.viewfinderpanoramas.org`). The different raster files of the hydrogeological layers were derived by layer-wise spatial interpolation of existing bore hole data (Heilongjiang Research Institute for Environmental Sciences(HRIES), 1983). This approach was feasible due to the horizontal layering within the study area and the absence of faults. The groundwater recharge is based on the average annual precipitation in the area of 515 mm.

The boundaries of the study area and the river course of Ashi River have been calculated using watershed analysis. The interested reader is directed to the OGS-*Tutorial: Computational Hydrology I* (Sachse et al., 2015) for further information about watershed delineation using GIS software.

The location of the groundwater wells and the abstraction rates are provided by local authorities. Land cover data was obtained by satellite data from China's GlobeLand30 data set.

2.1.2 Software requirements

The first step in order to start our numerical modelling will be to download all the necessary softwares and the needed input files. For this tutorial, we use only open access software which is easily available for any user from different web sources. Please download the softwares individually from the following sources considering your user system (32-Bit or 64-Bit).

1. *OGS* version 5.7.0 : https://docs.opengeosys.org/download5
2. *OGS Data Explorer* version 6: https://docs.opengeosys.org/download
3. *GMSH*: http://gmsh.info/#Download
4. *QGIS*: http://www.qgis.org/en/site/forusers/download.html
5. *ParaView*: http://www.paraview.org/download/
6. *Notepad++*: https://notepad-plus-plus.org/download/v6.7.8.2.html
7. Input Files: https://docs.opengeosys.org/books/computational-hydrology-ii-groundwater-flow-modeling

Chapter 3
Stationary Groundwater model

3.1 Meshing

3.1.1 2D Meshing

The mesh creation process via the *OGS Data Explorer* requires the selection of geometric data sets and the parametrization of those elements by the graphical user interface of the *OGS Data Explorer*.

The mesh generation should be done with great care since it influences both the quality and time of the solution of the equation system. Setting up a new model usually starts with the import of a number of geographic and hydrogeological datasets which were provided as GIS shape data.

Firstly, open the *OGS Data Explorer* and click on `File` →`Import files` →`Shape Files` to integrate the model geometry into the data explorer. Please import all shape files within the project folder ...\files\Topography into the *OGS Data Explorer*. Note that the shape file which includes point data can be imported both as geometric or station points. The station points can be checked if the points contain additional information such as observation sites of data loggers or boreholes. The import as the stations is useful for boreholes records.

- Ashi_River.shp (as polylines)
- boundary_line.shp (as polylines)
- Fanjia_River.shp (as polylines)
- Suspicious_site_3D.shp (as station points)
- wellfield_bottom.shp (as station points)
- WW_WWTP_3D.shp (as station points)

The visualized results are shown in Fig. 3.1. The *OGS Data Explorer* provides several tools to visualize data which are documented in the previous tutorial (Sachse et al., 2015).

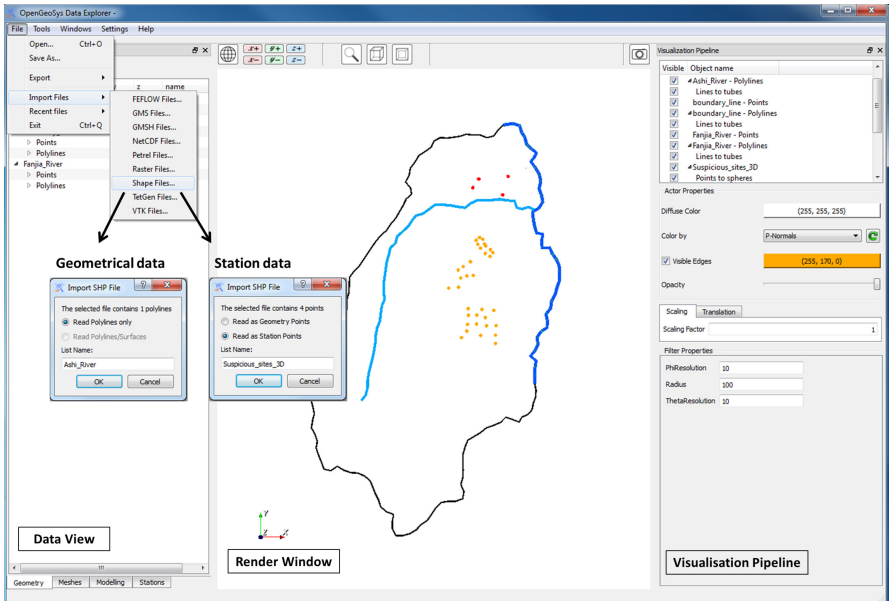

Fig. 3.1: Uploaded Geometries in *OGS Data Explorer*

The meshing in *OGS Data Explorer* requires external finite element mesh generators and supports either *GMSH* or *Tetgen* mesh generator. For our example, please make sure that you have downloaded the *GMSH* executable and set a full path to the *GMSH* folder in the data explorer by clicking on `Settings` →`Data Explorer Settings` →`Path to` *GMSH*.

Next, click on `Tools` and select `Create Mesh From Input Data` in order to start the 2D meshing. In the appearing window move all available geometry information to the right side and press on the label `Advanced` for meshing options.

In principle, two meshing options are available:

1. *Adaptive Meshing:* The element density increases towards the geometric features. The physically location of input points and lines is precisely represented by nodes within the mesh. The three given options can be used to define how refined the mesh should be close to input points (max. number of points in a quadtree leaf) and how fine the mesh density should be in general (mesh density scaling for points and stations).
2. *Homogeneous Meshing*: Mesh elements have roughly the same size. Physical points contained in lines are represented by mesh nodes, but geographical point information such as wells is not.

The designing of the mesh is a very critical step in applying a groundwater model. A finer mesh provides a more accurate spatial solution but needs more

computation time. For this case study, we choose homogeneous meshing with a relatively large element size of 500 m. The meshing procedure may take several seconds depending on the options and your CPU. Finally, a triangulated mesh named "tmp_gmsh" appears in the *Meshes Data View* (Fig. 3.2). Save the mesh_file as "Ashi_2D.vtu" using the disk symbol right above the *Meshes Data View*.

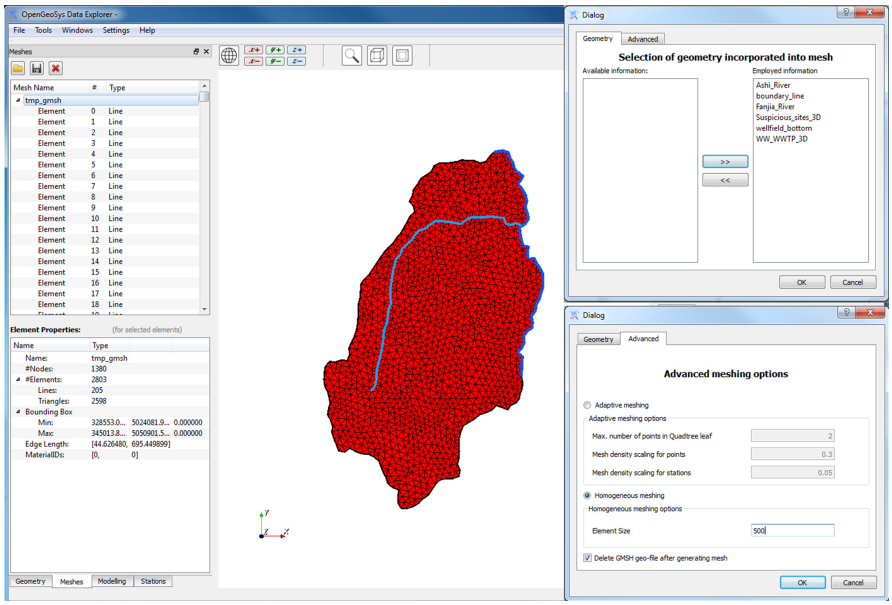

Fig. 3.2: Planar meshing procedure

The element properties can be displayed by selected the mesh in the *Meshes Data View*. The 2D mesh should contain about 2840 elements and about 1380 nodes, although this number may slightly vary in your case.

3.1.2 Volume Meshing

For generating a 3D mesh of our study area, the 2D mesh which z-component is zero has to be extruded by adding the surface and geological information mapped as raster files. From top to bottom, these are the lower boundaries of the loess layer (unc.asc), the aquitard (aqd.asc) and the confined gravel aquifer (conf.asc). To extrude the mesh, follow the instructions:

- Right-click on the 2D mesh in the *Meshes Data View*

- Click on `Edit Mesh`
- Specify in the appearing dialogue the number of mesh layers, which should be attached to the 2D mesh. Due to the geology of the study area we have to add three layers and press `Next`.
- Activate `Add layers based on raster files` and click `OK`.
- Choose the file DEM_-1.asc as the surface and the subsequent geological layers. The one meter lowered DEM has to be used in order to add a topsoil layer later (chapter 3.1.3).
- Choose `Prisms` element as output and a minimum thickness of 2 m in order to avoid quasi planar 3D elements.
- Finally press `OK`.

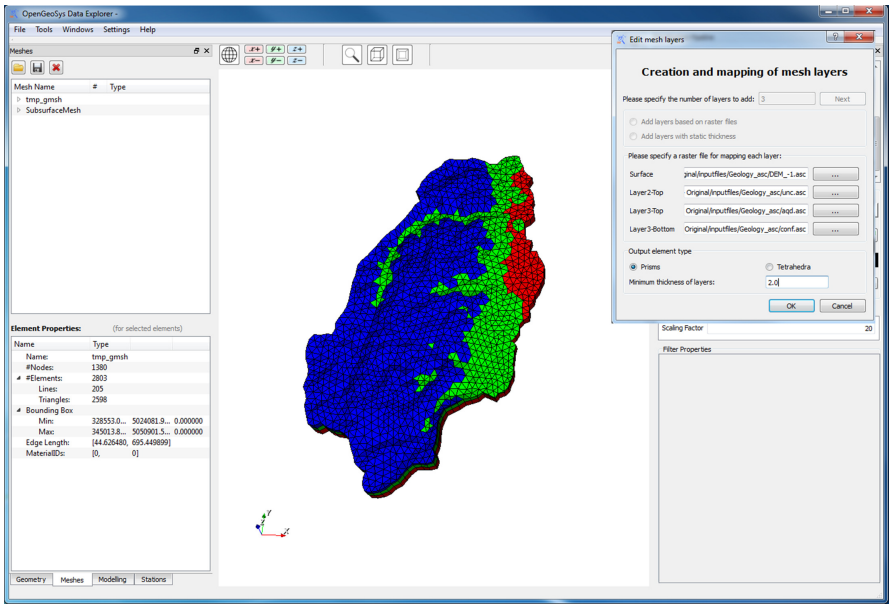

Fig. 3.3: Final 3D mesh of the study area with outcropping geological layers

For better exploring details of the three dimensional mesh, which should contain about 4800 nodes and 6800 elements, the scaling factor should be set to 20 in the *Visualization Pipeline*. The final mesh matches with the previous qualitative description of the geology (chapter 1.1.4). The loess layer is eroded in the valleys of the study area and the usually confined aquifer becomes unconfined in the flood plain (Fig. 3.3).

3.1.3 Adding soil layer

In reality, the geological layers do not outcrop to the topographical surface but are covered by a thin soil layer which properties depend on the type of land cover/land use. In order to account for that we will add a 1 m thick soil layer on our 3D mesh with the help of a tool called `Add Layers`. First, click on the right mouse button on the produced 3D mesh ("SubsurfaceMesh") in the *Meshes Data View* and select `Add Layers`. Choose `at the top of the mesh` and define 1m for `Thickness of new layer`.

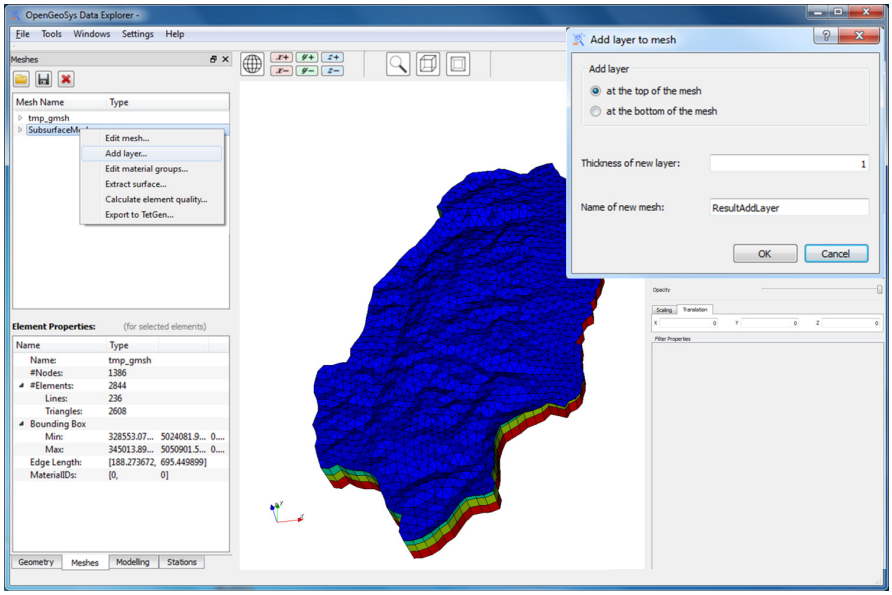

Fig. 3.4: 3D mesh with added soil layer

3.1.4 Mesh Quality

As mentioned above, the accuracy and reliable of numerical results highly depend on the quality of the finite element mesh. The *OGS Data Explorer* provides several tools to evaluate the mesh quality (Fig. 3.5). For qualitative evaluation, please click on the upper tool bar and click on `Tools` and `Analyze Mesh`. In the appearing window selected the "ResultAddLayer" mesh and start the analysis. As an optimum, no nodes or elements should be listed in any field. Some problems such as collapsible nodes and elements without

volume will lead to a failure in the conduction of the numerical simulation whereas other like the wrong node order may have a minor impact on the flow simulation but significantly the spatial allocation of boundary conditions by using *OGS Data Explorer*. The *OGS Data Explorer* further provides options to quantify the mesh quality by clicking right on the selected mesh and choose `Calculate Mesh Quality`. Several parameters are available to evaluate the shape of the elements. If either the qualitative or the quantitative Mesh analysis shows significant problems of the mesh, the mesh should be created again, using a different resolution or meshing option.

