FACULTAD POLITÉCNICA
UNIVERSIDAD NACIONAL DE ASUNCIÓN

INFORME DE AVANCE DE
MARZO A AGOSTO DE 2016

PROYECTO

MONITOREO Y SIMULACIÓN DE TRANSPORTE DE CONTAMINANTES EN ZONAS URBANAS DEL ACUÍFERO PATIÑO

ANEXO 4

Modeling and Simulation of the Patiño Aquifer

Monitoring and Simulation of the Contaminant Transport in Urban Areas of the Patiño Aquifer

Modeling and Simulation of the Patiño Aquifer

Monitoring and Simulation of the Contaminant Transport in Urban Areas of the Patiño Aquifer — Project: 14-INV-190

August 8, 2016

Jhabriel Varela, Ch.E.
Juan Pablo Nogues, Ph.D.
jhabriel@gmail.com

Facultad Politécnica - Universidad Nacional de Asunción
San Lorenzo - Paraguay

Outline of the presentation

Aim of the work

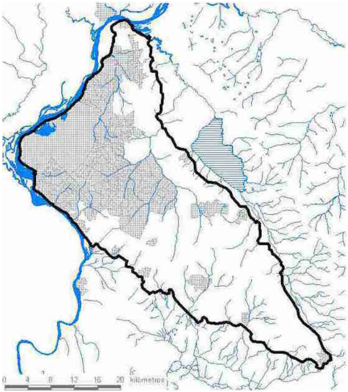


Figure 1: Patiño Aquifer.
Source: Roger Monte Domec. Tercer Congreso Paraguayo de Población.

Simulate the groundwater flow of the Patiño Aquifer using PMWIN, including **topography**, **bathymetry**, **heterogeneity**, and **recharge**.

Motivation

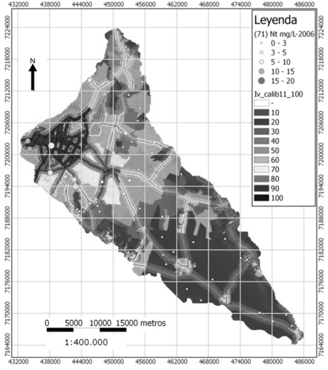


Figure 2: Patiño Aquifer Contamination Map.

Source: Liz Baez, et. al., IV Congreso Paraguayo de Recursos Hídricos.

The simulation of the Patiño Aquifer will allow us to:

- Approximate the water table level in order to control overexploitation of the groundwater.
- Analyse potential contamination scenarios and predict the displacement of the contaminants.
- Predict the optimal location of remediation wells in real contamination scenarios.

Research Methodology

FP - UNA - 2016

Jhabriel Varela, Ch.E.

4

1. Field Data Pre-processing (ILWIS)
2. Modeling and Simulation (PMWIN)
3. Calibration (PEST)
4. Sensitivity Analysis (OAT)

Research Methodology

4

1. Field Data Pre-processing (ILWIS)
2. Modeling and Simulation (PMWIN)
3. Calibration (PEST)
4. Sensitivity Analysis (OAT)

Research Methodology

1. Field Data Pre-processing (ILWIS)
2. Modeling and Simulation (PMWIN)
3. Calibration (PEST)
4. Sensitivity Analysis (OAT)

Research Methodology

1. Field Data Pre-processing (ILWIS)
2. Modeling and Simulation (PMWIN)
3. Calibration (PEST)
4. Sensitivity Analysis (OAT)

ILWIS

Integrated Land and Water Information System

- ILWIS is a remote sensing and GIS software which integrates image, vector and thematic data in one unique and powerful package on the desktop.
- ILWIS delivers a wide range of features including import/export, digitizing, editing, analysis and display of data, as well as production of quality maps.

Figure 3: ILWIS Software.

Source: Official ILWIS's Web Page.

ILWIS

Integrated Land and Water Information System

- ILWIS is a remote sensing and GIS software which integrates image, vector and thematic data in one unique and powerful package on the desktop.
- ILWIS delivers a wide range of features including import/export, digitizing, editing, analysis and display of data, as well as production of quality maps.

Figure 3: ILWIS Software.

Source: Official ILWIS's Web Page.

DEM visualization

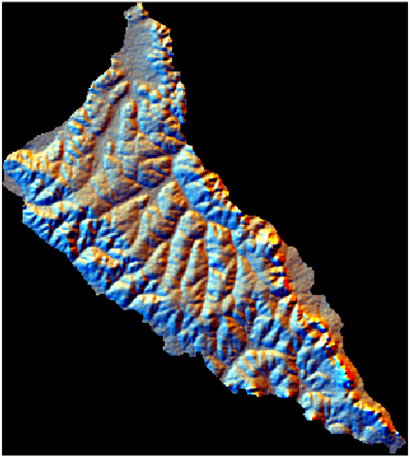


Figure 4: Digital Elevation Model Visualization of the Patiño Aquifer.

