UNIVERSIDAD AUTÓNOMA DE SAN LUIS POTOSÍ

FACULTAD DE CIENCIAS QUÍMICAS, INGENIERÍA Y MEDICINA

PROGRAMAS MULTIDISCIPLINARIOS DE POSGRADO EN CIENCIAS AMBIENTALES

THESIS TO OBTAIN THE DEGREE OF

DOCTORADO EN CIENCIAS AMBIENTALES

GROUNDWATER USE IN THE MÉRIDA-PROGRESO REGION, YUCATÁN, AND ITS IMPLICATIONS IN THE COASTAL AREA ECOSYSTEMS REQUIREMENTS

BY

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INSTITUTIONAL CREDITS

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1. Introduction

1.1. Importance of groundwater

Groundwater has been since ancient times an important source of supply for population, either by the use or uptake of springs (including rivers water receptors) or directly accessing the saturated level by wells (Custodio 1995). So amazing and abundantly used, sometimes its origin and processes are hardly known, so it is quite vulnerable to misunderstandings, which lies largely, in its physical position (below ground surface) and therefore can't be seen (Moore *et al.* 2005).

Price (2003), estimated the balance of water in the world and predicted a volume of water in the planet indicating that the total available drinking water in good condition for human consumption, 95% corresponds to groundwater.

It is very common that the water resources management is not governed with technical and scientific criteria, although it has a large amount of existing knowledge, impacting in inappropriate harvesting strategies (Vargas & Mollard 2005).

With the continuous development of society and science, population uses water resources increasingly, leading to negative effects such as depletion and pollution of groundwater, which motivates the interest and concern of governments, social organizations and scientific groups looking for the conservation and protection of water (Batista 2001).

Such interest has been reflected in increased research on variables that affect the hydrological cycle and as a result there is a boom in the study of groundwater water balances in several ways like quantifications in natural water discharges (Smith & Nield 2003), catchment areas (Cardille *et al.* 2004), recharge estimations (Healy & Cook 2002; Flint *et al.* 2002; Edmunds *et al*. 2002; Lewis & Walker 2002; Carrera & Gaskin 2008), studies of groundwater levels caused by extractions (Carrera & Gaskin 2007) and climate change (Kirshen 2002).

Also, in the last years it has emerged the need to predict the behavior of groundwater levels to different particular cases, incorporating the most important influences in accordance with the purpose of study and have given way to the groundwater flow modeling to meet potential impacts to several natural situations and patterns of groundwater extraction that has influence in the behavior of the variables that governing the groundwater movement (Guvanasen & Wade 2000; Ramirez 2000; CEAG 2001; Sanford 2002; Vallner 2003; Jaworska-Szulc 2004, McPhee & Yeh 2004; Ökten & Yazicigil 2005; Vásquez 2005; Abderrahman *et al*. 2007;. Rojas 2007; Weiss & Gvirtzman 2007; Rocha 2009).

1.2. Problem statement (state-of-the-art)

1.2.1. Karstic morphology

Karstification is a complex geological phenomenon related with geological media compounds of limestone, dolomite, gypsum, halite and other soluble rocks, which have very specific hydrogeological characteristics. This process, which involves the dissolution of the rocks may occur naturally or artificially under the action of water and followed by chemical, physico-chemical, geological and climatic conditions in the time, causing openings, destruction and alteration of rock structures, formations, groundwater movement, drainage network regimes and topographical features (Assaad & Jordan 1994; Darnault 2008).

In karstic terrains, the effective porosity is due to a combination of high secondary porosity fissures and tertiary porosity in areas where the system of fissures ducts has been enlarged by chemical dissolution effects. As a result, the groundwater flow in karstic aquifers can occur in some areas as diffuse and sometimes as flow through ducts, and can be present both cases adjacently (Teutsch & Sauter 1991).

Karst land cover between 12% (KWI, 2008) and 25% (Ford & Williams 2007; LaMoreaux *et al*.1997) of the total land surface of the planet (Figure 1) and 25% of the total world population is supplied either partially or completely by water from karst aquifers (Darnault 2008; Green *et al.* 2006).