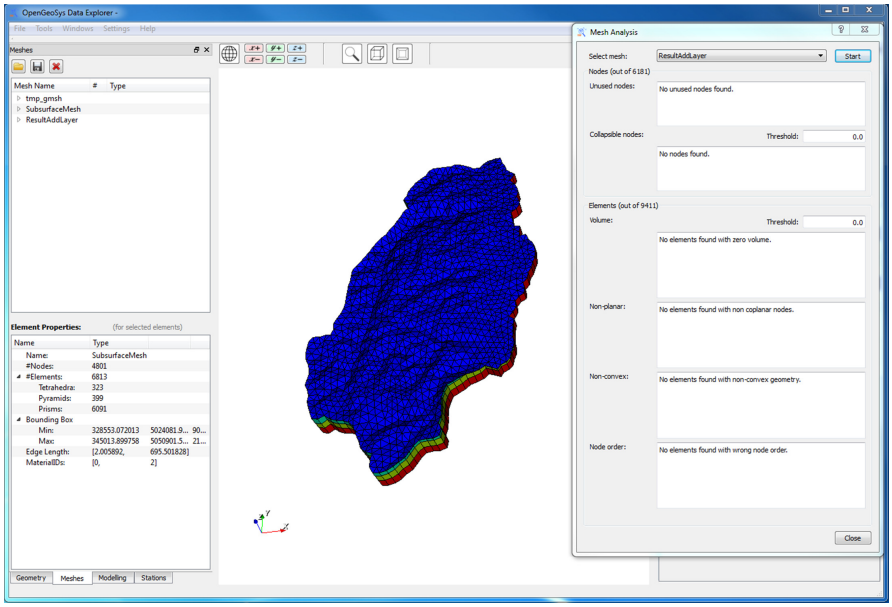

Fig. 3.5: Mesh Quality Analysis using the *OGS Data Explorer*

3.2 File Transformation into *OGS* input files

OpenGeoSys follows an object orientated approach and takes the input data for the simulation from ASCII input files with specified filename extensions. The number of files depends on the simulated process. Some files can be generated from the *OGS Data Explorer* but others have to be created manually using *Notepad++* or similar software (e.g. *Notepad*). After set-up our geometry and mesh, we need to transfer our files into ASCII code which can be used as an input data of the *OGS* 5 executable.

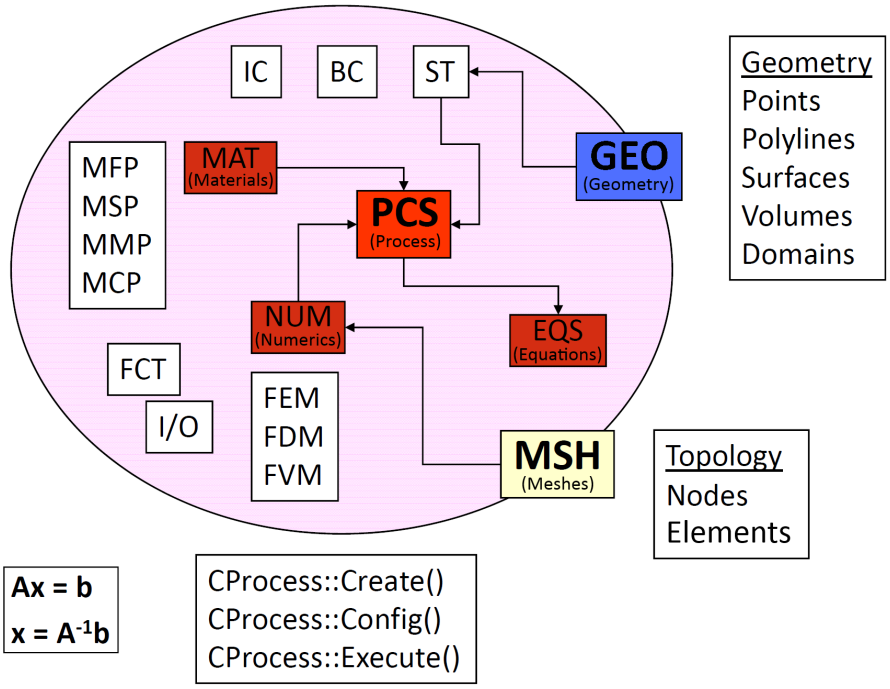

Fig. 3.6: Object-orientated structure of *OpenGeoSys* Version 5 (Kolditz et al., 2012)

Before converting the geometry in the *Data Explorer* in an *OGS* 5 input file we have to name the specific points of the geometry because the attribute tables of the shape files could not be imported by the *OGS Data Explorer*. Note that it may be necessary to import all shape files as geometry points. Please set names according to Tab. 3.1 by clicking right on the specific point and choosing `Set name`.

After entering all names, please merge all objects in the *Geometry Data View* by clicking on `Tools` from the main menu and then and `Merge geometry`. Name the new geometry data simply "Ashi" and save the new data as "Ashi.gml" using the disk symbol in the *Geometry Data View*. The file conversion of the gml geometry-files and the msh-files is conducted by the *OGS File Converter*. Click on `Tools` →`File Converter` and convert both geometry (Ashi.xml) and mesh (Ashi_3Ds.vtu) to ASCII file format one after another. Please create a new folder called "Stationary_GW_Flow" and transfer all existing ASCII files (Ashi.gli, Ashi.msh) into this folder, which should be used to save any following *OGS* input file created for the stationary groundwater flow model.

Table 3.1: Assigning names for geometric objects

File	Point	Name
Wellfield_top	0	Well1_t
...	...	...
Wellfield_top	33	Well34_t
Wellfield_bottom	0	Well1_b
...	...	...
Wellfield_bottom	33	Well34_b
Suspicious_sites	0	Coal power plant
Suspicious_sites	1	Wood treatment facility
Suspicious_sites	2	Textile manufacturing facility
Suspicious_sites	3	Steel works
WW_WWTP	0	Water works
WW_WWTP	1	Waste water treatment plant
File	Polyline	Name
Ashi_River	Line0	Ashi_River
boundary_line	Line0	boundary_line
Fanjia_River	Line0	Fanjia_River

3.3 Boundary conditions

3.3.1 Source terms

Before we leave the interface of the *OpenGeoSys Data Explorer* and switch to the easily manually editable *OGS*5 input files, we will use the potential of an older version of the *OGS Data Explorer* (V.6.00) to set up boundary conditions on mapped surfaces, in our case the groundwater recharge.

For each surface element, the water balance equation for groundwater recharge is:

$$R = P - ET - S \tag{1}$$

P is the average precipitation, ET the total evapotranspiration, S the surface runoff and R the groundwater recharge. This means that only a part of the rainfall will recharge the aquifer. The ratio depends mostly on climate factors (temperature, wind speed, etc) and land cover/land use related factors (soil type, vegetation, impervious and compacted surfaces, irrigation pattern, etc.).

A study in the Songhua floodplain in northern Jilin provinces, which shares a similar climate (Paul, 2006) estimates groundwater recharge ratios r in dependence on the land cover (Tab. 3.2). Due to the climatic similarities we can use this data to delineate groundwater recharge in our study area related to land cover by simplifying equation 1 to:

Table 3.2: Recharge ratio depending on land cover in southern Songhua-River Basin

Land-use type	Recharge ratio r [–]
Water	0
Grasland	0.28
Farmland	0.37
Rural settlement	0.39
Urban settlement	0.19
Forest	0.6

$$R = r \cdot P \tag{2}$$

Please open the *ogs_gui.exe* of the data explorer 6.00 version[1] and load the "Ashi_3Ds" mesh into the *Meshes Data View*. Then click right on the mesh and choose `DIRECT Conditions` →`load`. In the appearing window choose the correct descriptions from the pop-up menus according to Fig. 3.7 and press on *calculate values*. In the new window select the "Recharge.asc" file, which contains the land cover dependent in the demonstration area, as raster input and select the calculation method *integrate over the mesh elements* with a scaling factor of 31536000000. *OGS* uses SI standard units such as second, meter and kg for its calculation but recharge is given in mm/year. Hence, the factor 31536000000 is needed to convert mm/a to m/s. Please press two times OK to conduct the calculation and to close the windows. Save the result "Ashi.cnd" by selecting `Modelling` in the *Data View* and then right click on `Groundwater model` and choose `Save FEM`. Similarly to the geometry and mesh data, convert the cnd-file into ASCII-files by using the *OGS Data Explorer* and the option `XML conditions to ASCII`. Finally, close both versions of the *OpenGeoSyS Data Explorer*. Subsequently two new files, "Ashi.st" (*OGS* 5 input file) and "direct_value0.txt" file emerge in the specific folder. The "direct_value0.txt" file consists of two columns. The first column contains all nodes which are located on the surface of the 3D Mesh (node numbers from 0 to about 1380) and the second column the corresponding recharge for each node which defines a local Neumann boundary condition. The values should be in a range of $\sim 10^{-3}$ m/s and depend on the size and orientation of each mesh cell. Please rename the file to "recharge.txt" and copy both files into your Stationary_GW_Flow-folder.

The already created "Ashi.st" file can be used to add the groundwater pumping rates as additional source terms. Please open the "Ashi.st" file and have a look on the structure:

[1] Please note that the new features of the DataExplorer are currently available. For more information, updates and useful links, please visit our webpage: `https://docs.opengeosys.org/docs/tools/getting-started/overview`.

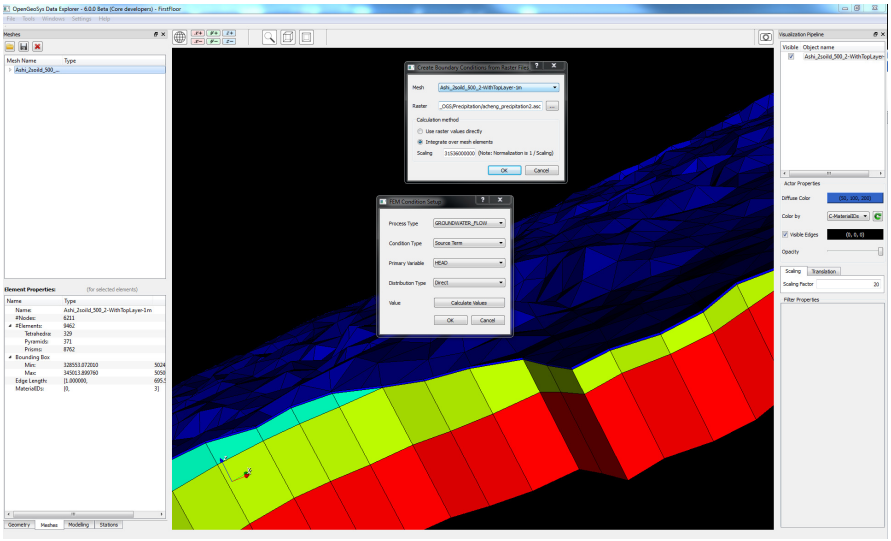

Fig. 3.7: Assigning direct FEM conditions with *OGS Data Explorer*

Listing 3.1: Source term File (Ashi.st)

```
GeoSys-ST: Source Terms--------------------------
#SOURCE_TERM
$PCS_TYPE
GROUNDWATER_FLOW
$PRIMARY_VARIABLE
HEAD
$DIS_TYPE
DIRECT direct_values0.txt
#STOP
```

The first line is a header line and can be ignored. The `#SOURCE_TERM` keyword indicates the beginning of a source/sink term description. Each process related description ends with the beginning of a new block, i.e. another `#SOURCE_TERM`. The last block ends with the file input terminator `#STOP`. In our case, only one block is defined, which is related to groundwater recharge. The first-subkeyword `PCS_TYPE` enables the specification of the process to which the following source term belongs. In our case, it is `GROUNDWATER_FLOW`. The keyword `PRIMARY_Variable` is needed to define the units of the calculation, for `GROUNDWATER_FLOW`, the primary variable is always hydraulic `HEAD`. `DIS_TYPE` specifies the way of how data are distributed over the defined geometric object. In our case `Direct` is defined as discharge type which means that the source/sink term values are assigned to nodes directly by reading them from an external file. The path and name of the file are given in the next line. Please replace the command line C : \...\...\...\...\`Boundaries/direct_values0.txt` by the simple ex-

pression `recharge.txt`. This is sufficient as long as both files are in the same folder.

Next, we will add new data blocks above the `#STOP` in order to implement the drinking water wells. The wells 1-19 abstract at an average rate of $-2.3 \cdot 10^{-2}\,\mathrm{m}^3/\mathrm{s}$ and the remaining wells 20-33, which refer to wellfield 2, have an abstraction rate of about $-7.7 \cdot 10^{-3}\,\mathrm{m}^3/\mathrm{s}$. Keep in mind that we define each well with two points on the top and at the bottom of the aquifer layer. Hence, the actual pumping values for each point are $-1.065 \cdot 10^{-2}\,\mathrm{m}^3/\mathrm{s}$ and $-3.85 \cdot 10^{-3}\,\mathrm{m}^3/\mathrm{s}$. Therefore add for each well point the following data block:

Listing 3.2: Source term File (POINT well1_t)

```
#SOURCE_TERM
$PCS_TYPE
GROUNDWATER_FLOW
$PRIMARY_VARIABLE
HEAD
$GEO_TYPE
POINT well1_t
$DIS_TYPE
CONSTANT -1.065e-002
```

In total, 66 data blocks should be added. You can use copy and paste but pay attention to changing name and pumping rates.

In contrast to the previous boundary conditions, the sub-keyword `GEO_TYPE` is used in the new data block. It describes for which type of geometry (0D-Point, 1D-Polyline, 2D-Surface, 3D-domain) the conditions are defined. In all cases except of domain, the name of the specific geometry has to be added as a second word in the line (e.g. `POINT Well1_t`). The parameter `CONSTANT` after the sub-keyword `DIS_TYPE` assigns the constant flux to the geometry.

Finally, proof that only the last line of the file contains the `#STOP` expression and save the file.

3.3.2 Boundary conditions

Beside of the definition of specified fluxes as source terms (*.st), it is additionally possible to define values for the primary variable (e.g. head, temperature, concentration) itself on certain areas of the model domain within a Boundary Condition File (*.bc). All surfaces of the model domain for which no boundary condition are defined, are treated as no flow boundaries. According to our definition of the study area as a sub catchment all surfaces except the one referring to the river course of Ashi River are no flow boundaries. In reality, the water level of Ashi River is variable in space and time. For our very first stationary groundwater model, we will neglect these variations and assume a constant head of 137 m, which is the spatially and temporarily averaged head of Ashi River in the study area. Furthermore it is assumed that no upwelling or down-welling conditions occur in the river bed, which means that

surface water levels equal groundwater heads in the vertical direction. The consideration of the river slope will be added in a later part of the tutorial (see Chap. 5) by the help of the software *QGIS*.