Image Processing (Upscaling)

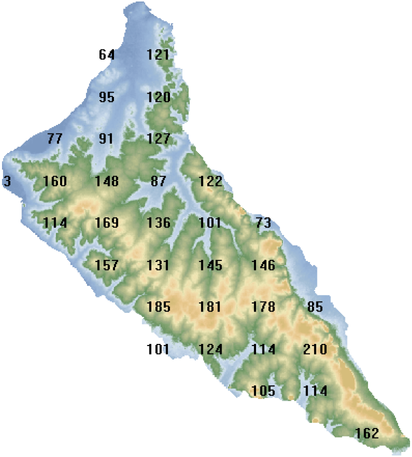


Figure 5: Upscaled DEM map.
· Fine-grid pixel size: 87.431 [m]
· Upscaled-grid pixel size: 175.931 [m]

Flow Determination
Filling Sinks

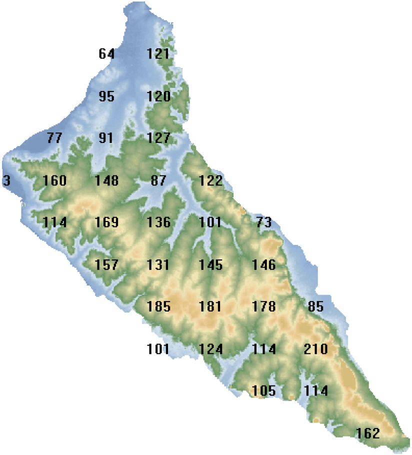


Figure 6: Upscaled DEM map with sinks filled.

Flow Determination
Flow Direction

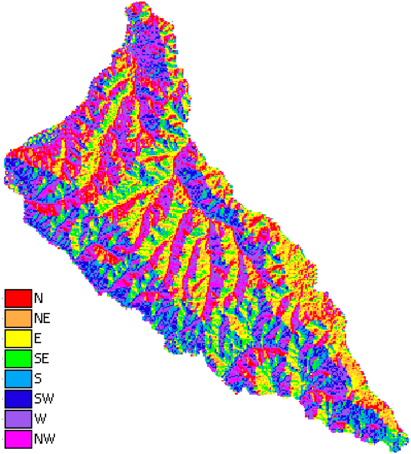


Figure 7: Flow Direction.

Flow Determination

Flow Acummulation

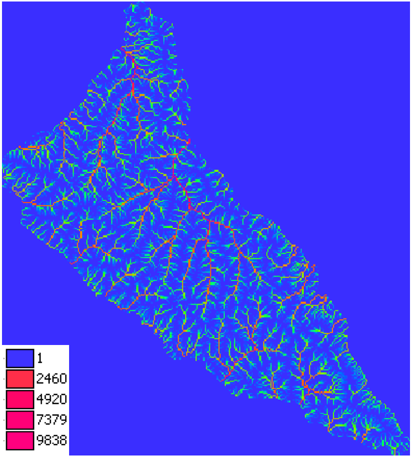


Figure 8: Flow Accumulation.
The output map contains cumulative hydrologic flow values that represent the number of input pixels which contribute to the outlets.

Drainage Network Extraction

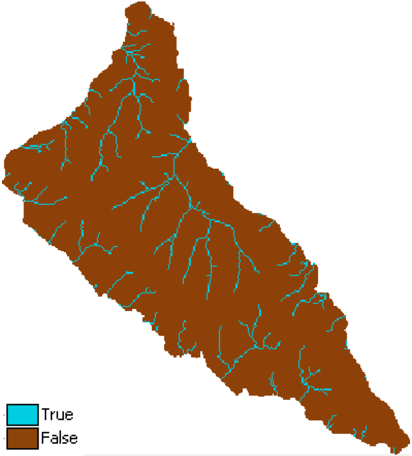


Figure 9: Drainage Network Extraction.
With this pre-processing procedure it is possible to capture the primary, secondary and tertiary streams that are connected to the aquifer.

Governing Equations

Three Dimensional, transient groundwater flow equation (General Case)

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)=S_s\frac{\partial h}{\partial t}\pm Q \qquad (1)$$

Three Dimensional, steady-state groundwater flow equation (Simulated Case)

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)=\pm Q \qquad (2)$$

PMWIN

What is PWMIN?

13

- PMWIN is one of the most complete groundwater simulation systems in the world.
- It provides a sophisticated and integrated groundwater modeling system with the hope that the very user-friendly implementation.

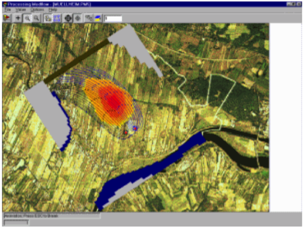


Figure 10: Three-dimensional simulation in PWMIN.

Source: Official PMWIN's Web Page.

PMWIN
What is PWMIN?

13

- PMWIN is one of the most complete groundwater simulation systems in the world.
- It provides a sophisticated and integrated groundwater modeling system with the hope that the very user-friendly implementation.

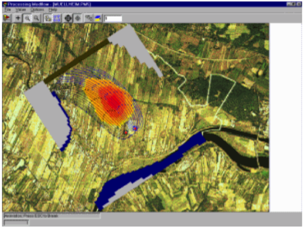


Figure 10: Three-dimensional simulation in PWMIN.
Source: Official PMWIN's Web Page.