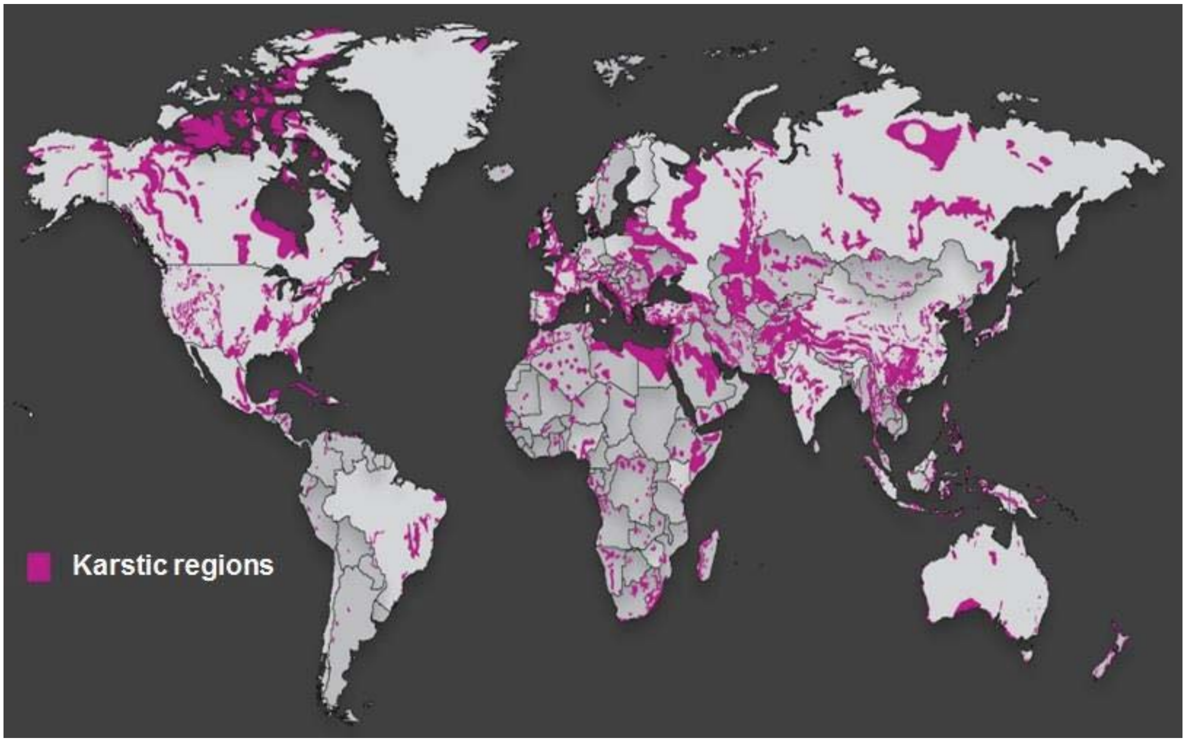


Figure 1. Karstic regions in the world (modificated of Circle of Blue 2010).

México has a karst area of 391 700 km^2 (Figure 2) in the different provinces of the country (Gunn 2004), where there are different types as "plateau platform karst" in the Yucatán Peninsula (YP), in the “Planicie Norte” and in the northern portion of the “Planicie Costera del Golfo”. The "karst plateau by staggered faults" is found only in the eastern part of the “Planicie Norte” of the YP. The "lower elevations folded karst and fold block” corresponds to the “Planicies y Lomeríos del Sur” of the YP. The "tilt table karst" appears in a small region of the Sierra Madre Oriental (Espinasa 1990).

Figure 2. Karstic regions of México (modificated of “Instituto de Geografía”, UNAM 2012).

The rest of the karstic regions of México correspond to the type of folded mountain elevations and fold-block in different variants (alpine, tropical, subtropical, fossil, mixed, etc.) so it covers areas of the provinces of the “Sierra Madre Oriental”, “Sierra Madre del Sur”, “Mesa Central”, “Chiapas” and “Depresión del Balsas”. Some provinces have not karst development (although in some of them there are few outcrops of limestone which form a potential karst) as the “Baja California” Peninsula, the “Sierras Sepultadas de Sonora”, the “Planicie Costera del Pacífico Occidental”, the “Sierra Madre Occidental”, the “Cinturón Neovolcánico Transversal”, the “Planicie del Noreste” and the “Planicie Costera del Golfo de México” (Espinasa 1990).