Please open *Notepad++* and open a new form and add the following lines which are almost similar to the source term definition file. Subsequently save the file as "Ashi.bc".

Listing 3.3: Boundary condition

```
#BOUNDARY_CONDITION
$PCS_TYPE
GROUNDWATER_FLOW
$PRIMARY_VARIABLE
HEAD
$GEO_TYPE
POLYLINE Ashi_River
$DIS_TYPE
CONSTANT 137
#STOP
```

3.3.3 Initial Conditions

The initial conditions (*.ic) are simply the values of the primary variable (hydraulic head in our case) specified at a certain location in the model domain at the starting time of the simulation. Initial conditions in the range of the expected results help to save computation time. In our case an initial head of 175 m for the entire study area (domain) is reasonable considering the average altitude of the study area.

Please set-up the initial condition by creating an "Ashi.ic" file with *Notepad++*. The following code has to be entered into the file:

Listing 3.4: Initial condition

```
#INITIAL_CONDITION
$PCS_TYPE
GROUNDWATER_FLOW
$PRIMARY_VARIABLE
HEAD
$GEO_TYPE
DOMAIN
$DIS_TYPE
CONSTANT 200
#STOP
```

3.4 Material properties

Material parameters required for the simulation are specified in an *.mmp file. As we have defined 4 geological layers in our mesh we have to write 4 material-property blocks. The blocks are ordered from bottom to top and the first block refers to the finite elements having the Material-ID 0. The permeability values of the 4 geological layers were derived from hydrogeological data and calibration with PEST software using plausible parameter ranges. It is important to mention that the permeability value of the topsoil layer highly depends on the land cover. For instance, a sealed surface has a permeability of nearly zero. According to Darcy law this would result in a hydraulic head approaching infinity as the groundwater process simulation does not include surface runoff. Furthermore, the loess layer is treated as a saturated zone in *OGS* by using the process groundwater flow although unsaturated flow is implemented in *OGS*, too (process type `Liquid flow`). Hence, the real (saturated) permeability of the loess layer may differ.

Thus, we decided to choose permeability value for both layers which are most likely not realistic but lead to a good correlation between simulated and measured hydraulic heads.

Table 3.3: Permeability values referring to the geological layers

Layer	Material_ID	Permeability $[m/s]$
Soil	0	$1 \cdot 10^{-4}$
Loess	1	$1 \cdot 10^{-4}$
Aquitard	2	$1 \cdot 10^{-6}$
Aquifer	3	$2 \cdot 10^{-3}$

For the porosity and tortuosity, values of 0.3 and 1, respectively are assumed for each layer.

Please create an “Ashi.mmp” file and add the following text-block 4 times for each geological layer. The order is important and should be from bottom of the geological model to the top.

Listing 3.5: Medium properties file: Ashi.mmp

```
#MEDIUM_PROPERTIES
 $NAME
 Aquifer
 $GEOMETRY_DIMENSION
 3
 $GEOMETRY_AREA
 1.000000000000e+000
 $POROSITY
 1      0.3
 $PERMEABILITY_TENSOR
 ISOTROPIC      .00100000000
 $TORTUOSITY
```

```
 ISOTROPIC 1
#MEDIUM_PROPERTIES
 [..]
#MEDIUM_PROPERTIES
 [..]
#MEDIUM_PROPERTIES
 [..]
#STOP
```

3.5 Additional *OGS* Input files

Beside the already defined geometry, material parameters and process boundaries, *OGS* needs additional files dealing with:

1. the simulated process (*.pcs),
2. the numerics (*.num),
3. time discretization (*.tim)
4. output (*.out.)

3.5.1 Process specification

Our process is `GROUNDWATER_FLOW` which can be described by adding the following lines in a new txt-file and save it as "Ashi.pcs":

Listing 3.6: Process file: Ashi.pcs

```
#PROCESS
$PCS_TYPE
GROUNDWATER_FLOW
#STOP
```

3.5.2 Numerics

The numerical file (Ashi.num) defines and controls the numerical solver. For each process specified in the "Ashi.pcs" file, one set of numerical parameters is required in a "Ashi.num" file:

Listing 3.7: Numeric parameters file: Ashi.num

```
#NUMERICS
$PCS_TYPE
GROUNDWATER_FLOW
$LINEAR_SOLVER
```

```
; method convergence criteria error_tolerance max_iterations theta
    preconditioning storage
2 1 1.000000000000e-14 2000 1.0 100 4
#STOP
```

The keyword linear solver enables the set up for numerically solving linear problems e.g. groundwater flow. The comment line (indicated by a semicolon) explains the meaning of the line below. For further information, the interested reader is referred to the input file documentation (http://www.opengeosys.org/help/documentation/).

3.5.3 Time stepping

Next, we will define the time stepping in the file "Ashi.tim". For each process one data set has to be defined. For our stationary groundwater model, only one time step with a time length of one second is necessary for the simulation run.

Listing 3.8: Time discretisation file: Ashi.tim

```
#TIME_STEPPING
$PCS_TYPE
GROUNDWATER_FLOW
$TIME_START
0
$TIME_STEPS
1 1
$TIME_END
1
#STOP
```

3.5.4 Output

Finally, it has to be defined in an "Ashi.out" file how and when simulation results are written. For our groundwater flow model the output should be defined as:

Listing 3.9: Example output parameterisation file: ammer.out

```
#OUTPUT
$PCS_TYPE
GROUNDWATER_FLOW
$NOD_VALUES
HEAD
VELOCITY_X1
VELOCITY_Y1
VELOCITY_Z1
$GEO_TYPE
```

```
DOMAIN
$DAT_TYPE
VTK
$TIM_TYPE
STEPS 1
#STOP
```

For our model, we want to get head values and velocity field data from each node (`NOD_VALUES`) for the whole domain (`GEO_TYPE`) at the time step 1 (`TIM_TYPE`) as output data. Possible output data types are ASCII-tecplot-files (TEC), Visualization Toolkit files (VTK) and *ParaView* data files (PVD).

3.6 Model Execution

After setting up all input files, our model is ready for the simulation. Please proof that all required input files (Tab. 3.4) are within one folder. Next, add the executable *ogs.exe* [2] to the folder containing the input files

Table 3.4: Required files for groundwater flow simulation with *OpenGeoSys*

Type of file	File name
Geometry	Ashi.gli
Mesh	Ashi.msh
Initial Condition	Ashi.ic
Boundary Condition	Ashi.bc
Material Properties	Ashi.mmp
Source Term	Ashi.st; recharge.txt
Process Control	Ashi.pcs
Time Step Control	Ashi.tim
Numeric File	Ashi.num
Output Control	Ashi.out

and open the executable. In the command line enter the word `Ashi` and press Enter (Fig. 3.8). The calculation starts and will be conducted within seconds. As results the files "Ashi_GROUNDWATER_FLOW0000.vtk" and "Ashi_GROUNDWATER_FLOW0001.vtk" should appear in your data folder. The latter one contains the calculated flow field after a simulation time of one second.

Unfortunately, *OGS* 5 neither records the output lines in the command window nor has an adequate error output. Starting *OGS* with a batch file help to overcome these problems. Create a "Ashi.bat" file with *Notepad++* which consist of one line:

[2] Please download the OGS executable (Version 5.6): https://docs.opengeosys.org/books/computational-hydrology-ii-groundwater-flow-modeling

`ogs.exe Ashi >Ashi_Protocoll.txt`

By clicking double on the Ashi.bat file, *OGS* will conduct the simulation and the *OGS* process output is stored in the txt-file called "Ashi_protocoll.txt".

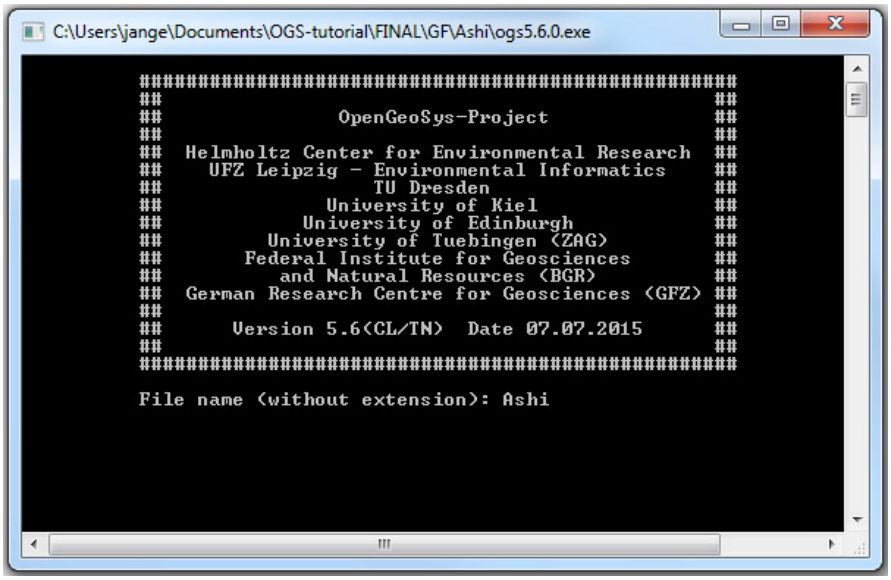

Fig. 3.8: Command window of the *OpenGeoSys* executable

3.7 Results

For the visualization of our first results, we will use the Open Source Software *ParaView*, which is applied in a multitude of scientific research fields (Fig. 3.9). Please open *ParaView* and click on `File` →`Open` in the main toolbar. Please locate the *OGS* project folder and open the file "Ashi_GROUNDWATER_FLOW0001.vtk" which will appear in the pipeline browser. Click on the data set and press `Apply` in the properties window. The study site should appear in the layout window. In the colouring sub-menu click on `Show` to see the range of head values. The result show that the head is less in the floodplain and higher in the southeastern part of the study area. Thus, the head distribution in general aligns with the altitude of the study area. Head differences and subsequently hydraulic gradients are rather small in most parts of the study area which is typical for a lowland aquifer. On the other hand, the hydraulic head variations do not mimic the smaller scale topography of the

area which includes several valleys. One reason is the relatively large distance between surface and groundwater level in the plateau of about $20 - 30\,\mathrm{m}$ at well field1, but also uncertainties in the geology, the coarse mesh resolution, and the lacking of measured water tables outside the well fields may also contribute to this result.

Additonally, *ParaView* allows us to visualize the velocity field of the study area. Please split the *Layout View* by clicking on the icon `Split horizontal` in the upper right corner. Choose `Create 3D View` from the following dialog. A new empty window should appear. In the pipeline browser mark the "Ashi_Groundwater_Flow0001.vtk" data set and select from the main toolbar: `Filters` →`Common` →`Glyph`. A new data set called "Glyph1" will appear in the *Pipeline Browser*. Select the empty window and click on `Apply` in the "Glyph1" data set properties. Now, the velocity field is visible in the *Layout View*. A better visibility is reached by choosing the scale mode `Scalar` with the scaling factor 10 in the *Properties Menu*.

Velocities at most nodes are on average in a magnitude of $10^{-6}\,\mathrm{m/s}$ which is about $0.1\,\mathrm{m/d}$. The flow direction is from south-west to north-east to the river which means that the river is under gaining conditions within the entire domain.

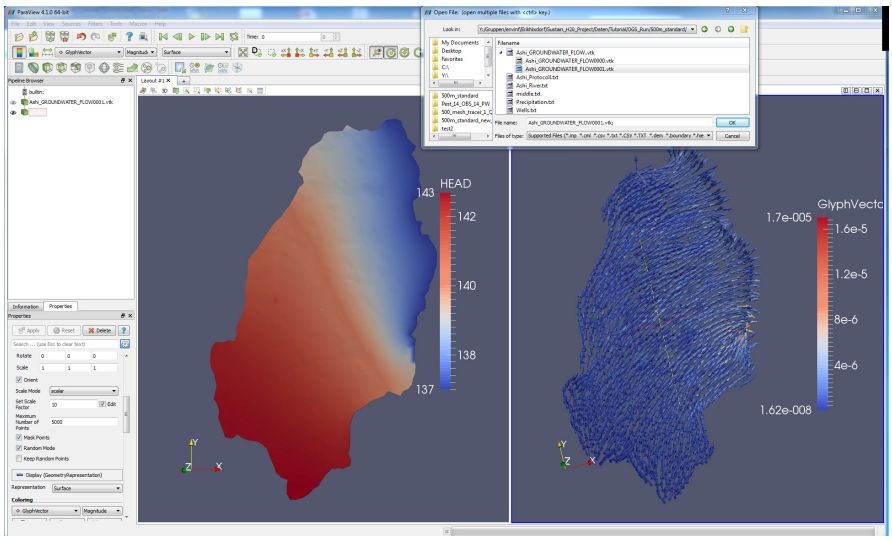

Fig. 3.9: Result visualization with *ParaView*

Chapter 4
Reactive Nitrate transport model

One of the main applications of numerical groundwater models is to predict future field behavior. For our study area, we want to use the already established stationary groundwater flow model to forecast the development of nitrate pollution in the aquifer for the next 20 years. Hence, we will superimpose matter transport on the steady groundwater flow field.

4.1 Nitrate allocation and degradation in the subsurface

In general, the change in concentration of each species within a volume of groundwater can be described by the advection-dispersion equation:

$$\nabla \cdot (\mathbf{v} C_i) + \nabla \cdot (D \nabla C_i) + R\left(C_1, ...C_i, ...\right) = \frac{\partial C_i}{\partial t} \tag{1}$$

The equation contains (from left to right) two conservative transport terms (advective transport and dispersive transport), a reaction term which could include effects of various chemical processes and a rate change in concentration term. *OGS* calculates the two conservative terms and the reactive term separately using an iterative two steps sequential approach. This allows the use of different mathematical solvers and the possibility of decoupling time scales for transport and chemistry.

Although the conservative transport is similar for each species as long as the concentration do not affect the flow field (e.g. density-dependent flow), the reaction term can incorporate species dependent processes and reactions such as precipitation and re-dissolution, f locculation, redox-reactions, adsorption, ion exchange, complexation, nuclear decay, etc. Hence, we have to specify in which reactions Nitrate is involved within the saturated zone.

In general, nitrate is degraded in the subsurface to the end-product nitrogen. This process occurs in the presence of organic carbon compound (denoted CH_2O) and or reduced iron sulphide compounds whereas the first reaction

path is thermodynamically favored (e.g Pauwels (1994)):

$$CH_2O + \frac{4}{5}NO_3^- + \frac{4}{5}H^+ \overset{Denitrifier}{\rightarrow} CO_2 + \frac{2}{5}N_2 + \frac{7}{5}H_2O \tag{2}$$

The degradation is carried out by some microbial species (denitrifier) which are able to cover their oxygen demand from the oxygen bound in the nitrate, if free oxygen molecules are available in low concentrations (<2-5 mg/l), only (Wendland, 1994).