PMWIN

Capabilities and Limitations

- PMWIN 5.3.1 is a **freeware** than runs under Windows XP and Windows Vista.
- Provides several packages for simulation purposes, including **Drainage**, **Evapotranspiration**, **Recharge**, **Reservoirs**, **Stream-flow routing**, **Rivers** and **Wells**.
- Well documented.
- Maximum number of rows per layer = 2000.
- Maximum number of columns per layer = 2000.
- Maximum number of cells = 250,000.
- Not possible to perform several simulations.

PMWIN

Capabilities and Limitations

- PMWIN 5.3.1 is a **freeware** than runs under Windows XP and Windows Vista.
- Provides several packages for simulation purposes, including **Drainage**, **Evapotranspiration**, **Recharge**, **Reservoirs**, **Stream-flow routing**, **Rivers** and **Wells**.
- Well documented.
- Maximum number of rows per layer = 2000.
- Maximum number of columns per layer = 2000.
- Maximum number of cells = 250,000.
- Not possible to perform several simulations.

PMWIN

Capabilities and Limitations

- PMWIN 5.3.1 is a **freeware** than runs under Windows XP and Windows Vista.
- Provides several packages for simulation purposes, including **Drainage**, **Evapotranspiration**, **Recharge**, **Reservoirs**, **Stream-flow routing**, **Rivers** and **Wells**.
- Well documented.
- Maximum number of rows per layer = 2000.
- Maximum number of columns per layer = 2000.
- Maximum number of cells = 250,000.
- Not possible to perform several simulations.

- PMWIN 5.3.1 is a **freeware** than runs under Windows XP and Windows Vista.
- Provides several packages for simulation purposes, including **Drainage**, **Evapotranspiration**, **Recharge**, **Reservoirs**, **Stream-flow routing**, **Rivers** and **Wells**.
- Well documented.
- Maximum number of rows per layer = 2000.
- Maximum number of columns per layer = 2000.
- Maximum number of cells = 250,000.
- Not possible to perform several simulations.

PMWIN
Capabilities and Limitations

- PMWIN 5.3.1 is a **freeware** than runs under Windows XP and Windows Vista.
- Provides several packages for simulation purposes, including **Drainage**, **Evapotranspiration**, **Recharge**, **Reservoirs**, **Stream-flow routing**, **Rivers** and **Wells**.
- Well documented.
- Maximum number of rows per layer = 2000.
- Maximum number of columns per layer = 2000.
- Maximum number of cells = 250,000.
- Not possible to perform several simulations.

PMWIN

Capabilities and Limitations

- PMWIN 5.3.1 is a **freeware** than runs under Windows XP and Windows Vista.
- Provides several packages for simulation purposes, including **Drainage**, **Evapotranspiration**, **Recharge**, **Reservoirs**, **Stream-flow routing**, **Rivers** and **Wells**.
- Well documented.
- Maximum number of rows per layer = 2000.
- Maximum number of columns per layer = 2000.
- Maximum number of cells = 250,000.
- Not possible to perform several simulations.

PMWIN

Capabilities and Limitations

- PMWIN 5.3.1 is a **freeware** than runs under Windows XP and Windows Vista.
- Provides several packages for simulation purposes, including **Drainage**, **Evapotranspiration**, **Recharge**, **Reservoirs**, **Stream-flow routing**, **Rivers** and **Wells**.
- Well documented.
- Maximum number of rows per layer = 2000.
- Maximum number of columns per layer = 2000.
- Maximum number of cells = 250,000.
- Not possible to perform several simulations.

PMWIN

Research and publications with PMWIN

- **A Survey of Methods for Analysing Groundwater Recharge in Arid & Semi-arid Region.** (United Nations Environmental Programme; Year of publication: 2002; 5,905 KB).
- **A System to support decision making for peatland management in the humid tropics.** By Henk Ritzema, Dana Veltman, and Henk Wösten. Published in: J. Paivanen (Ed). Wise use of peatlands. Proceedings 12th Int. Peat Congress, 6-11 June 2004, Tampere, Finland, Vol I: 720-725.
- **Comparision of an analytic and a numerical approach for tracer transport in a fractured geothermal reservoir.** By Aniko Toth, Peter Szucs and Elemer Bobok. PROCEEDINGS, Thirty-Fourth Workshop on Geothermal Reservoir Engineering. Stanford University, Stanford, California, February 9-11, 2009.

PMWIN

Research and publications with PMWIN

- **Complex Scientific Analysis in Geothermal Exploration in the Pannonian Basin.** By Elemer B, Peter Sz, Aniko T, and Attila K. Proceedings World Geothermal Congress 2010. Bali, Indonesia, 25-29 April 2010.
- **Development of Steady State Groundwater Flow Model in Lower Walawa Basin - Sri Lanka.** (Integrating GIS, Remote Sensing, and Numeric Groundwater Modelling). By Amarasingha Arachchillage Anoja Kumudu Kumari Senevratne, March 2007)
- **Evaluation of groundwater resources in the Geba basin, Ethiopia.** By Kibrewossen Tesfagiorgis, Tesfamichael Gebreyohannes, Florimond De Smedt, Jan Moeyersons, Miruts Hagos, Jan Nyssen and Jozef Deckers. Bulletin of engineering geology and the environment DOI: 10.1007/s10064-010-0338-3