Due to the complexity of karstic aquifers, concepts related to groundwater movement and occurrence, methods of exploration and development of water, engineering safety practices in all types of construction and environmental safety, can’t be based on a comparable regulations with another types of aquifers (LaMoreaux *et al.* 1997).

Karstic aquifers exploitation contemplates the concept of the close relationship between surface water and groundwater with the karstification process for the management and protection of water resources against overexploitation and pollution (Darnault 2008).

1.2.2. Groundwater contamination in karstic aquifers

Karstic aquifers have very different characteristics of the porous media aquifers: quick hydraulic responses, high velocities of flow and transport through ducts and channels which makes them particularly vulnerable to spills of contaminants (Green *et al.* 2006).

Karst areas are susceptible to higher ranks problems of environmental impact than any other type of terrain (Ford & Williams 2007). The karstic groundwater pollution depends of the conditions in the catchment areas and the potential of the contaminant; furthermore, the spreading of contaminants is faster than in the porous media aquifers due to higher flow velocities, which does not give much time for contaminants to be retarded by chemical reactions or other attenuation mechanisms (Kaçaroğlu 1999).

Possible contaminants that can be found in groundwater are unlimited and can be classified into organic and inorganic chemicals, biological, physical and radiological, while the main sources of these can be categorized as municipal, industrial and agricultural, combined with the growth urban areas, altering the conditions of groundwater quality and quantity (Kaçaroğlu 1999).

There are different karst areas in the world where exist pollution problems in karstic aquifers and which have conducted various studies to characterize the problems as: domestic, industrial, agricultural processes, services and mining, sewage infiltration deposited directly in the ground without treatment (Bodhankar & Chatterjee 1994; Drew 1996; Kaçaroğlu 1999; Green *et al*. 2006; De Waele 2009; Kelly *et al*. 2009;. Lúcia *et al*. 2012; Qiao *et al.* 2011), the behavior of the distribution and transport of hydrocarbons (Zhu *et al.* 2000), the spatiotemporal variation groundwater quality (Jiang *et al.* 2006), the groundwater quality due to water table fluctuations in karstic media (Rudzianskaite & Sukys 2008) and the determination of protection zones for sustainable use of water resources (Biondić *et al*. 2006;. Qian *et al.* 2006).

1.2.3. Freshwater/Saltwater interaction

Although the intensive use and pollution of groundwater represent frequent problems, the freshwater-seawater interaction creates a unique problem in terms of sustainability called saline intrusion. This phenomenon consists in the entrance of seawater into freshwater aquifers, causing changes in the quantity and quality of groundwater discharge to coastal systems (Barlow & Reichard 2010). As a result, coastal aquifers are characterized by spatiotemporal salinity variations, a condition that justify a special research treatment in the flow and quality characteristics (Post & Abarca 2009). In México like in many other countries, there are large lengths of coastline. The development of several economic activities, generates a groundwater exploitation which causes constant changes in relationships freshwater-saltwater (Custodio & Llamas 1976). The analysis of the relationship between freshwater-saltwater (Figure 3) in coastal regions creates a state of equilibrium called brackish water interface; its location and dimensions depend on the hydrogeological characteristics and density of seawater. The brackish water interface is dynamic and depends on variations in groundwater recharge and extraction (Custodio & Llamas 1976).