Considering these 4 species and regarding their different occurrence in different phases i.e. the mobile pore water, the biophase and the aquifer material, Kinzelbach et al. (1991) listed 16 equations (8 transport equations and 8 explicit source terms) which has to solved to calculate nitrogen degradation rates. Although *OGS* is able to solve this or even more complex kinetic reaction systems by using a coupling interface between *OGS* and *IPhreeqc* (e.g. (He et al., 2015)), we will simplify the nitrate degradation reaction to one equation based on multi-parameter Monod-kinetics which is commonly used in environmental engineering to calculate denitrification rates in waste water treatment systems (e.g. (Batchelor, 1982; Wang et al., 2009)) but has also been already applied to describe denitrification in the groundwater (Holzbecher, 2012; Kinzelbach et al., 1991):

$$\frac{\partial C_{NO3}}{\partial t} = \left(-\mu_{Denit\_m}\frac{C_{Denit}}{Y_{Denit}}\right) \cdot \frac{C_{NO3}}{K_{NO3}^{Denit} + C_{NO3}} \cdot \frac{C_{OC}}{K_{OC}^{Denit} + C_{OC}} \cdot f\,(DO) \tag{3}$$

The first part of the equation contained in the brackets describes the maximum degradation rate of nitrate k_{NO3_m}.

$$k_{NO3\_m} = -\mu_{Denit\_m} \cdot \frac{C_{Denit}}{Y} \tag{4}$$

It depends on the maximum biomass growth (μ_{Denit}), the biomass concentration of the denitrifiers (C_{Denit}) and the yield coefficient (Y) which describes how much biomass is produced per unit nitrate.

$$k_{NO3\_m} = -\mu_m \cdot \frac{C_{Denit}}{Y} \tag{5}$$

Assuming a constant biomass concentration over time, both the maximum biomass growth and the maximum nitrate degradation rates are constant values (Bekins et al., 1998). The two monod terms approach one at high concentrations of nitrate and dissolved organic matter and zero at low concentrations. The reaction is inhibited by sufficient amount of oxygen. The oxygen dependence can be for instance described by a monod-like inhibition term (Holzbecher, 2012) or by a DO-dependent weight function (Kinzelbach et al., 1991).

The monod half-saturation coefficients concentrations K_{NO3}^{Denit} and K_{OC}^{Denit}, the reaction dependence on dissolved oxygen $f(DO)$ and the maximum biomass growth rate μ_{max} depend on many factors (such as aquifer properties, microbial community, pH, temperature, ...) and may vary in space and time at the field site. Hence, they either have to be obtained from literature or lab experiments.

The monod kinetics equation mathematically reflects the research results that for small nitrate concentrations, nitrate reduction is to be first-order kinetics and for nitrate concentrations larger 20 mg/l, the denitrification seems to be zero order kinetics, independent from the actual nitrate concentration (Wang et al., 2009). Furthermore, microbial denitrification rates are more sensitive to organic matter concentration than nitrate concentration, which means that K_{OC} should be larger than K_{NO3}. Concerning the time scale for denitrification, for German aquifer, half-life times for nitrate freshly recharged to groundwater vary in a range between 2 and 35 years (Wendland, 1994).

Under aerobic conditions, the metabolism of organic matter depletes the dissolved oxygen in groundwater:

$$CH_2O + O_2 \overset{Decomposer}{\rightarrow} H_2O + CO_2 \tag{6}$$

For further simplifications we assume that carbon decay is following a first order decay which means that the rate of metabolism of the bacteria (Decomposer) is directly proportional to the concentration of utilizable organic matter (e.g. Holzbecher (2012); La Scala Jr. et al. (2009)):

$$\frac{\partial C_{CO}}{\partial t} = k_{OC\_m}^{1st} \cdot C_{OC} \cdot C_{DO} \tag{7}$$

This first order kinetics equation can be rewritten as a monod kinetics assuming that the half saturation constants are significantly larger than the substrate concentrations.

$$\begin{aligned} \frac{\partial C_{CO}}{\partial t} &= \frac{k_{OC\_m}^{1st}}{K_{OC}^{Decom} \cdot K_{OC}^{Decom}} \cdot C_{OC} \cdot C_{DO} \\ &= \left(-\frac{\mu_{Decom\_m}}{K_{OC}^{Decom} \cdot K_{OC}^{Decom}} \cdot \frac{C_{Decom}}{Y_{Decom}} \right) \cdot C_{OC} \cdot C_{DO} \\ &= k_{OC\_m} \cdot C_{OC} \cdot C_{DO} \end{aligned} \tag{8}$$

Similarly to the denitrification, decomposer concentration is assuemd to be constant over time.

The maximum bacteria growth rates for Decomposers are higher than for Denitrifiers (Liwarska-Bizukojc et al., 2012):

$$\frac{\mu_{NO3\_m}}{\mu_{OC\_m}} = \eta_g = 0.15...1 \tag{9}$$

4.2 Media characterization

In order to simulate the reactive subsurface transport of matter (e.g. nitrate) in the groundwater a new process ("mass transport") has to be defined for each species and additional data blocks have to be added in almost every *OGS* input file as well as new files are needed. It is suggested to create a new folder called *Stationary_GW_NO3_Model* and to copy all files from the existing stationary groundwater flow model into this folder.

4.2.1 Material component parameters

For the simulation of mass transport processes, the six species (named: Nitrate, DO, OC, Decomposer, Denitrifier, and Tracer) has to be defined in an "Ashi.mcp" (material component properties) file. The two microbial groups (Decomposer and Denitrifier) should be defined as immobile and their transport phase is the biophase. The other four species are mobile and are transported in the aqueous phase. For the molecular diffusion, a value of $10^{-10}\,\mathrm{m}^2/\mathrm{s}$ is assumed for each species.

Listing 4.1: Component Properties File (*.mcp)

```
#COMPONENT_PROPERTIES
$NAME
Nitrate
$MOBILE
1; MOBIL-Flag: 0=immobile, 1=mobile/transported
$DIFFUSION
1 1.0e-10 ; diffusion model type, diffusion constant
$TRANSPORT_PHASE
0 ; 0=aqueous phase, 1=solid phase,  2=biophase
#STOP
```

OGS allows to specify decay rates for each species individually in the *.mcp file by using the keyword `$DECAY`. Both first order decay and monod decay are implemented. Nevertheless, in our scenario, decay rates of one species depends on other species which requires a more complex reaction model considering multi-reactants rate laws (see section 4.3).

4.2.2 Material properties

Next is to adapt the existing "Ashi.mmp" file in order to add additional medium properties for the mass transport simulation. Please add for all four layers the following sub-keyword in order to determine the longitudinal and transversal dispersivities.

Listing 4.2: Material Proporties File: Mass Dispersion (*.mmp)

```
$MASS_DISPERSION
1 10 1; 1=Disp. on; 10=long. Disp., 1=transv. Disp.
```

We assume equal dispersivities in all layers, as the main impact factors of dispersivity, tortuosity and porosity are also assumed to be equal (Gutierrez-Neri, 2009).The values are in the typical range for field-scale dispersivities (Gelhar et al., 1992).

Next, we have to add a volume for the biophase for each layer in order to determine the space where our two microbial species live. In our case we assume that 1 % of the total volume is reserved for biota which means that, considering the porosity of 0.3, the remaining 69 % of total volume is filled with solids. Add the data block below the porosity definition for each layer:

Listing 4.3: Material Properties File: Biophase Volume (*.mmp)

```
$VOL_BIO
1 0.01
$VOL_MAT
1 0.69
```

4.2.3 Material solid properties

For mater transport simulation, the material density of each layer is required as well which has be added in a new “Ashi.msp” (material soil properties) file. Assuming a constant and similar density for each layer, the file should be consist of four data blocks which only differ in the name of the `$SOLID_TYPE`:

Listing 4.4: Material Solid Properties File (*.msp)

```
#SOLID_PROPERTIES
$SOLID_TYPE
Aquifer
$DENSITY
1 2.00000e+003
#SOLID_PROPERTIES
[..]
#SOLID_PROPERTIES
[..]
#SOLID_PROPERTIES
[..]
#STOP
```

4.2.4 Material fluid properties

OGS also allows to simulate flow for several fluids which properties have to be defined in a fluid property file (*.mfp). As we defined our process as groundwater flow, deionized water is assumed to be the standard fluid and no “Ashi.mfp” file was needed to conduct the stationary groundwater flow simulation. On the other hand, the extension of the model to reaction matter transport needs the fluid properties explicitly specified in an “Ashi.mfp” file. Please create this file by adding the following data block in *Notepad++*:

Listing 4.5: Fluid Properties File (*.mfp)

```
#FLUID_PROPERTIES
$FLUID_TYPE
LIQUID
$PCS_TYPE
HEAD
$DENSITY
1 1000.0
$VISCOSITY
1 1e-3
#STOP
```

4.3 Kinetic reaction definition

There are several ways apply chemical reaction kinetics usable in *OGS*. One option is to couple *OGS* with *IPhreeqc* by using an *.pqc input file and an *OGS* executable in which *IPhreeqc* source code is implemented (see Appendix and (He et al., 2015). Alternatively, we will simulate the biodegradation reactions using in a new file called “Ashi.krc”. First, a general block starting with the keyword `#KINREACTIONDATA` has to be entered which determines the solver settings for the kinetics:

Listing 4.6: Kinetic Reaction File: Biodegradation Reaction (*.krc)

```
#KINREACTIONDATA
$SOLVER_TYPE
1 ; Solver type
$RELATIVE_ERROR
1.e-6 ; rel. Error
$MIN_TIMESTEP
1.e-6 ; min Timestep
$INITIAL_TIMESTEP
1.0 ; init Timestep
$BACTERIACAPACITY
1000.0
```

Beside the numerical definitions, a high bacteria capacity value of 1000 ensures no limitation in this simulation. In general, however, it depends on

the bacteria concentration. The capacity is an additional Monod-term for bacteria concentration. As the bacteria concentration is constant, the keyword `$BACTERIACAPACITY` can be omitted and this will result in no limitation as well.

Next, each reaction has to be defined by using the keyword `#REACTION`. In total, we have four reactions. First is the metabolism of organic matter based on equation 6 and 7 which can be added to the file by the following code block:

Listing 4.7: Kinetic Reaction File: Organic Matter (*.krc)

```
#REACTION
$NAME
Decomposition
$TYPE
monod
$BACTERIANAME
Decomposer
$EQUATION
1 OC + 1 DO = 8 CO2 + 5 H2O;
$RATECONSTANT
1.0e-5 1.0
$GROWTH
1; 1= growth allowed
$PRODUCTIONSTOCH
OC -1
DO -1
$MONODTERMS
OC 10000 1.0; for each monod term: species concentration order
DO 10000 1.0
```

First, we have to name the reaction and define the reaction type as monod. Then, we define the involved bacteria group for the oxic organic matter decay which is allowed to grow in concentration. Following the keyword `$EQUATION`, we have to add the reaction equation according to eq.6. It is important to leave one space around each mathematical operator. The product concentrations of H_2O and CO_2 are not calculated because they are not defined as species in the "Ashi.mcp" file and not of particular interest.

The rate constant represents the maximum growth rate constant value μ_{NO3_m} which is determined to 10^{-5}/s and is a first order term. Setting the `$GROWTH` to 0 ensures that bacterial mass will not increase by reaction. The sub-keyword `$PRODUCTIONSTOCH` allows to consider differences in stoichiometry and product yield ratios. Finally, sub-keyword `$MONODTERMS` is added which allows to specify the half-saturation concentrations of oxygen and organic carbon in the monod.kinetics. These constants have to be chosen to be significantly larger in order to obtain similar results to the calculation by first-order kinetics (see equation 8).

The second reaction keyword describes the denitrification reaction process. Two main changes can be observed in comparison to the previous equation. First, a sub-keyword `$MONODTERMS` is added which allows to specify the half-saturation concentrations of Nitrate and organic carbon in the monod-kinetic (equation 3). Second, the `$INHIBITIONTERMS` allows to determine in which

way the reaction is inhibited by the occurrence of oxygen. For simplification we assume that above an oxygen concentration of 3 mg/l, no denitrification can taken place.

Listing 4.8: Kinetic Reaction File: Denitrification (*.krc)

```
#REACTION
$NAME
Denitrification
$TYPE
monod;
$BACTERIANAME
Denitrifier
$EQUATION
1 OC + 0.8 Nitrate +0.8 H = 1 CO2 + 1.4 H2O 0.4N2;
$RATECONSTANT
2.0e-6 1.0
$GROWTH
0; 0= growth not allowed
$MONODTERMS
OC 8.33e-5 1.0 ; for each monod term: species concentration order
Nitrate 3.13e-5 1.0
$PRODUCTIONSTOCH
OC -1
Nitrate -0.8
$INHIBITIONTERMS
DO 3 1.0 ; species, concentration, order
```

Finally, we do not need to implement the decay of biomass by additional kinetic reactions as we assume a constant concentration of biomass which means that decay rates and growth rates are equal at each time step.

4.4 Boundary conditions

4.4.1 Initial conditions

Additional lines have to be added to the initial conditions file (Ashi.ic) to determine the matter concentrations at the beginning of the simulation. Microbiota has to be available in order to ensure the conduction of the defined kinetic reactions. Therefore, for both species, a small initial concentration of 10^{-6} mg/l is used for the entire domain. The tracer concentration should be zero for the entire domain:

Listing 4.9: Initial Condition File (*.ic)

```
#INITIAL_CONDITION
$PCS_TYPE
MASS_TRANSPORT
$PRIMARY_VARIABLE
Denitrifier
$GEO_TYPE
DOMAIN
$DIS_TYPE
```

```
CONSTANT 1e-6
#INITIAL_CONDITION
$PCS_TYPE
MASS_TRANSPORT
$PRIMARY_VARIABLE
Decomposer
$GEO_TYPE
DOMAIN
$DIS_TYPE
CONSTANT 1e-6
```

For nitrate, we assume an initial concentration of 8.64 mg/l which fits to the currently measured values in the groundwater of the region. As an initial condition, this value is assumed to be valid for the whole domain. The tracer should have the same initial concentration in order to allow us to evaluate the degradation process.