PMWIN

Research and publications with PMWIN

- **Groundwater Availability Models of Texas: A great number of groundwater availability models (GAMs) has been developed since early 2000's for major and minor aquifers of the State of Texas with Processing Modflow**. Documents and datasets of the models are available from the website of the Texas Water Development Board. GAMs include comprehensive information on each aquifer, such as recharge (amount of water entering the aquifer); geology and how that conveys into the framework of the model; rivers, lakes, and springs; water levels; aquifer properties; and pumping.
- **Groundwater flow section modelling of salinisation processes in the Champhone Catchmen**t, Savannakhet Province, Lao PDR. By Iwona Wiszniewski and Rungruang Lertsirivorakul. Proceedings of the 2005 International Conference on Simulation and Modelling.
- **Groundwater Modeling Course. Material of a short course that utilizes PMWIN**. By Arlai Phatcharasak, University Rajabhat Pathom Nakhon and Manfred Koch, University of Kassel.

Creation of the mesh

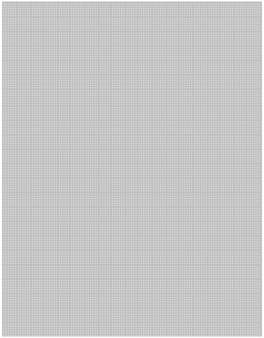


Figure 11: Part of the mesh used for the simulation.

- Number of columns: 309
- Size of the columns: 174.931 [m]
- Total horizontal length: 54,054 [m]
- Number of rows: 343
- Size of the rows: 174.931 [m]
- Total vertical length: 60,001 [m]
- Number of cells: 105,987
- Number of inactive cells: 67,318 (63.5 %)
- Number of active cells: 38,669 (36.5 %)

Type of Layers

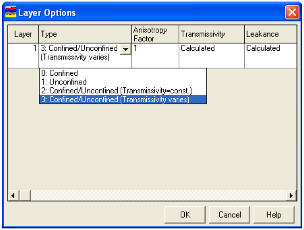


Figure 12: Layer Options.

PMWIN deals with four type of layers:

- Strictly confined
- Strictly unconfined
- Confined or unconfined with **constant** transmissivity
- Confined or unconfined with **variable** transmissivity

For our model, we select the last type, in order to handle variations of the water table.

Boundary Conditions

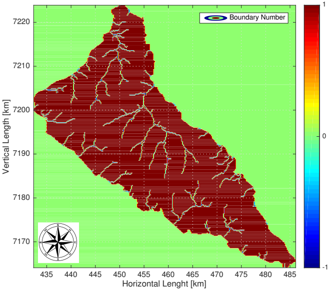


Figure 13: Boundary Conditions.

PMWIN deals with three types of boundary conditions:

- 0 No flux or **inactive cells**.
- 1 Active cells.
- -1 Fixed head cells.

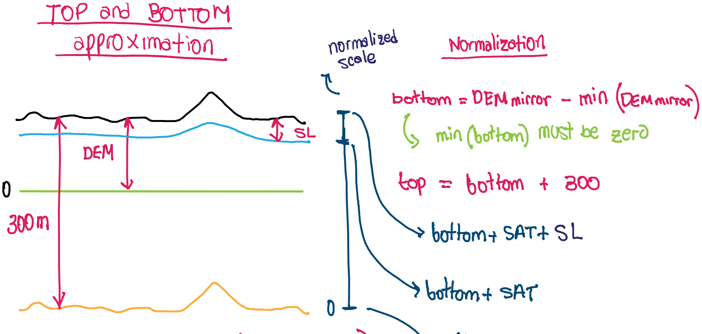
The hydraulic head of the active cells will change during the simulation.

The hydraulic head of the fixed head cells will remain constant.

Inhere, we set the Paraguay River and all the streams as fixed cells.

Bottom and Top Of Layers

In order to approximate the top and the bottom of the aquifer, we suggest the following strategy:



DEM mirror = DEM − 300 (Negative values)

SAT = 300 − SL (saturated zone thickness)

$$\boxed{\text{CHECK} \rightarrow (\text{bottom} + \text{SAT} + \text{SL}) - \text{top} = 0}$$

Bottom and Top Of Layers

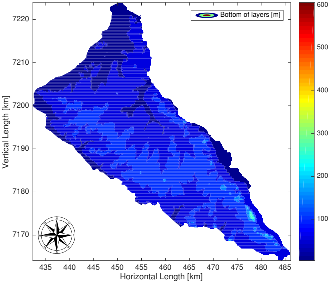


Figure 14: Bottom of the aquifer.

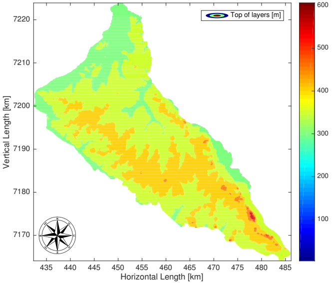


Figure 15: Top of the aquifer.

Time parameters

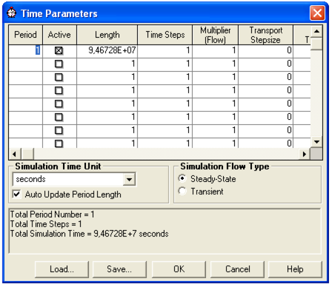


Figure 16: Time parameters.