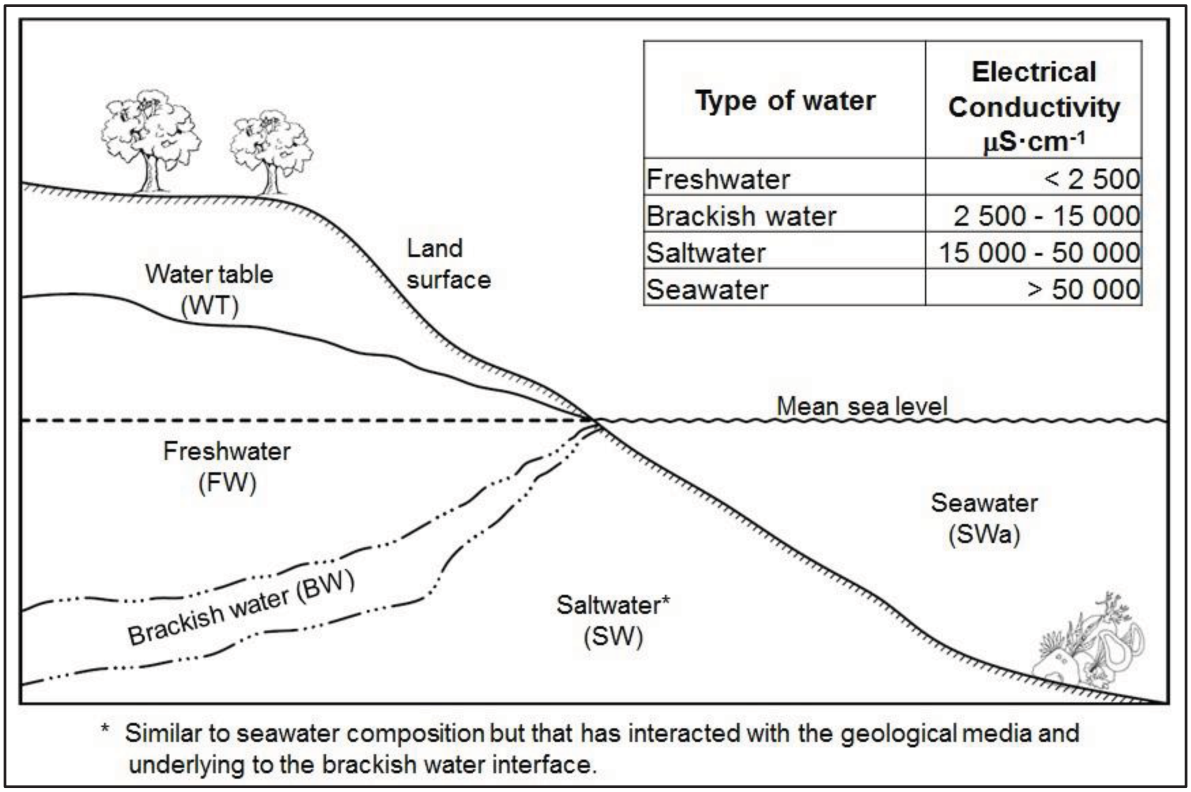


Figure 3. General definition of types of water into coastal aquifers (applicable to this thesis).

Coastal karstic aquifers generate great interest because its natural discharge supports diverse coastal ecosystems (mangroves, wetlands, etc.) and they are use like supply source for population. In these calcareous geological media geochemical processes can accelerate the increase of high permeability through the dissolution of ducts development. Applying chemical thermodynamic principles, it has been shown that simple mixing of two samples of water in equilibrium or even supersaturated with respect to calcite, can result in a mixture undersaturated with respect to the mineral (Hanshaw & Back 1979). Direct observations corroborate that there is an increase of karstification in the brackish water interface. Furthermore, the physicochemical process of water/aquifer interaction, play an important role in ion exchange processes (Ca/Na), dolomitization or magnesian fraction increasing of limestones, and may also be variable in the year due to the change of composition of freshwater (Fernández *et al*. 2003).

In México, the biggest problems of saline intrusion are located in the states of “Sonora”, “Baja California” and “Baja California Sur”, while problems of lesser magnitude have been identified in the YP, “Veracruz”, “Sinaloa” and “Nayarit” (Barlow & Reichard 2010). Have been reported salinization phenomena due to diagenetic effects by interaction with groundwater low salinity, changes in the flow regime as a result of pumping rate and percolated effluents produced by agricultural activities in the coastal aquifer of “Valle de Santo Domingo” (“Baja California Sur”, México, Cardona, Carrillo-Rivera, Huizar-Álvarez & Graniel-Castro 2004); saltwater intrusion problems in more than 30 km inland into the aquifer “Costa de Hermosillo” (“Sonora”, México; Rangel *et al*. 2002); and effects on water quality at supply sites in “Ensenada” city because of saline intrusion as a result of pumping in the aquifer “Maneadero” (“Baja California”, México; Daesslé *et al.* 2005). In all of these investigations, the location of the saltwater interface was not identified.

Due to the high hydraulic conductivities of the coastal plains of the Pliocene (10-86 000 $m \cdot day^{-1}$, depending on the scale of analysis; Worthington & Ford 2009), where the water table elevations of freshwater are under 2 masl, in large areas of the YP, saline intrusion effects occur (Bauer-Gottwein *et al.* 2011).