Listing 4.10: Initial Condition File: Tracer (*.ic)

```
#INITIAL_CONDITION
$PCS_TYPE
MASS_TRANSPORT
$PRIMARY_VARIABLE
Nitrate
$GEO_TYPE
DOMAIN
$DIS_TYPE
CONSTANT 8.64
#INITIAL_CONDITION
$PCS_TYPE
MASS_TRANSPORT
$PRIMARY_VARIABLE
Tracer
$GEO_TYPE
DOMAIN
$DIS_TYPE
CONSTANT 8.64
```

For the organic carbon, we assume that dissolved organic carbon (DOC) is the exclusive source for denitrification as microorganisms are presumed unable to feed on adsorbed carbon in the soil matrix or organic fluids forming an own phase (Kinzelbach et al., 1991). From previous studies, DOC concentrations of water in the organic surface horizons, which is assumed to refer to our 1 m soil layer are in a range of 50 mg/l (Lal et al., 1997). In deeper layers, DOC concentrations generally decrease due to sorption and run-off processes. For dissolved oxygen (DO), the pattern should be similar with oxic ($\sim$ 10 mg/l) conditions in the soil layer and strictly anoxic conditions in the aquifer *OGS* provides the opportunity to define initial conditions individually (or other boundary conditions) for subdomains which are defined by different material IDs. Thus, enter the following two blocks to determine the initial distribution of organic carbon and dissolved oxygen in the model:

Listing 4.11: Initial Condition File: Organic Carbon and Dissolved Oxygen (*.ic)

```
#INITIAL_CONDITION
$PCS_TYPE
MASS_TRANSPORT
$PRIMARY_VARIABLE
OC
$GEO_TYPE
DOMAIN
$DIS_TYPE
FUNCTION
$GEO_TYPE
SUBDOMAIN
4
0 0
1 1
2 5
3 50
#INITIAL_CONDITION
$PCS_TYPE
MASS_TRANSPORT
$PRIMARY_VARIABLE
DO
$GEO_TYPE
DOMAIN
$DIS_TYPE
FUNCTION
$GEO_TYPE
SUBDOMAIN
4
0 0
1 1
2 5
3 10
#STOP
```

4.4.2 Source terms

For our model, we will set the matter input directly on the nodes, an approach which is similar to the implementation of the groundwater recharge. In contrast to the recharge, nitrate is only distributed to the surface covered with farmland. We will select the nodes referring to farmland by using the Software *QGIS*.

Please open *QGIS* and load the land cover shapefile related to farmland (farmland.shp) from the project folder by clicking on `layers` →`add layer` →`Add vector layer` and enter the path of the dataset. Finally press open in order to add the shapefile. If you want to visualize your geographic information you can import the shapefiles used for mesh generation (section 3.1) into *QGIS* as well. After uploading we see a coloured rectangle with white areas inside which simply refer to land covered differently. Next step is to upload the nodes of the mesh and the node specific precipitation file into *QGIS* in order to select the nodes which refer to the specific land cover. Please click on `layers` →`add layer` →`Add delimited text layer`. As the `file name`, enter the full path of the "Ashi.msh" file by clicking on `browse`.

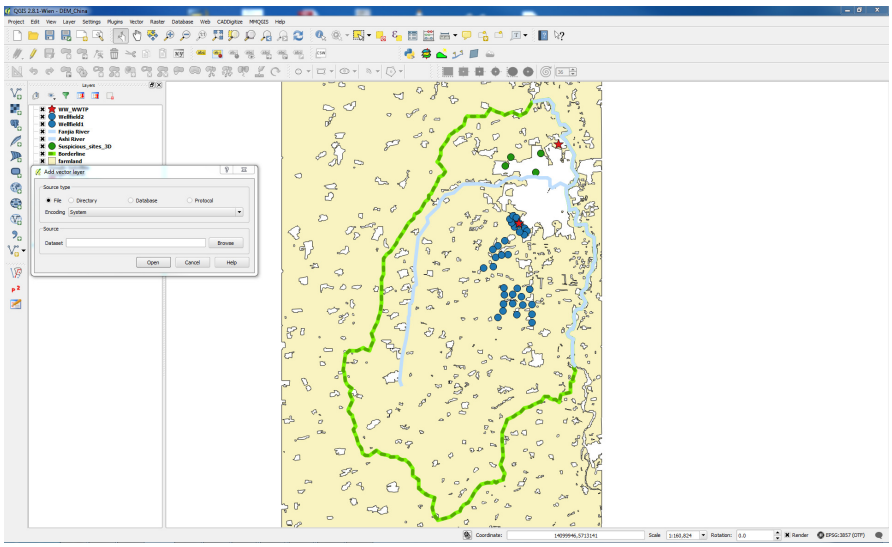

Fig. 4.1: Upload of land cover data into *QGIS*

The name of the new layer should be "Ashi_nodes". Next, choose `number of header lines to discard` as 4. Set up the geometry definition by using `point coordinates` and field_2 as the x-field and field_3 as the y-field. As you can see, *QGIS* in its recent version is only able to deal with planar 2D data. Finally press ok and ignore the error message. *QGIS* automatically georeferenced the new shapefile as WGS84, which is wrong but can be changed easily. Please click right and save the file as "Ashi_node" in your landuse folder selecting EPSG:32652 as CRS. After pressing ok, you should see a lot of points in the main view which cover the shape of the study area. The points have the position of the nodes in the 3D mesh. The imported node file has to be edited in order to calculate the groundwater recharge dependent on the land use. Hence, we open the attribute table by clicking right on the layer and selecting `Open Attribute table`. Please click on the pen on the upper left corner of the attribute table to select in the editing mode. Delete all excess columns by clicking on the icon `Delete Columns` and select all columns from field_5 to field_9.

The attribute table contains data of about 6030 nodes, but only about 1380 nodes belong to the surface (check the exact number of the last node from the recharge.txt file). Hence, nodes belonging to the surface have to be extracted. Click on the forth icon from the left called `Select features using an expression` in the attribute table and type in the edit field of the appearing window `field_1 <1380`. Next, press `select` and `close`. The nodes in your attribute table should be highlighted now. Click right on the "Ashi_nodes" data set in the layer view and save it again as "Ashi_nodes_surfaces". Take care

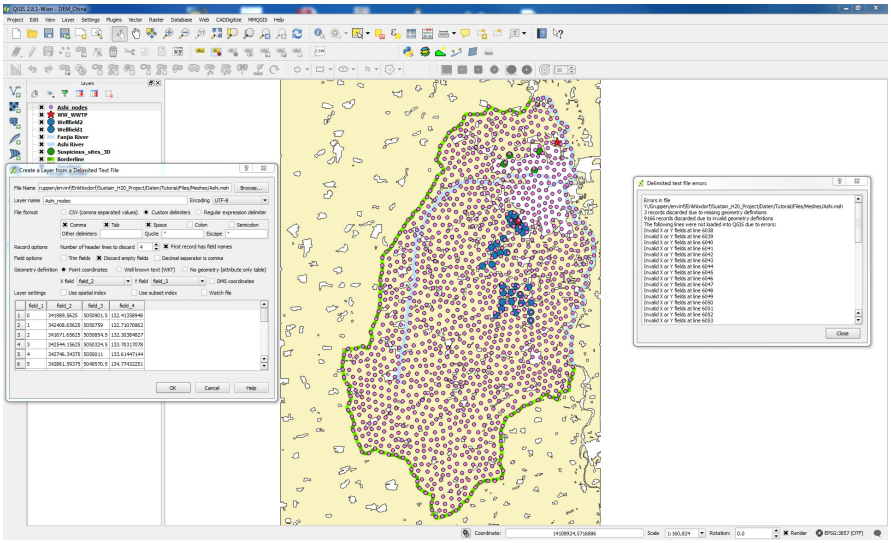

Fig. 4.2: Import of node-files into *QGIS*

that you mark the `Save only selected features` option. A new shape file appears in the layers view. Please leave the editing mode of the "Ashi_nodes" file by clicking on the pen again and agree to `Save all changes`. Finally,

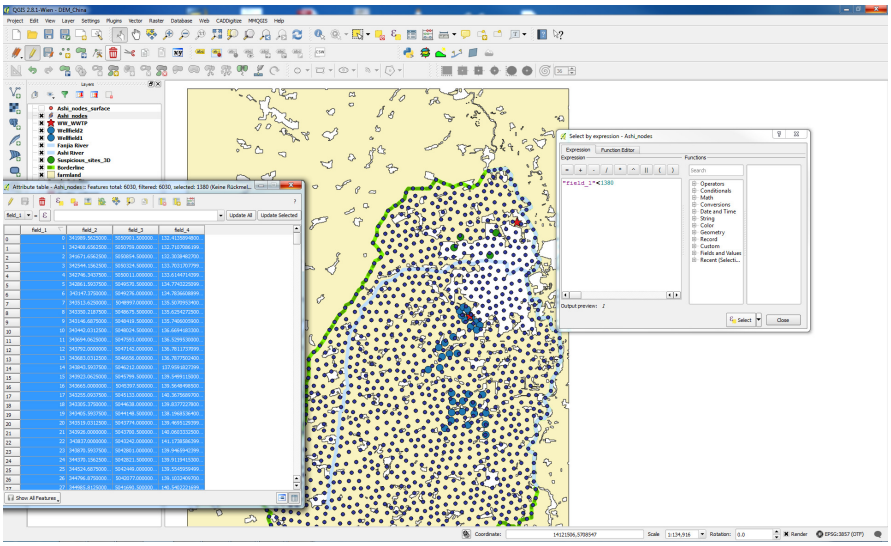

Fig. 4.3: Extraction of surface nodes

we will delineate the nodes which are located on the farmland. Therefore we have to download the *Spatial Query Plugin* in *QGIS*. Please click in the main tool bar on `Plugins` →`Manage and Install Plugins` and search for *Spatial Query Plugin*. Click on `Install`, mark the plugin and close the window. The tool icon will appear in the left tool bar.

The delineation and subsequent export of the data as an ASCII file will be done step by step:

1. Open the *Spatial Query Plugin*
2. Select "Ashi_nodes_surface" as source feature, `farmland` as the reference feature and `within` as the spatial selection mode and Press `Apply`. After finishing the calculation (which may take a while), the nodes within agricultural areas will be selected and marked in yellow.
3. Press on the `Create layers with list of items` icon in the *Spatial Query Plugin* and save the new shapefile has "Ashi_nodes_farmland".
4. Save changes.
5. Open the "Ashi_nodes_farmland" attribute table, select all rows and copy them by using ctrl+c from *QGIS* into a new *Notepad++* file and save it as "Nitrate.txt".
6. Save everything and close *QGIS*.

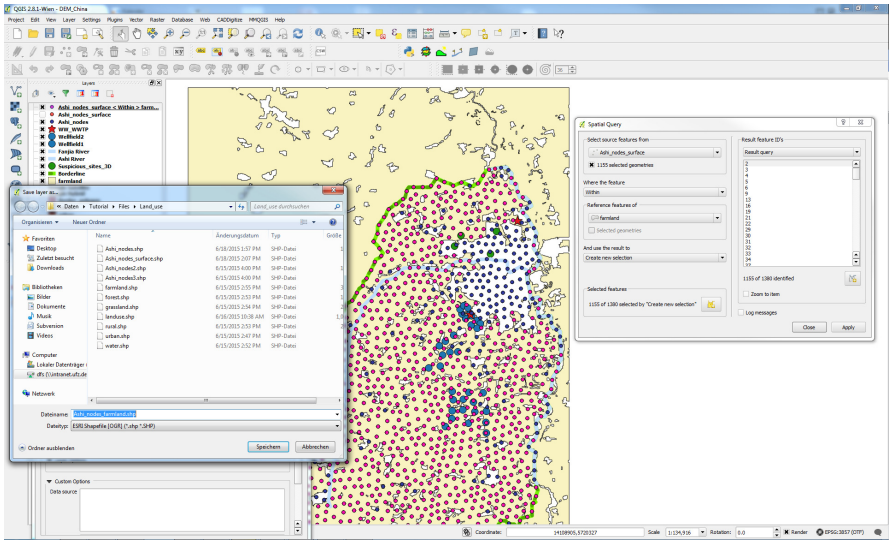

Fig. 4.4: Application of the Spatial Query Plugin in *QGIS*

The last step is to bring the Nitrate.txt file in a structure similar to the recharge.txt file with one column containing the specific nodes and the second

column the node values. First please delete the geographical information which is written in each line prior to the node. Using the column mode by holding “alt” during selection by mouse saves time. Next, delete the leading tab by clicking on `edit` →`Blank Operations` →`Trim leading space`.

For the second column we have to add the nitrate input on each node in the unit $\mathrm{mg} \cdot \mathrm{m}^{-2} \cdot \mathrm{s}^{-1}$. Although nitrogen fertilizer application depends on the individual crop requirement, we use for simplification purpose a spatially (and temporarily) uniform nitrogen distribution. Assuming a constant fertilizer input of 155 kg N/ha · a and a leaching rate of 20 %, about $3.54 \cdot 10^{-4}$ mg NO_3 enters the groundwater per square meter and second. Therefore we enter the expression 3.54e-04 in each line. Finally be careful that the file does not contain blank lines and save your changes. Finally we will use the created

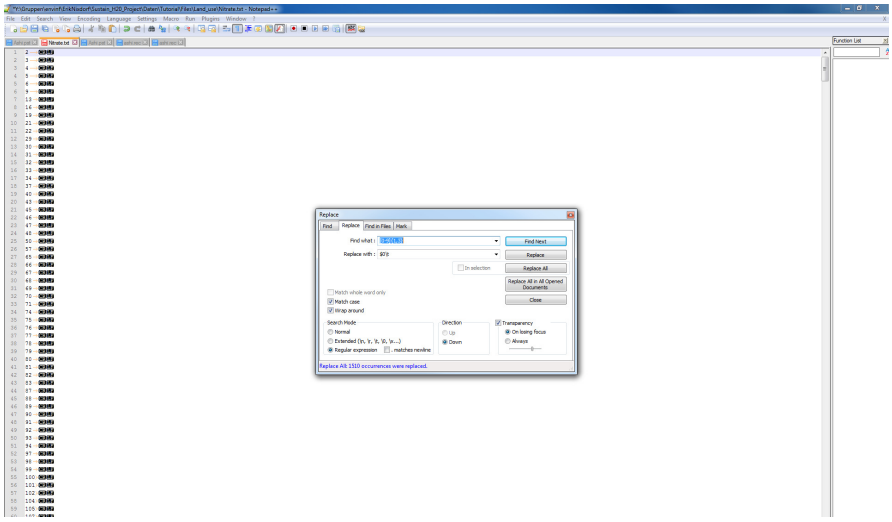

Fig. 4.5: Adaption of the Nitrate.txt-file with*Notepad++*

Nitrate.txt file to define our source terms for the Nitrate and the Tracer within the “Ashi.st” file. Please add below the definition for the groundwater flow process the following to data blocks.