PMWIN deals with two options regarding the time parameters:

- Steady-state simulation.
- Transient simulation.

As we said before, this simulation will be in steady-state in order to lower the complexity of the problem.

Initial Hydraulic Heads

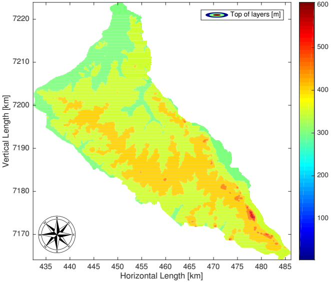


Figure 17: Initial Hydraulic Heads.

In PMWIN it is necessary to set initial hydraulic heads. Even though this is a steady-state simulation, it is mandatory to assign values of hydraulic heads to the Paraguay River and streams.

As a first attempt, we have tried to use the static level measurements, however, setting the top of layers as initial heads offers far more accurate results.

Horizontal Hydraulic Conductivity

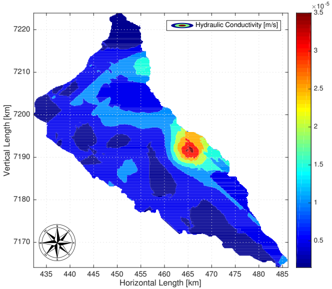


Figure 18: Horizontal Hydraulic Conductivity.

PMWIN can also take into account the effects of heterogeneity. The heterogeneity matrix is generated from field data and must be consistent with the units of the simulations, in this case [m/s].

Effective Porosity

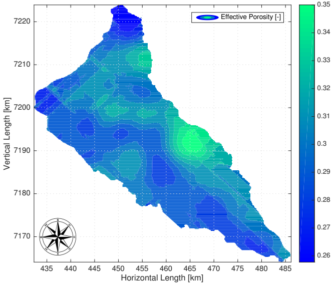


Figure 19: Heterogeneous porosity field.

The porosity field is generated with a correlation that relates the permeability and the porosity (Holtz, 2002).

$$\phi(k) = \left(\frac{k(md)}{7 \times 10^7}\right)^{\left(\frac{1}{9.606}\right)}. \quad (3)$$

Moreover, the permeability is related with the hydraulic conductivity via:

$$K = \frac{k\mu}{\rho g}, \quad (4)$$

where g is the acceleration of gravity and μ and ρ are the dynamic viscosity and density of water, respectively.

Recharge

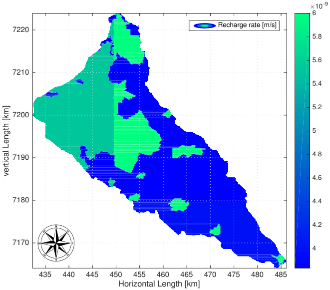


Figure 20: Recharge.

The recharge rate is set via a package from MODFLOW, which is external to PMWIN. The recharge map was generated considering the natural recharge from rain and the anthropogenic recharge due to agricultural activities (mainly).

The recharge rate must be imported in [m/s].

Wells

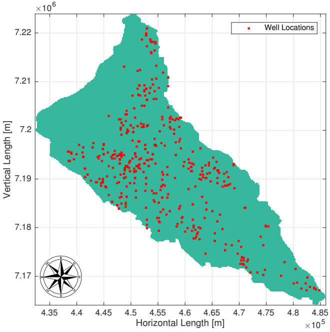


Figure 21: Positions of wells.

In PMWIN, we can also include extraction and injection wells by assigning its rates to the corresponding cell.

Discharge Wells Rates

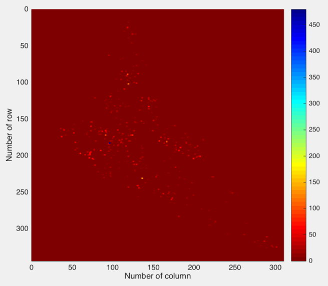


Figure 22: $x - y$ view of the extraction rates.

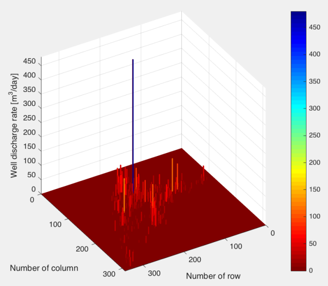


Figure 23: 3D view of the extraction rates..

Results

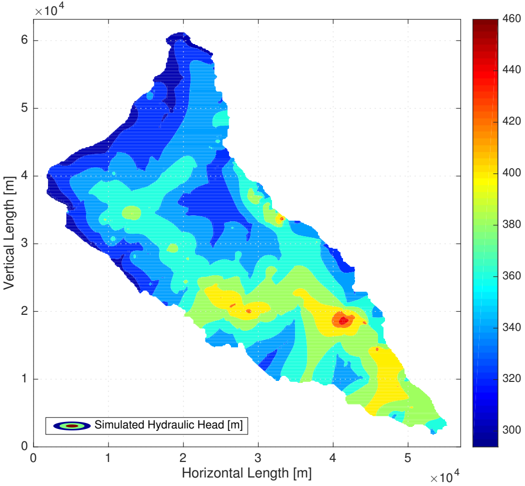


Figure 24: Steady-state distribution of the hydraulic head.