1.2.4. Nitrogen cycle

Nitrogen exists in many forms in the natural environment and is an essential nutrient for life (Biitner 2000). Nitrogen is an essential constituent of proteins that are a basic component of all living tissues. It is also the main constituent (79% by volume) of the atmosphere. The paradox is that in gaseous form (N_2), although it is abundant because of its inertness, is not harvestable by most life forms; before it can be used it should become in more reactive chemical forms. The transformation to these other forms is the one that occupies most of the nitrogen cycle (Smith & Smith 2001).

To be used, the free molecular nitrogen to be fixed. This fixation occurs in two ways. The first way, is a fixation by chemical action of high energy. Cosmic radiation, contrails meteorites and lightning provide the high energy needed to combine nitrogen with oxygen and water. Ammonia and the resulting nitrates are carried to the surface of the earth with rainwater. The second method of fixation is biological, which is carried out by nitrogen-fixing bacteria, some of them are symbiotic, which living in association with leguminous and non-leguminous plants that produce nodules on the roots, by free living aerobic bacteria and anaerobic conditions or cyanobacteria. Fixing divides molecular nitrogen (N_2) into two free N atoms. Free N atoms then combine with hydrogen to form two molecules of ammonia (NH_3) (Smith & Smith 2001).

Another source of Nitrogen is the organic matter. The dead organic matter decomposed by putrefaction, it releases nitrogen in the ecosystem as ammonia (ammonification) and is the starting point for other phases of the nitrogen cycle: the processes of nitrification and denitrification. In ammonification, decomposers break down the amino acids of dead organic matter for obtain energy releasing the amino groups in the form of ammonia. It is a unidirectional reaction and the released ammonia is then absorbed directly by the roots of plants and incorporated into their amino acids, which will go into the food chain. Nitrification is a biological process in which ammonia is oxidized by nitrifying bacteria to nitrites and nitrates, producing energy. Two groups of microorganisms are involved: the bacteria of the genus Nitrosomonas which using ammonia soil as their only source of energy and promote its transformation into nitrites and water. And the genus Nitrobacter, another group of bacteria which subsequently take these nitrites transforming in nitrates. Nitrogen in nitrate form can be transformed by the denitrification process in gaseous molecular nitrogen (N_2) by the action of denitrifying bacteria, represented by numerous species of the genus Pseudomonas and *Thiobacillus denitrificans* (Smith & Smith 2001).

These processes take place under certain conditions of temperature and pH, but it is essential the aerobic character of nitrification and anaerobic character of denitrification, the process in which NO_3^- is the terminal acceptor of electrons in the anaerobic respiratory chain (Smith & Smith 2001).

Combining these basic and necessary processes, it is possible to construct the nitrogen cycle. The main source of nitrogen under natural conditions is the biological fixation of atmospheric nitrogen to which additions of inorganic nitrogen are produced by rain, having originated with the help of lightning and volcanic activity. There is an ammonia absorption from the atmosphere by the plants and soil and an increase of nitrogen occurs from windblown aerosols, which containing both organic and inorganic forms of nitrogen. In terrestrial ecosystems, nitrogen, largely as ammonia or nitrates, it is absorbed by plants, which make in amino acids and proteins. Amino acids are transferred to consumers that make their own proteins. Finally, animal excrements, dead plants and dead animals are decomposed by bacteria and fungi with the release of ammonia. Ammonia can get lost in the atmosphere as a gas, become NO_3^- by the action of nitrifying bacteria, or be absorbed directly by plants. Nitrates can be used by plants by immobilization in the form of microbial biomass, linked to decaying organic matter, or leachates. The leached material comes through runoff to different streams, lakes and finally to the sea, where it is available for to be use in aquatic ecosystems (Smith & Smith 2001).

In aquatic ecosystems, nitrogen circulates similarly, except because there is not the large reservoir from the soil. Life in the water adds organic matter and dead organisms which suffer decomposition, releasing ammonia, which is subsequently converted to nitrites or reincorporated to biomass (Smith & Smith 2001).

Under natural conditions the nitrogen lost by ecosystems due to denitrification, volatilization, leaching, erosion and windblown aerosols it is compensated by biological fixation and other sources (Smith & Smith 2001).