Listing 4.12: Source Term File: Nitrate and Tracer (*.st)

```
SOURCE_TERM
$PCS_TYPE
MASS_TRANSPORT
$PRIMARY_VARIABLE
Nitrate
$DIS_TYPE
DIRECT Nitrate.txt
#SOURCE_TERM
$PCS_TYPE
```

```
MASS_TRANSPORT
$PRIMARY_VARIABLE
Tracer
$DIS_TYPE
DIRECT Tracer.txt
#STOP
```

4.4.3 Boundary conditions

We assume that a plenty of oxygen and organic carbon are continuously, from an infinitely large reservoir, provided by external inflow from the surface. Therefore we will define a constant value of 10 mg/l and 50 mg/l, respectively for each surface node. Please open the recharge.txt file and save two copies of it with the names "do.txt" and "oc.txt". Within these files, replace the second column by adding for each node a corresponding value of 10 in case of dissolved oxygen and of 50 in case of organic carbon. Finally open the existing "Ashi.bc" file and add the data block which defines the boundary conditions by using the created *.txt files:

Listing 4.13: Boundary Condition File (*.bc)

```
#BOUNDARY_CONDITION
$PCS_TYPE
GROUNDWATER_FLOW
$PRIMARY_VARIABLE
DO
$DIS_TYPE
DIRECT do.txt

#BOUNDARY_CONDITION
$PCS_TYPE
GROUNDWATER_FLOW
$PRIMARY_VARIABLE
OC
$DIS_TYPE
DIRECT oc.txt
#STOP
```

4.5 Adaptation of additional input files

4.5.1 Process specification

In the "Ashi.pcs" file three lines have to be added to define the mass transport process:

Listing 4.14: Process File (*.pcs)

```
#PROCESS; Species_name
$PCS_TYPE
MASS_TRANSPORT
#STOP
```

This input block has to be repeated for each species. In total, 6 transport processes must be defined, five for each species involved in the denitrification (Nitrate, DO,OC and the two bacteria species Decomposer and Denitrifier) and one for a conservative tracer which is used to check the correctness and numerical accuracy of the transport simulation. It is helpful to use the semicolon to delineate which process belongs to which species.

4.5.2 Time stepping

The "Ashi.tim" file has to be changed, as matter transport requires a transient simulation. Fortunately time stepping has to be added just once to cover all mass transport process. We are interested in a total simulation time of 20 years and a simulated time step of one year. The decision of an appropriate time step size does not depend only on the requirements of the specific task but also impacts numerical stability. A too coarse time stepping may lead to a violation of the courant criteria, particularly if the finite element size and the flow velocities are considered as fixed.Transferred to the SI-Unit second, please replace the existing data block by the following lines:

Listing 4.15: Time discretization File (*.tim)

```
#TIME_STEPPING
$PCS_TYPE
GROUNDWATER_FLOW
$TIME_START
0
$TIME_STEPS
20 31556926
$TIME_END
631138520
#TIME_STEPPING
$PCS_TYPE
MASS_TRANSPORT
$TIME_START
0
$TIME_STEPS
20 31556926
$TIME_END
631138520
#STOP
```

4.5.3 Numerics

For the numeric, just one additional block has to be added to the "Ashi.num" file which defines the numerical parameters for the mass transport process. The two sub-keywords`$ELE_MASS_LUMPING` and `$FEM_FCT` help to increase numerical stability of the solution.

Listing 4.16: Numeric File (*.num)

```
#NUMERICS
$PCS_TYPE
MASS_TRANSPORT
$ELE_MASS_LUMPING
1
$FEM_FCT
1 0
$LINEAR_SOLVER
2 5 1.0e-14 2000 1 100 4
```

4.5.4 Output

In the output file, concentrations of the transport parameters should be obtained by adding the corresponding names in the sub-keyword "NOD_VALUES" for the already selected output geometry:

Listing 4.17: Output File (*.out)

```
#OUTPUT // profile
$PCS_TYPE
GROUNDWATER_FLOW
$NOD_VALUES
HEAD
VELOCITY_X1
VELOCITY_Y1
VELOCITY_Z1
Nitrate
OC
DO
Tracer
Decomposer
Denitrifier
$GEO_TYPE
DOMAIN
$DAT_TYPE
VTK
$TIM_TYPE
STEPS 1
#STOP
```

4.6 Model Execution

After setting up all input files, our reactive transport model is ready for the simulation. Please proof that all required input files (Table 4.1) are within one folder and start the simulation in the same way as for the hydrological model.

Table 4.1: Required files for reactive matter flow simulation with *OpenGeoSys*. The newly added files are marked bolt.

Type of file	File name
Geometry	Ashi.gli
Mesh	Ashi.msh
Initial Condition	Ashi.ic
Boundary Condition	Ashi.bc, **oc.txt, do.txt**
Material Properties	Ashi.mmp
Soil Properties	**Ashi.msp**
Fluid Properties	**Ashi.mfp**
Material Component Properties	**Ashi.mcp**
Kinetic Reaction Components	**Ashi.krc**
Source Term	Ashi.st, **nitrate.txt, tracer.txt**
Process Control	Ashi.pcs
Time Step Control	Ashi.tim
Numeric File	Ashi.num
Output Control	Ashi.out

4.7 Model Results

For the post processing we use once more the software *ParaView*. Please locate the *OGS* project folder and open all VTK files inside together. After pressing apply the model appears in the *Layout View*. In the properties menu the file, change the colouring from head to Nitrate. Above the layout and pipeline browser you can find several toolbars. One of them is the Current time controls toolbar. By clicking the play button in this toolbar you can start the simulation to the temporary changes of your nitrate concentration in the subsurface. As you see, the Nitrate concentration is first increasing in farmland area. But with increasing time, advective transport distributes elevated Nitrate concentrations over the entire area. Nitrate levels are at the end of the simulation time in the range of about 9.5 mg/l, which means an increase of more than 10 %. Nevertheless, almost no additional nitrate could reach the aquifer within the simulation time due to low travel times from the topsoil to the aquifer.

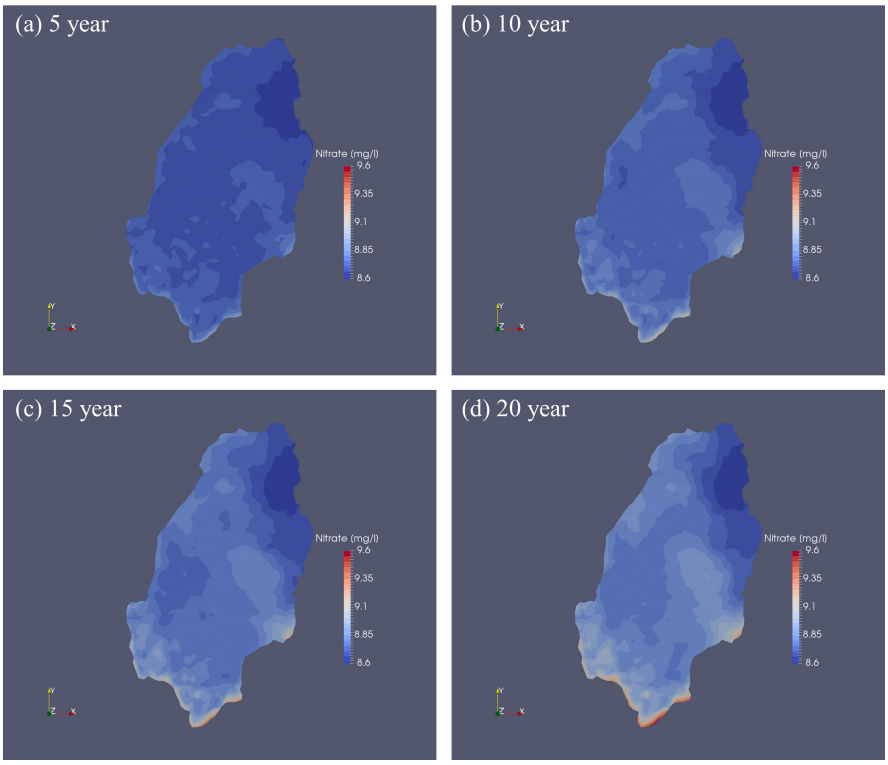

Fig. 4.6: Nitrate concentration after 5, 10, 15 and 20 years of simulation time

Chapter 5
Reactive point pollutants model within a transient flow field

In our last part of the simulation, we will forecast changes in groundwater regime impacted by increasing drinking water abstraction rates (section 1.2.3) and show how these changes might influence the pathways of potential groundwater pollutants (section 1.2.2). We will create the model based on our stationary groundwater flow model and our denitrification model.

Please create a new folder called `Transient_GW_MF_Model`. Copy the files **Ashi.num**, **Ashi.tim**, **Ashi.mmp**, **Ashi.msp**, **Ashi.mfp**, **Ashi.gli** and **Ashi.msh** from the previous from the `Stationary_GW_NO3_Model` folder of previous matter transport model (Chap. 4)) into the new folder. They do not need to be changed for the current simulation. Additionally, please copy from the stationary groundwater model folder `Stationary_GW_Model` the **Ashi.pcs**, **Ashi.bc**, **Ashi.ic, Ashi.st** (plus recharge.txt) and **Ashi.out** files into the new folder. We will extend some of these existing files to implement our transient groundwater and matter flow model. Furthermore we will create a completely new material component file **Ashi.mcp** in order to define the properties of the organic pollutants.

5.1 Process Definition

In the Ashi.pcs file, we have to define matter transport in order to simulate the transport of pollutants from point sources. We want to simulate four pollutants, which are likely to emit from the suspicious sites of the study area: **Phenol** emissions from the steel work, **Benzo(a)pyrene** from the coal piles of the coal power plant and the steel work, BTEX (e.g. **Benzene**) from the wood treatment facility and PCH (e.g. **Tetrachloroethylene**) from the textile manufacturing facility. Additionally we will let a conservative tracer emit from each suspicious site. Hence, please add the following data block five times below the groundwater flow definition and make sure that the `#STOP` is occurring in the last line, only.

Table 5.1: Average half-life constants for first-order decay

$NAME	K[l/s]	Reference
Phenol	$1.7 \cdot 10^{-07}$	(Aronson and Howard, 1997)
Benzpyren	$3.2 \cdot 10^{-07}$	(Kanaly et al., 1997)
Benzene	$2.3 \cdot 10^{-08}$	(Rifai and Newell, 1998)
PCE	$5.8 \cdot 10^{-08}$	(Schaerlaekens et al., 1999)

Listing 5.1: Process File (*.pcs)

```
#PROCESS; Species_name (Phenol, Benzpyren, Benzene, PCE or Tracer)
$PCS_TYPE
MASS_TRANSPORT
#STOP
```

5.2 Material component properties

For each species (five in total) a data block has to be added in a new Ashi.mcp file. All species are assumed to be mobile and to have a molecular diffusion in water of 10^{-10}. For simplification, we assume that the degradation of all species can be described as first-order-decay:

$$C_i(t) = C_i(t - t_0) \cdot e^{-k_i \cdot t} \tag{1}$$

This allows us to skip the definition of more complex kinetic reactions in the Ashi.krc file. The half-life-constants k for each species, the name and the reference are given in Table. 5.1.

Please add the data blocks for each component (including the tracer) into the Ashi.mcp file.

Listing 5.2: Component Properties File (*.mcp)

```
#COMPONENT_PROPERTIES
$NAME
Phenol
$MOBILE
1; MOBIL-Flag: 0=immobile, 1=mobile/transported
$DIFFUSION
1 1.0e-10 ; diffusion model type, diffusion constant
$TRANSPORT_PHASE
0 ; 0=aqueous phase, 1=solid phase,  2=biophase
$DECAY; 0 ; 0=no decay, 1=first-order decay,  2=Monod kinetics
1 1.7e-7
#COMPONENT_PROPERTIES
[..]
#COMPONENT_PROPERTIES
[..]
#COMPONENT_PROPERTIES
```

```
[..]
#COMPONENT_PROPERTIES
$NAME
Tracer
$MOBILE
1; MOBIL-Flag: 0=immobile, 1=mobile/transported
$DIFFUSION
1 1.0e-10; diffusion model type, diffusion constant
$TRANSPORT_PHASE
0 ; 0=aqueous phase, 1=solid phase,  2=biophase
$DECAY; 0 ; 0=no decay, 1=first-order decay,  2=Monod kinetics
0
#STOP
```

5.3 Initial and boundary conditions

5.3.1 Initial Conditions

We assume that the concentrations of all pollutants and the tracer are zero prior to the simulation. Please add the following data block (in total five times) below the existing initial conditions definition for the groundwater flow.

Listing 5.3: Initial Condition File (*.ic)

```
#INITIAL_CONDITION
$PCS_TYPE
MASS_TRANSPORT
$PRIMARY_VARIABLE
Phenol;
$GEO_TYPE
DOMAIN
$DIS_TYPE
CONSTANT 0
#INITIAL_CONDITION
[..]
#INITIAL_CONDITION
[..]
#INITIAL_CONDITION
[..]
#INITIAL_CONDITION
[..]
#STOP
```

5.3.2 Source terms

In the source term file Ashi.st no data blocks related to mass transport process have to be added. On the other hand we have to implement a variable

abstraction rate for each groundwater well. First change the constant abstraction rates for each well to 1. Next, add a new sub-keyword cms$TIM_TYPE in each source term data block referring to a well. In the line below write `Curve 1` for all wells with numbers from 1-19 and `Curve 2` for the remaining wells of well field 2. The word curve defines the type of time dependence and the number 1 or 2 refers to the applied curve.