Difference between input and output

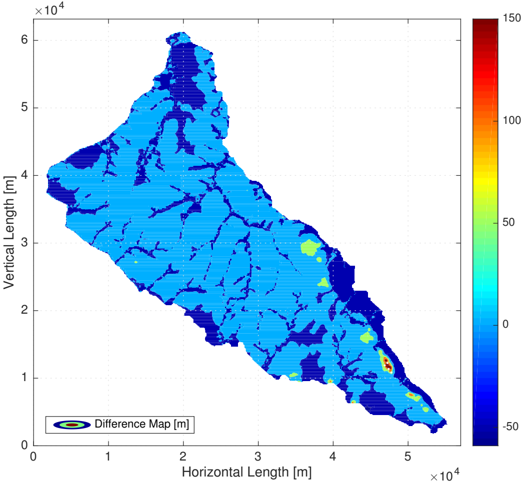


Figure 25: Difference Map: Static Level (Field Data) - Simulated Heads

Cuts and profiles

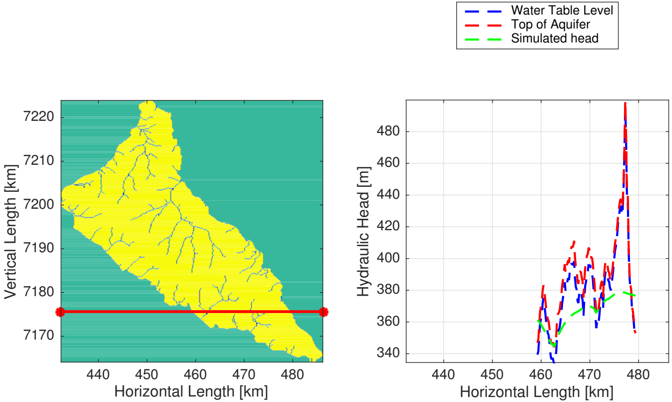


Figure 26: Cut at y = 7176 [km]

Cuts and profiles

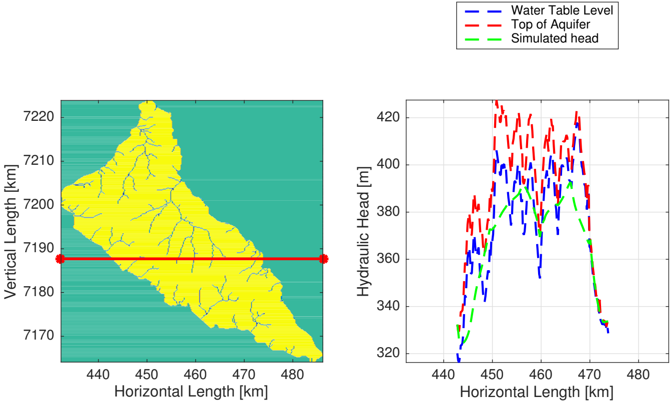


Figure 27: Cut at y = 7188 [km]

Cuts and profiles

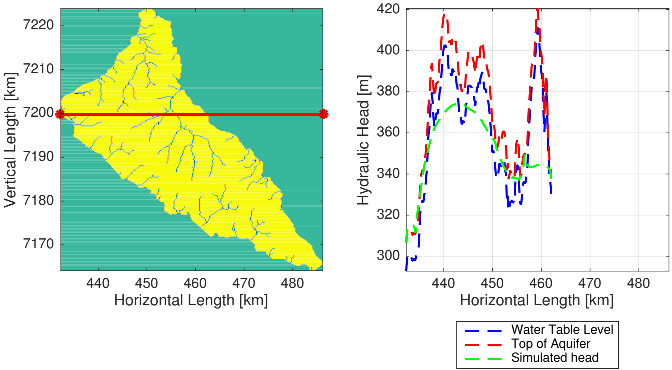


Figure 28: Cut at y = 7200 [km]

Cuts and profiles

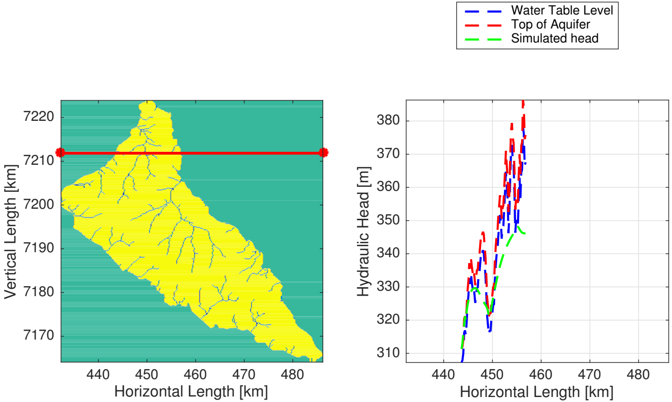
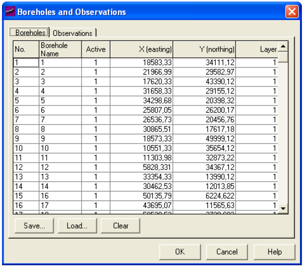