Artificial sources of $N\text{-}NO_3$ emission are the use of fertilizers, livestock (animal excreta mainly) and municipal, industrial and transport wastewaters (Pacheco & Cabrera 2003). This was one of the reasons why the $N\text{-}NO_3$ was chosen to be modeled in the study region. Mérida-Progreso, Yucatán, as well as virtually all the YP regions, has drainage systems consisting of septic tanks, so that the entire study region translates into an artificial source of N-NO_3 which could cause various alterations in the ecosystems of the coastal zone.

1.2.4.1. Nitrate in groundwater

Nitrate (NO_3^-) forms in the environment from nitrogen (N), which is a nutrient used for plant growth (Gross 2008). The four primary forms of nitrogen include organic nitrogen, ammonia nitrogen (NH_3), nitrite (NO_2^-), and nitrate (Canter *et al.* 1987). Organic nitrogen is converted to nitrate through a process called nitrification (Gross 2008; Canter *et al.* 1987). Nitrification involves an aerobic reaction that is principally carried out by obligate autotrophic organisms, which are organisms that are able to synthesize their own food from simple organic material (Canter *et al.* 1987). Through this process, microorganisms transform organic nitrogen into inorganic ammonium, nitrifying bacteria convert ammonium ions to nitrite, and nitrite is converted to nitrate by another bacterial form (Makuch & Ward n.d.; Canter *et al.* 1987).

Nitrogen enters the landscape via both nonpoint and point sources. Nonpoint sources include contamination areas of large extent (Winter *et al.* 1998). Point sources represent a single point of discharge, such as a small area with a concentration of livestock or a facility burning fossil fuels (Winter *et al.* 1998; Canter *et al.* 1987; Driscoll & Lambert 2003).

Once nitrate reaches the land surface and leaches into groundwater, it is capable of traveling significant distances as long as the lithologic materials are permeable and contain dissolved oxygen (Canter *et al.* 1987). This process becomes hindered when nitrate is not capable of reaching groundwater supplies, which occurs through immobilization and denitrification (Canter *et al.* 1987; Knox & Moody 1991).

Excess concentrations of nitrate in groundwater can generate negative impacts like eutrophication in discharge areas, specifically in surface water bodies and drinking water quality, thus leading to the identification of nitrate as a primary water contaminant (Gross 2008; Killingstad *et al.* 2002).

Eutrophication can alter the physical, chemical, and biological characteristics of entire aquatic ecosystems. The increased algal growth causes decreases in species diversity, often favoring grazing resistant cyanobacteria over small edible algae (Hall & Smol 2001). Decreased light penetration associated with increased primary productivity can result in decreased macrophyte growth, which in turn alters the habitat and food available for other organisms. With increased algal growth, decomposition and respiration increase, thereby depleting oxygen in the hypolimnion and causing declines in fish habitat and changes in internal cycling and biogeochemical processes (Smol 2008). Increased algal productivity can enhance biodegradation of pollutants such as pesticides and petrochemicals, but can also increase biological cycling of contaminants like Polychlorinated Biphenyls (PCBs) (Smith & Schindler 2009). Many of these issues lead to water taste and odor problems and increase water toxicity (Hall & Smol 2006).

The maximum contaminant level (MCL) set by the EPA is 10 $mg \cdot L^{-1}$, (Focazio *et al.* 2006).

Consumption of nitrates can have several detrimental health effects. One adverse health effect is methemoglobinemia. Another adverse effect of nitrate consumption in drinking water is from the increased risks of certain types of cancer like gastric, esophageal, and stomach cancer (Bittner 2000).

In México the maximum concentration of NO_3^- is 10 $mg \cdot L^{-1}$ as $N\text{-}NO_3$, but household or domestic wells used by many property owners are not regulated or monitored.

1.2.5. Groundwater as unique supply source

In many coastal regions, groundwater is the main source of water for humans. However, due to population growth, tidal effects and intensive extraction, many coastal aquifers present seawater intrusion, especially in karst areas where high porosities and permeabilities of geological media facilitate this phenomenon (Vera *et al.* 2012) for example, in the United States of America, México and Australia (Walther *et al.* 2012). Seawater intrusion, resulting in an increase of freshwater-saltwater interface and therefore degradation of the water quality (Khomine *et al.* 2011).