Listing 5.4: Source Term File (*.st)

```
#SOURCE_TERM
$PCS_TYPE
GROUNDWATER_FLOW
$PRIMARY_VARIABLE
HEAD
$GEO_TYPE
POINT well1_t
$DIS_TYPE
CONSTANT 1
$TIM_TYPE
CURVE 1
[..]
#SOURCE_TERM
$PCS_TYPE
GROUNDWATER_FLOW
$PRIMARY_VARIABLE
HEAD
$GEO_TYPE
POINT well33_b
$DIS_TYPE
CONSTANT 1
$TIM_TYPE
CURVE 2
#STOP
```

Additionally to these changes in the Ashi.st file, we have to define the curves to which the `$TIM_TYPE` keyword refers to. This is done in an additional Ashi.rfd file which is created using *Notepad++*. The Ashi.rfd file consists of two curves, which are delineated by the keyword `#CURVES`. The curve is defined by two columns, one containing the time and the second column the corresponding value. This time dependent value acts as a multiplier of the constant abstraction values in the Ashi.st file. By defining the constant value to 1, we are able to write the time-dependent abstraction rates directly in the Ashi.rfd file. Based on our water demand forecast (chapter 1.2.3) it is expected that the total abstraction rate of the well fields has to increase by the factor 7.9 within 20 years in order to satisfy the increasing demand. Furthermore, we assume that the increase is linearly and equally for each well. This scheme can be implemented in the Ashi.rfd input file by adding the following data blocks:

Listing 5.5: RFD (*.rfd)

```
#CURVES
0       -0.0107
31556926        -0.0142
[..]
```

```
631138520        -0.0820
#CURVES
0        -0.00385
31556926         -0.0051
[..]
631138520        -0.02964
#STOP
```

5.3.3 Boundary Conditions

In the Ashi.bc boundary condition file we will define our pollutant emissions from the suspicious sites. We assume that the pollutants are emitting with a constant rate during the entire simulation time from an infinite reservoir at the location of the respective sites. For the concentrations we take the highest concentrations measured at similar field sites (chapter 1.2.1). Furthermore it needs to be considered that coal piles exist on both the steel work and the coal power plant which are both sources for Benzo(a)pyren emissions. For the tracer, we assume that it emits with a constant concentration of 1 mg/l from each suspicious sites. Summarizing, nine data blocks have to be added to the Ashi.bc file:

Listing 5.6: Boundary Condition File (*.bc)

```
#BOUNDARY_CONDITION
$PCS_TYPE
MASS_TRANSPORT
$PRIMARY_VARIABLE
Phenol ; other species: 2*Benzpyren, Benzene, PCE, 4x Tracer
$GEO_TYPE
POINT Steel_work ; others: Coal power plant, Wood treatment facility,
    Textile manufacturing facility
$DIS_TYPE
CONSTANT 1500; Benzpyren=0.03; Benzene=0.6; PCE=4; Tracer=1
[..]
```

For our transient groundwater flow model, we expect changes in flow direction and velocity with time. In order to get a more realistic representation of the groundwater flow path we have to improve the groundwater flow boundary connected to the head of Ashi River. Until now, the river boundary is defined by a constant head of 137 m. We will improve that by implementing a linearly river slope into that boundary condition with the help of *QGIS* and a spreadsheet software (e.g. *Excel*).

Please open *QGIS* and load the file Ashi_nodes_surfaces.shp which you created in the previous denitrification model (chapter 4.4.2). Additionally open the shapefile Ashi.shp which describes the river course by a polyline. Select all nodes which are on the polyline by pressing the button `Select features by area or by single click` and clicking on all nodes holding the control key. All select nodes should be marked yellow afterwards. Open

the attribute table of the shapefile and press control+c in order to copy the information of the selected rows. Open a spreadsheet software and paste

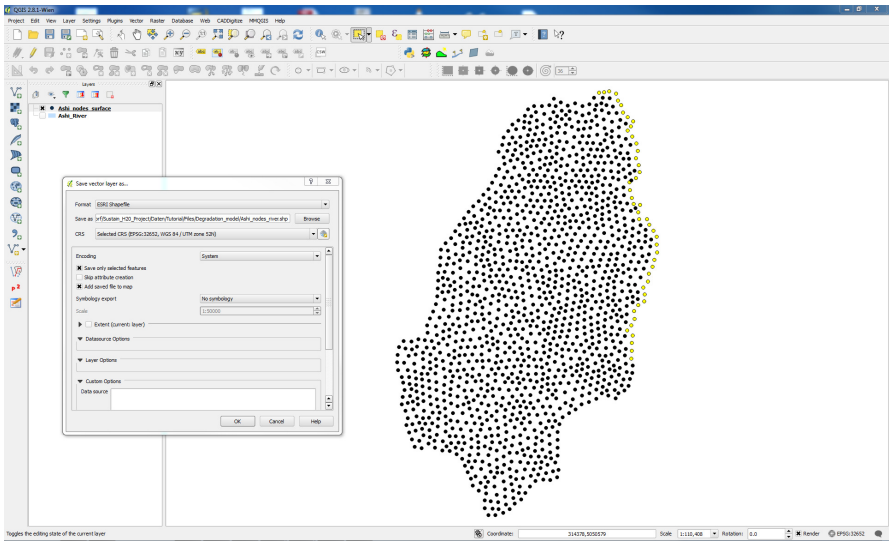

Fig. 5.1: Selecting nodes refering to the localation of Ashi River

the copied columns into a new sheet. The column with the header “field_1” consists of the node number and the columns “field_2”, “field_3” and “field_4 contain the node position in x, y and z-direction. If the nodes are numbered correctly the node numbers will increase towards upstream direction. If this is not true, please order the rows manually from downstream to upstream. Theoretically, the z-values should increase continuously from downstream to upstream but, due to the coarse DEM and an even coarser mesh resolution, this is usually not the case. Therefore, the river slope has to be implemented by changing the z-value of each node manually:

1. First, the distance of each node from its downstream predecessor has to be calculated by:

$$d_i = \sqrt{((x(i) - x(i-1))^2 + ((y(i) - y(i-1))^2} \tag{2}$$

2. Sum up the all n node distances in order to get the total length L of the river reach.:

$$L = \sum_{i=1}^{n} d(i) \approx 23000\,\mathrm{m} \tag{3}$$

3. Calculate the linear river slope r using realistic boundary altitudes of 143 m upstream and 132 m downstream:

$$r = \frac{z(max) - z(min)}{L} = \frac{145\,\mathrm{m} - 132\,\mathrm{m}}{L} \approx 0.0006 \tag{4}$$

4. Change the z-value of the upstream and downstream border nodes to the given values above and interpolate the z-values in between:

$$z(i) = z(i-1) + r \cdot d(i) \tag{5}$$

5. Copy the two columns containing the node number and the z-value into a new file Ashi_River.txt using *Notepad++*. Delete the header line and save it in the project folder.

Finally we have to replace the old groundwater flow boundary condition with the new based on the direct node values in the Ashi_River.txt file. Replace the existing data block with the following lines:

Listing 5.7: Boundary Condition File (*.bc)

```
#BOUNDARY_CONDITION
$PCS_TYPE
GROUNDWATER_FLOW
$PRIMARY_VARIABLE
HEAD
$DIS_TYPE
DIRECT Ashi_River.txt
```

Make sure that the last line of the Ashi.bc file consists of the `#STOP` expression and save the file.

5.4 Model execution

Before starting the simulation, the five new species have to added in the Ashi.out file below the sub-keyword `$NOD_Values`.

Similarly to the previous scenarios, proof that the folder "Transient_GW_MF_Model" contains all files listed in table 5.2 and start the *OGS* simulation by either using the ogs executable directly or by clicking on the Ashi.bat file. In comparison to the previous stationary groundwater simulation, the computation time will be significantly longer.

5.5 Model Results

For the results, please open *ParaView* and load all vtk files which emerged in the project folder. Next, upload the position of the wellfields and of the suspicious sites in *ParaView*. Both are located in the "CSV_DATA" folder of the data provided for the tutorial. After pressing apply, both files are first

Table 5.2: Required files for point source pollutants simulation in a transient flow field

Type of file	File name
Geometry	Ashi.gli
Mesh	Ashi.msh
Initial Condition	Ashi.ic
Boundary Condition	Ashi.bc, **Ashi_River.txt**
Material Properties	Ashi.mmp
Soil Properties	Ashi.msp
Fluid Properties	Ashi.mfp
Material Component Properties	Ashi.mcp
Source Term	Ashi.st; recharge.txt **Ashi.rfd**
Process Control	Ashi.pcs
Time Step Control	Ashi.tim
Numeric File	Ashi.num
Output Control	Ashi.out

integrated in the Pipeline Browser as tables. The filter “table to points”, which can be found in the filers menu of the toolbar has to be applied on both tables and the correct columns containing the x-y-z coordinates have to be selected. After pressing apply the locations should appear on the layout view as points.

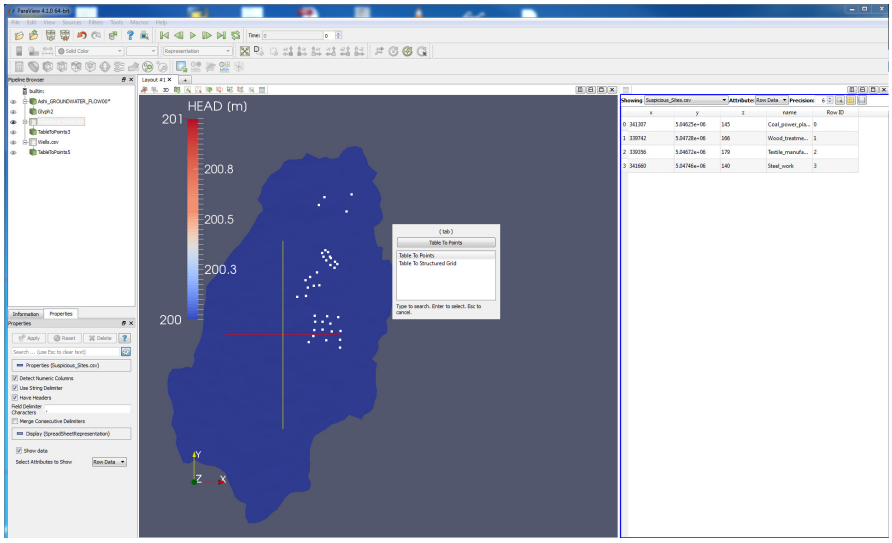

Fig. 5.2: Set up for Postprocessing with *ParaView*

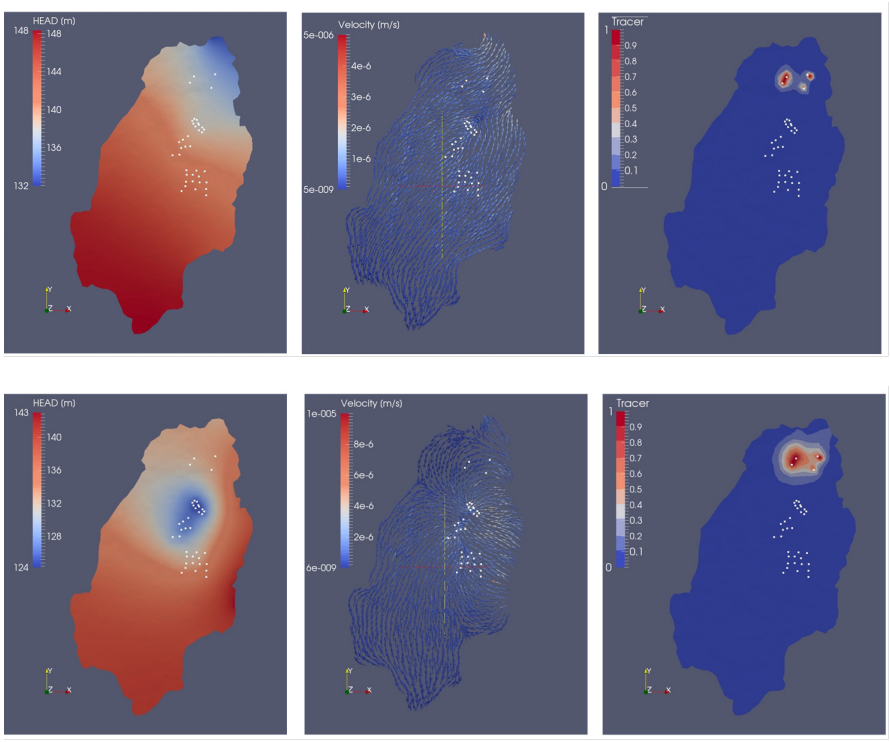

Fig. 5.3: Head distribution (left), flow field(middle) and tracer concentration(right) in a transient flowfield after one year (first column) and 20 years (bottom column) of simulation time.

After uploading the necessary files, we will look on our transient modelling results. By pressing the green play button, you can observe the changes in the head distribution with time. With increasing time, the drawdown in the vicinity of the well fields increases (Fig. 5.3). After 20 years, the groundwater level at the northern part of wellfield 1 is about 15 meters lower than at the beginning of the simulation. Next, we will apply the glyph tool to see how the velocity flow field changes with increasing water abstraction rates (Fig. 5.3). At the beginning of the simulation, water flows from south-west to north-east following the ground slope. Only in the vicinity of the well fields, groundwater is relocated which means that the cone of depression has a relatively small size. The cone of depression increases with time and water from further areas is redirected towards the well fields and the exchange conditions between river and aquifer change from gaining to losing. Additionally it can be seen that even at the catchment boundaries flow paths change which means that the size of the chosen study area is too small to cover the entire aquifer volume

which is influenced by the increasing abstraction rates. Finally we will take a look how the potentially emitted pollutants are affected by the changes of the flow field. One simple option is to track the changes by switching the coloring of the loaded vtk files from head to the specific pollutant and press play. Fortunately, not even the conservative tracer is able to reach the drinking water wells within 20 years, although the velocity field changed in the direction of the wells. This is due to the low groundwater velocities which are in the range of less than 50m/a in the vicinity of the suspicious sites.