Figure 29: Cut at y = 7212 [km]

Boreholes

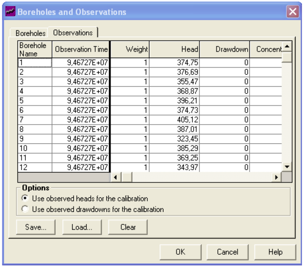


No.	Borehole Name	Active	X (easting)	Y (northing)	Layer
1	1	1	18583,33	34111,12	1
2	2	1	21966,99	29582,97	1
3	3	1	17620,33	43390,12	1
4	4	1	31658,33	29155,12	1
5	5	1	34298,68	20398,32	1
6	6	1	25807,05	26200,17	1
7	7	1	26536,73	20456,76	1
8	8	1	30865,51	17617,18	1
9	9	1	18573,33	49999,12	1
10	10	1	10551,33	35654,12	1
11	11	1	11303,98	32873,22	1
12	12	1	5828,331	34367,12	1
13	13	1	33354,33	13990,12	1
14	14	1	30462,53	12013,85	1
15	16	1	50135,79	6224,622	1
16	17	1	43695,07	11565,63	1

Figure 30: Allocation of boreholes (field data)

PMWIN allow us to set boreholes in order to include information regarding hydraulic head (water table level) or concentration. We need to pass the information as a `.bor` containing the X and Y coordinate of the borehole and its corresponding layer.

Observation Wells



Borehole Name	Observation Time	Weight	Head	Drawdown	Concent
1	9,46727E+07	1	374,75	0	
2	9,46727E+07	1	376,69	0	
3	9,46727E+07	1	355,47	0	
4	9,46727E+07	1	368,87	0	
5	9,46727E+07	1	396,21	0	
6	9,46727E+07	1	374,73	0	
7	9,46727E+07	1	405,12	0	
8	9,46727E+07	1	387,01	0	
9	9,46727E+07	1	323,45	0	
10	9,46727E+07	1	385,29	0	
11	9,46727E+07	1	369,25	0	
12	9,46727E+07	1	343,97	0	

Figure 31: Observation wells with their corresponding hydraulic head values.

The information of the value (in this case hydraulic head) is set in the Observation Windows. Several parameters can be set, in this case the only values that concern us are the *observation time*, *weight*, and *head*. The observation time corresponds to the final simulation time (in steady state), the weight is set as 1 and the head is the field measurement. All the other parameters are set as 0.

Observation Wells Map

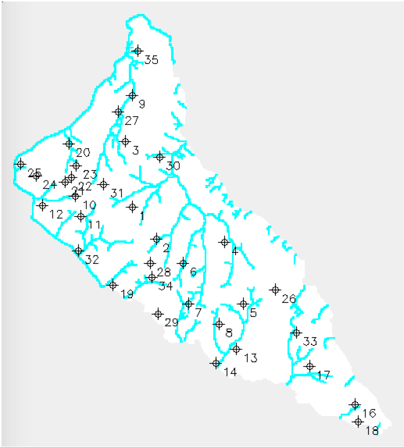


Figure 32: Domain showing the locations of the observation wells.

Observed vs. Calculated heads

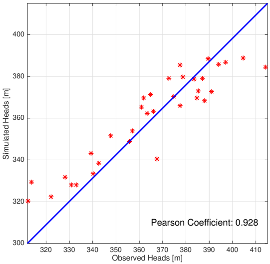


Figure 33: Simulated heads [m] vs. Observed heads[m]

Now, we plot the simulated heads (results) against the observed heads (data field) in order to demonstrate the accuracy of the model. We quantify the relation between the parameters via the Pearson Coefficient. A Pearson coefficient close to 1 will show a strong linear correlation.

Calibration

Modflow offers a calibration package called PEST (Parameter Estimation). PEST takes as inputs specific parameters (as recharge zones, conductivities zones, well rates, etc) which are optimized via an algorithm in order to minimize the difference between **observed hydraulic head** values and **simulated hydraulic head values**.

How does it work?

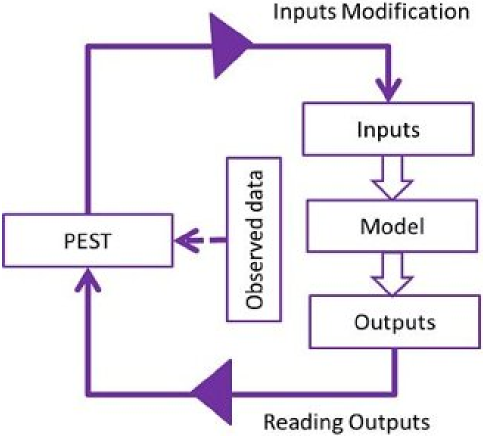


Figure 34: General Algorithm Necessary for Calibration.

Variable to calibrate

- Calibrated Variable: Recharge rate
- Number of Regions: 6
- Goal: Minimize difference between calculated hydraulic heads values and data field measurements (boreholes)

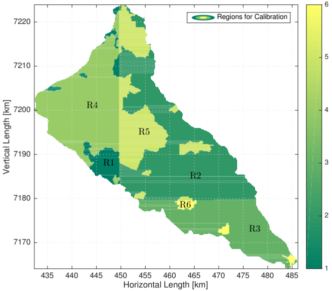


Figure 35: Regions to calibrate.