1.2.6. Importance of mangrove ecosystems

Mangroves are the only intertidal wetland ecosystems found along the shores of the limits of estuaries in tropical and subtropical regions. Mangroves act as a transit zone between terrestrial and marine environments, covering between 60% and 70% of the total of coast area in tropical regions, developing in the area where there is not waves, where sediments accumulate and sludge are anoxic, extending inland to the highest tide line where only be flooded periodically (Smith & Smith 2001).

These ecosystems provide several natural features of great ecological and economic importance, are habitats of fishes, crustaceans, mollusks, reptiles, mammals and birds; are sites of accumulation of carbon and nutrients, function as an environment of renewal of marine biomass and protection against coastal erosion (Santos *et al.* 2011). The dominant plants are mangroves, including eight families and twelve genres predominantly Rhizophora, Avicennia, Sonneratia and Briguiera. Growing among them, there are other salinity-tolerant plants, especially shrubs (Smith & Smith 2001).

Despite mangroves are great ecological and economic importance, they are one of the main ecosystems threatened by human activities such as timber harvesting (intensive or illegal), fishing, urbanization (construction of ports, industrial and tourist areas), extension of agricultural areas; also they have been used as disposal sites for waste, garbage, domestic, agricultural and industrial wastewater, accidental spills of toxic agents in combination with reducing freshwater flows (Smith and Smith 2001; Gopal & Chauhan 2006; Nordhaus *et al*. 2009; Santos *et al*. 2011).

At the same time, it has been tried to understand the status of water quality in the mangroves by analysis of chemical and biological parameters (Tripathy *et al*. 2005) and hydrochemical and isotopic characterizations to define types of aquifers and connectivities with coastal areas (Larsen & Cox 2011).

In addition, the growth and primary production of mangroves are strongly influenced by climatic variables such as solar radiation, temperature, precipitation and evapotranspiration (Drexler *et al.* 2001). This type of ecosystems is among the most threatened due to global climate changes, particularly by rising sea level (Gopal & Chauhan 2001), hurricanes (Castañeda-Moya *et al.* 2009) and erosion (Mazda *et al.* 2002), which can cause significant impacts on the continuity of such ecosystems.

With the study of these problems, there has been generating scientific basis for the management of mangrove resources under the direction of integrated management of coastal areas through understanding the behavior of ecosystems under different environmental conditions and usage scenarios (Berger *et al*. 1999) through conservation, recovery and protection methodologies (Chauhan & Gopal 2001; Santos *et al*. 2011), development of cross-disciplinary research involving the participation of academics, government agencies, Non-Governmental Organizations (NGO's) and local communities (Farley *et al*. 2010.), by spatiotemporal studies (Nordhaus *et al.* 2009) and through of developing of multivariable vulnerability models, geographic information systems, considering environmental and socioeconomic criteria (Omo-Irabor *et al.* 2011).

Ecosystems dependent on groundwater in karst environments have been recognized as important ecosystems and are the target of protection and restoration efforts as they are extremely vulnerable to pollution (Gondwe *et al.* 2010).

1.2.7. Climate change

Climate change is one of the challenges currently humanity confronts. Among the direct consequences, probably will rise further global average temperature, causing effects like an increase in evapotranspiration as well as a decreasing in precipitation and consequently in runoff, superficial storages and groundwater recharge (Vaccaro 1992), especially in arid and semi-arid areas due to the their close relationship climate variations (Lloyd 1986; Allison *et al*. 1985; Stephens & Knowlton 1986), thus affecting the water availability for any use.

Evaporation will be affected by climate change, including both that occurs on the ground, as originating in lakes and reservoirs (Morales *et al.* 2008). Changes in precipitation will benoticeable in their average annual value, but also in their patterns of temporal occurrence, registering variations in torrential runoff or avenues, as well as the frequency and intensity of droughts (Martínez 2007).

Climate change is an ongoing process and that it begins to have a significant impact in México on the availability of water resources by altering phenomena as precipitation (Sánchez 2008), temperature (Montero & Pérez 2008), evaporation and evapotranspiration (Martínez *et al.* 1998). Already have been generated reports on possible scenarios, based on global models of the atmosphere where have analyzed the effects of climate change on water demand (Martínez & Mundo 1995) and the possible effects on agriculture (Ojeda *et al*. 2008; Mundo 2008).