Additionally, visual data integration became an important tool to establishing and validating data. The Visualization Center *TESSIN VISLab* (Vislab) can be used to explore and analysis complex and heterogeneous spatial data sets (Fig. 5.4). More detailed information is available through: https://www.ufz.de/index.php?en=37716

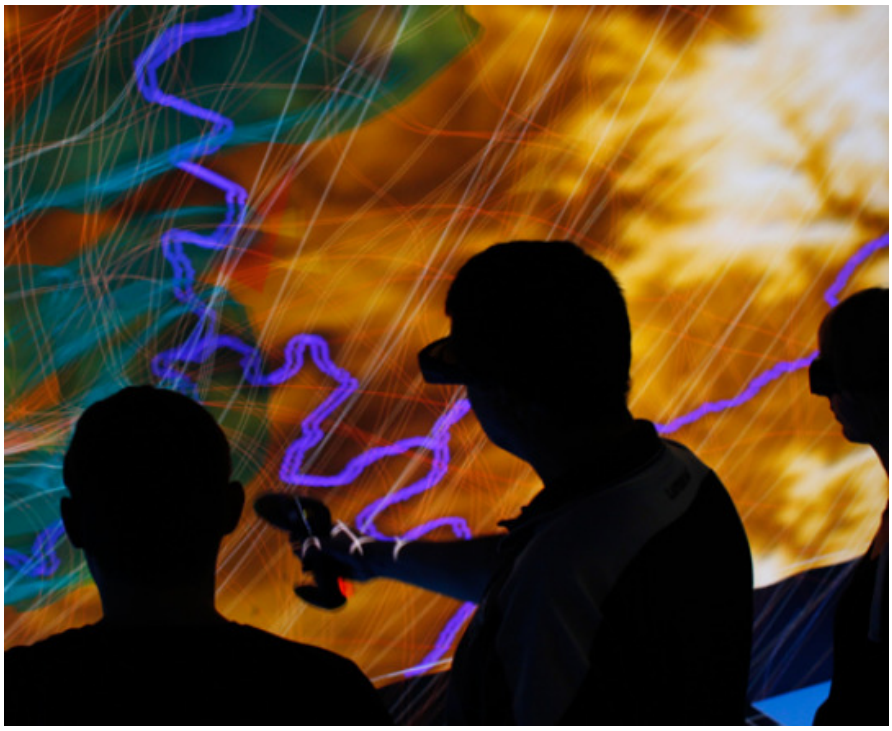

Fig. 5.4: Visualization center VISLab of the UFZ (Leipzig, Germany)

Appendix A
Symbols

Table A.1: Table of Symbols

Symbol	Parameter	Unit
Latin symbols		
$\mathbf{A}$	Global system matrix	
a	Heat transfer coefficient	$\mathrm{W \cdot K^{-1} \cdot m^{-2}}$
$\mathbf{b}$	Right-hand-side vector	
c	Specific heat capacity	$\mathrm{J \cdot kg^{-1} \cdot K^{-1}}$
Cr	Courant number, criteria	
$\mathbf{D}$	Diagonal matrix	
e	Specific energy	$\mathrm{J \cdot kg^{-1}}$
e_k	Iteration error	
$\mathbf{g}$	Gravity acceleration vector	$\mathrm{m \cdot s^{-1}}$
h	Specific enthalpy	$\mathrm{J \cdot kg^{-1}}$
$\mathbf{j}_{\mathrm{adv}}$	Advective heat flux	$\mathrm{W \cdot m^{-2}}$
$\mathbf{j}_{\mathrm{diff}}$	Diffusive heat flux	$\mathrm{W \cdot m^{-2}}$
$\mathbf{j}_{\mathrm{disp}}$	Dispersive heat flux	$\mathrm{W \cdot m^{-2}}$
$\mathbf{J}$	Jacobian	
$\mathbf{k}$	Permeability tensor	$\mathrm{m^2}$
k_{rel}	Relative permeability	$-$
$\mathbf{K}^{(e)}$	Element conductivity matrix	
$\mathbf{L}$	Differential operator	
$\hat{L}$	Approximation operator	
$\mathbf{L}$	Lower matrix	
$L^{(e)}$	Element length	
m	Mass	kg
n	Porosity	$\mathrm{m^3 \cdot m^{-3}}$
$\mathbf{N}^{(e)}$	Element shape function	
Ne	Neumann number, criteria	

Symbol	Parameter	Unit
q^i	Internal heat source	$\mathrm{J \cdot kg^{-1} \cdot s^{-1}}$
$\mathbf{q}$	Darcy flux, velocity	$\mathrm{m \cdot s^{-1}}$
Q	Amount of heat	J
Q_T	Heat production term (volumetric)	$\mathrm{J \cdot m^{-3} \cdot s^{-1}}$
q_T	Heat production term (specific)	$\mathrm{kg^{-1} \cdot s^{-1}}$
$\mathbf{R}$	Residuum vector	
S	Saturation	–
t	Time	s
T	Temperature	K
u	Internal energy	$\mathrm{J \cdot kg^{-1}}$
$u(t, x)$	Unknown field function of time and space	
u_j^n	Unknown field function approximation at time level n in node j	
$\mathbf{U}$	Upper matrix	
$\mathbf{v}$	Velocity vector	$\mathrm{m \cdot s^{-1}}$
V	Volume	$\mathrm{m^3}$
$\mathbf{x}$	Solution vector	
Greek symbols		
$\boldsymbol{\alpha}$	Diffusivity	$\mathrm{m^2 \cdot s^{-1}}$
$\boldsymbol{\lambda}$	Thermal conductivity	$\mathrm{W \cdot K^{-1} \cdot m^{-1}}$
ρ	Density	$\mathrm{kg \cdot m^{-3}}$
$\boldsymbol{\Delta}$	Difference	–
ϵ	Volume fraction	–
ϵ_j^n	Approximation error at time level n in node j	–
ψ	Conservation quantity	–
σ	Stress tensor	Pa
μ	Viscosity	$\mathrm{Pa \cdot s}$
Exponents, indices		
i, j	Node numbers	
k	Non-linear iteration number	
n	Time level	
s	Solid	
l	Liquid	
w	Water	
f	Fluid	
α	All phases	
γ	Fluid phases	

Appendix B
Keywords

This section provides a wrap-up compendium of the OGS keywords used in this tutorial. A more comprehensive compilation of OGS keywords you can find at www.opengeosys.org/help/documentation/.

B.1 GLI - geometry

Listing B.1: GLI keyword

```
#POINTS                // points keyword
0 0 0 0 $NAME POINT0   // point number | x | y | z | point name
1 1 0 0 $NAME POINT1   // point number | x | y | z | point name
#POLYLINE              // polyline keyword
 $NAME                 // polyline name subkeyword
  LINE                 // polyline name
 $POINTS               // polyline points subkeyword
  0                    // point of polyline
  1                    // dito
#STOP                  // end of input data
```

OGS Weblink:
http://www.opengeosys.org/help/documentation/geometry-file

B.2 MSH - finite element mesh

Listing B.2: MSH keyword

```
#FEM_MSH      // file/object keyword
$NODES        // node subkeyword
61            // number of grid nodes
0 0 0 0       // node number x y z
1 0 0 1       // dito
```

```
...
59      0       0       59
60      0       0       60
$ELEMENTS      // element subkeyword
60             // number of elements
0       0       line    0       1  // element number | material group
    number | element type | element node numbers
1       0       line    1       2  // dito
...
58      0       line    58      59 // dito
59      0       line    59      60 // dito
#STOP              // end of input data
```

OGS Weblink:
http://www.opengeosys.org/help/documentation/mesh-file

B.3 PCS - process definition

Listing B.3: PCS keyword

```
#PROCESS              // process keyword
  $PCS_TYPE           // process type subkeyword
    HEAT_TRANSPORT    // specified process(es)
    GROUNDWATER_FLOW  // dito
    LIQUID_FLOW       // dito
                ...
#STOP                 // end of input data
```

OGS Weblink:
www.opengeosys.org/help/documentation/process-file

B.4 NUM - numerical properties

Listing B.4: NUM keyword

```
#NUMERICS         // process keyword
  $PCS_TYPE       // process type subkeyword, see PCS above
  $LINEAR_SOLVER  // linear solver type subkeyword, see table below
         Parameters     // 7 parameters, see table below
#STOP             // end of input data
```

Numerical properties

- Linear solver type (its C++ ;-) numbering -1)
  1. SpGAUSS, direct solver
  2. SpBICGSTAB
  3. SpBICG

4. SpQMRCGSTAB
5. SpCG
6. SpCGNR
7. CGS
8. SpRichard
9. SpJOR
10. SpSOR

- Convergence criterion (its C++ ;-) numbering -1)

1. Absolutely error $||r|| < \epsilon$
2. $||r|| < \epsilon||b||$
3. $||rn|| < \epsilon||rn - 1||$
4. if $||rn|| < 1$ then $||rn|| < \epsilon||rn - 1||$ else $||r|| < \epsilon$
5. $||rn|| < \epsilon||x||$
6. $||rn|| < \epsilon \max||rn - 1||, ||x||, ||b||$

- Error tolerance ϵ, according to the convergence criterion model above
- Maximal number of linear solver iterations
- Relaxation parameter $\theta \in [0, 1]$
- Preconditioner

0 No preconditioner,
1 Jacobi preconditioner,
100 ILU preconditioner.

- Storage model

2 unsymmetrical matrix,
4 symmetrical matrix.

OGS Weblink:
http://www.opengeosys.org/help/documentation/numeric-file

B.5 TIM - time discretization

Listing B.5: TIM keyword

```
#TIME_STEPPING     // timt stepping keyword
  $PCS_TYPE        // process subkeyword
    HEAT_TRANSPORT // specified process
  $TIME_STEPS      // time steps subkeyword
   1000 390625e+0  // number of times steps | times step length
  $TIME_END        // end time subkeyword
    1E99           // end time value
  $TIME_START      // starting time subkeyword
    0.0            // starting time value
 $TIME_UNIT        // specified time unit
    DAY            // SECOND, DAY, YEAR
#STOP              // end of input data
```

OGS Weblink:
http://www.opengeosys.org/help/documentation/time-step-control-file

B.6 IC - initial conditions

Listing B.6: IC keyword

```
#INITIAL_CONDITION  // initial conditions keyword
 $PCS_TYPE          // process subkeyword
  HEAT_TRANSPORT    // specified process
 $PRIMARY_VARIABLE  // primary variable subkeyword
  TEMPERATURE1      // specified primary variable
 $GEO_TYPE          // geometry subkeyword
  DOMAIN            // specified geometry: entire domain (all nodes)
 $DIS_TYPE          // distribution subkeyword
  CONSTANT   0      // specified distribution: constant value 0 at DOMAIN
    geometry
#STOP               // end of input data
```

OGS Weblink:
http://www.opengeosys.org/help/documentation/initial-condition-file

B.7 BC - boundary conditions

Listing B.7: BC keyword

```
#BOUNDARY_CONDITION // boundary condition keyword
 $PCS_TYPE          // process type subkeyword
  HEAT_TRANSPORT    // specified process
 $PRIMARY_VARIABLE  // primary variable subkeyword
  TEMPERATURE1      // specified primary variable
 $GEO_TYPE          // geometry type subkeyword
  POINT POINT0      // specified geometry type | geometry name
 $DIS_TYPE          // boundary condition type subkeyword
  CONSTANT   1      // boundary condition type | value
#STOP               // end of input data
```

OGS Weblink:
Weblink: http://www.opengeosys.org/help/documentation/boundary-condition-file

B.8 ST - source/sink terms

Listing B.8: ST keyword

```
#SOURCE_TERM            // source term keyword
 $PCS_TYPE              // process type subkeyword
  LIQUID_FLOW           // specified process
 $PRIMARY_VARIABLE      // primary variable subkeyword
  PRESSURE1             // specified primary variable
 $GEO_TYPE              // geometry type subkeyword
  POINT POINT0          // specified geometry type | geometry name
 $DIS_TYPE              // boundary condition type subkeyword
  CONSTANT_NEUMANN 1E-6 // source term type | value
#STOP                   // end of input data
```

OGS Weblink:
http://www.opengeosys.org/help/documentation/source-term-file

B.9 MFP - fluid Properties

Listing B.9: MFP keyword

```
#FLUID_PROPERTIES        // fluid properties keyword
 $DENSITY                // fluid density subkeyword
  4 1000 0 -0.2          // type (4: temperature dependent) | 2 values
 $VISCOSITY              // fluid viscosity subkeyword
  1 0.001                // type (1: constant value) | value
 $SPECIFIC_HEAT_CAPACITY // specific heat capacity subkeyword
  1 4200.0               // type (1: constant value) | value
 $HEAT_CONDUCTIVITY      // thermal heat conductivity subkeyword
  1 0.65                 // type (1: constant value) | value
#STOP                    // end of input data
```

Table B.1: Density models

Model	Meaning	Formula	Parameters
0	curve	RFD file	
1	constant value	ρ_0	value of ρ_0
2	pressure dependent	$\rho(p) = \rho_0(1 + \beta_p(p - p_0))$	ρ_0, β_p, p_0
3	salinity dependent	$\rho(C) = \rho_0(1 + \beta_C(C - C_0))$	ρ_0, β_p, C_0
4	temperature dependent	$\rho(p) = \rho_0(1 + \beta_T(T - T_0))$	ρ_0, β_T, T_0
...	...	...	...

OGS Weblink:
http://www.opengeosys.org/help/documentation/fluid-properties-file
See table B.1.

B.10 MSP - solid properties

Listing B.10: MSP keyword

```
#SOLID_PROPERTIES // solid properties keyword
  $DENSITY        // solid density subkeyword
    1 2500        // type (1: constant value) | value
  $THERMAL        // thermal properties subkeyword
    EXPANSION:    // thermal expansion
    1.0e-5        // values
  CAPACITY:       // heat capacity
    1 1000        // type (1: constant value) | value
  CONDUCTIVITY:   // thermal conductivity
    1 3.2         // type (1: constant value) | value
#STOP             // end of input data
```

OGS Weblink:
TBD

B.11 MMP - porous medium properties

Listing B.11: MMP keyword

```
#MEDIUM_PROPERTIES      // solid properties keyword
 $GEOMETRY_DIMENSION    // dimension subkeyword
  1                     // 1: one-dimensional problem
 $GEOMETRY_AREA         // geometry area subkeyword
  1.0                   // value in square meter if 1D
 $POROSITY              // porosity subkeyword
  1  0.10               // type (1: constant value) | value
 $STORAGE               // storativity subkeyword
  1  0.0                // type (1: constant value) | value
 $TORTUOSITY            // tortuosity subkeyword
  1  1.000000e+000      // type (1: constant value) | value
 $PERMEABILITY_TENSOR   // pemeability subkeyword
  ISOTROPIC   1.0e-15   // tensor type (ISOTROPIC) | value(s)
 $HEAT_DISPERSION       // porosity subkeyword
  1  0.0e+00 0.0e+00    // type (1: constant values) | longitudinal |
    transverse
                            // thermal dispersion length
#STOP                   // end of input data
```

OGS Weblink:
http://www.opengeosys.org/help/documentation/material-properties-file

B.12 OUT - output parameters

Listing B.12: OUT keyword

```
#OUTPUT           // output keyword
 $PCS_TYPE        // process subkeyword
  HEAT_TRANSPORT  // specified process
 $NOD_VALUES      // nodal values subkeyword
  TEMPERATURE1    // specified nodal values
 $GEO_TYPE        // geometry type subkeyword
  POLYLINE ROCK   // geometry type and name
 $TIM_TYPE        // output times subkeyword
  STEPS 1         // output methods and parameter
#STOP             // end of input data
```

OGS Weblink:
http://www.opengeosys.org/help/documentation/output-control-file

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