Calibration of the model

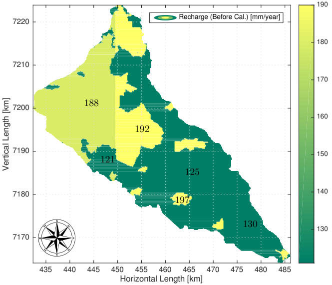


Figure 36: Recharge Map before calibration.

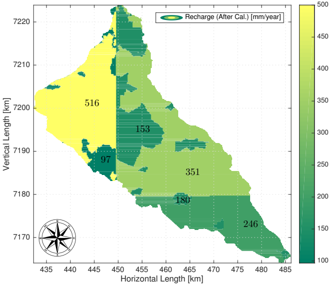


Figure 37: Recharge Map after calibration.

Results after the calibration process

FP - UNA - 2016

Jhabriel Varela, Ch.E.

44

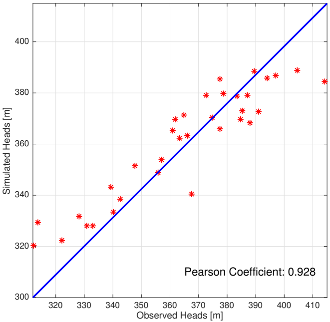


Figure 38: Calculated Heads vs. Observed Heads (before calibration).

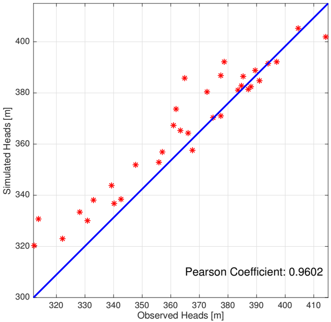


Figure 39: Calculated Heads vs. Observed Heads (after calibration).

What's Sensitivity Analysis?

FP - UNA - 2016

Jhabriel Varela, Ch.E.

Sensitivity analysis is the study of how the uncertainty in the output of a mathematical model or system (numerical or otherwise) can be apportioned to different sources of uncertainty in its inputs.

Types of Sensitivity Analysis

- One-at-a-time (OAT/OFAT)
- Local methods
- Scatter plots
- Regression analysis
- Variance-based methods
- Screening

One-at-a-time method

One of the simplest and most common approaches is that of changing one-factor-at-a-time (OFAT or OAT), to see what effect this produces on the output. OAT customarily involves:

- Moving one input variable, keeping others at their baseline (nominal) values, then,
- Returning the variable to its nominal value, then repeating for each of the other inputs in the same way.

Despite its simplicity however, this approach does not fully explore the input space, since it does not take into account the simultaneous variation of input variables. This means that the OAT approach cannot detect the presence of interactions between input variables.

Inputs and Outputs Variables

Input Variables

- Horizontal Hydraulic Conductivity
- Effective Porosity
- Recharge Rate
- Well's Extraction Rates

Output Variable

- Water fraction[1]

[1] The Water fraction is defined as the total volume of water within the aquifer per void volume within the aquifer.

Sensitivity Analysis Table

% Change	ΔW_f Hyd. Cond.	ΔW_f Porosity	ΔW_f Recharge
-80	Non-conv.	0	-2.4721
-60	Non-conv.	0	-1.8411
-40	Non-conv.	0	-1.2191
-20	0.5497	0	-0.6055
0	0	0	0
$+20$	-0.3709	0	0.5980
$+40$	-0.6382	0	1.1888
$+60$	-0.8398	0	1.7727
$+80$	-0.9975	0	2.3502

Sensitivity Analysis Plots

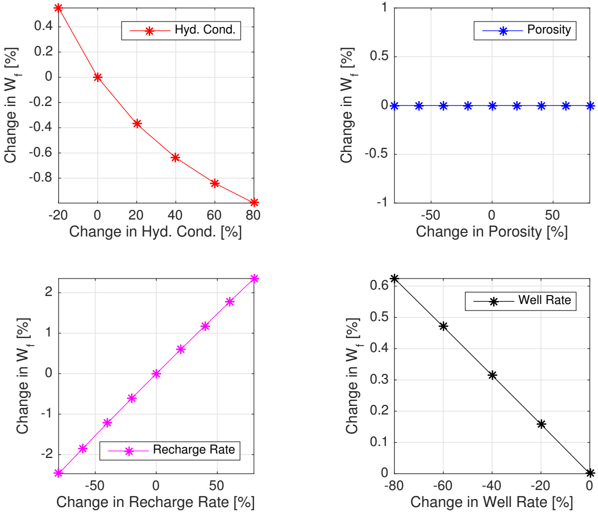


Figure 40: Results of the sensitivity analysis.

Conclusions

- The model that has been presented provides an useful tool for analyzing the groundwater flow of the Patiño Aquifer.
- The results after the calibration process show a strong correlation between the field measurements and the simulated hydraulic heads.
- Regardless the assumptions made along the modeling process, this work represents a robust starting point for future works.
- The possibility to add the effects of contamination to the model is highly feasible with the modules provided by PMWIN.