1.2.8. Groundwater modeling

The correct use of groundwater requires a precise knowledge of flow and water table levels to various natural external actions and as a result of human activities. At the same time, an aquifer is an element, consisting of physical, geometrical components and external actions, laws and own operating characteristics within a more complex water resources system (Custodio & Llamas 1976).

Mathematically, aquifers can be represented by a set of parameters and variables through a model, developed based on a conceptual representation that join several characteristics which constitute a likeness of a field situation (Anderson & Woessner 1992) and it is more representative if it has the ability to reproduce faithfully the behavior or states of reality, considering actions on it and the laws that govern it (Custodio & Llamas 1976).

A mathematical model of an aquifer, simulates the groundwater flow through a governing equation which represents the physical process that occurs in the system, obtaining a solution by analytical or numerical procedure. Most efforts on groundwater modeling are aimed at predicting future conditions from a proposed action, and consequently in the generation of regulatory policy frameworks of groundwater use. They are also used as an interpretation tool, organizational field data systems and analysis of hypothetical hydrological systems (Anderson & Woessner 1992).

Karstic aquifers are extremely heterogeneous with a permeability distribution that includes many orders of magnitude, often containing, flow paths conduits with hydraulic characteristics more like surface streams, having a component of turbulent flow, which represents a problem in most numerical models based on Darcy's law, which assumes laminar flow (Scanlon *et al.* 2003), it has caused the groundwater modeling in karst media not so completely successful (White 2002).

In practice, the problem of karstic aquifers modeling is the translation of the conceptual model from the physical schema to the set of differential equations that describes the processes of groundwater flow and transport together with the boundary conditions imposed by the geological environment (White 2003).

The study of the spread of pollutants in karstic and fractured aquifers exhibits uncertainties caused by the conditions of anisotropy of the geological media and the presence of cavities and waste products that could result in a more diluted flow and transport unexpected solutes. Therefore, in fractured and fissured aquifers, it is necessary to represent the conditions of flow and transport of contaminants, considering the high heterogeneity, to determine the preferential flows and to propose remediation strategies actions (Cherubini 2008).

Kovács (2003) mentions that two types of basic approaches can be distinguished in the study of karst and fractured aquifers: The discrete approach and continuous approach. The first one, considers the groundwater flow within fractures like individual conduits while the second one threats heterogeneities in terms of effective modeling parameters and their spatial distribution.

To model karstic aquifers, it is necessary to know the purpose of study. That is, it should be formulated the conceptual model of the problem before to construct or implement the model (White 2003).

Normally, the biggest problem encountered in karstic aquifers modeling, resulting from the handling of information at different scales, for example, measuring a hydraulic parameter taken at a specific location, but taken it at different scales could have different hydraulic behavior.

According to Dagan (1986), three different scales should be considered in groundwater modeling: (1) the domain length scale of flow and transport (L); (2) the length scale of the flow dominant heterogeneities (I) and; (3) the length scale of monitoring of the method used (D). Handling large scale field can generate parameters that appear to be almost homogeneous, whereas for small scales measurements in the same aquifer may seem highly heterogeneous; therefore, only the combination of methodologies in different scales can provide a comprehensive overview of relevant processes of groundwater flow in the aquifer (Teutsch & Sauter 1991).

Using a hierarchical scale approach, Teutsch & Sauter (1991) presented a classification of groundwater problems in karst media, according to approaches that can be applied for modeling the hydrodynamic conditions in karstic media: Discrete Fracture Network (DFN), Discrete Channel Networks (DCN), Equivalent Porous Media (EPM), Double Continuity (DC) and Combined Discrete-Continuous (CDC).

In the DFN approach, only some fracture systems are considered as permeable. The matrix is assumed with depreciable permeability. This simplification summarizes the system in a bi-dimensional network of fractures, the movement is expressed in terms of the "cube law". The DCN approach simulate flow modeling in a one-dimensional pipe network that representing the intersections of fractures and conduits in karstic media. The geometry of the pipe network can be generated statistically, or may be represented by actual field situation, this method is analyzed by the "Hagen-Poiseuille’s law" (laminar flow in unidimensional ducts). "The DC approach represents the combination of pipe network and fissured media (without detailed knowledge of geometry) by continuous equations. The exchange of water and solutes in continuous networks is calculated on the basis between the differences in hydraulic head, in terms of linear exchange (Cherubini 2008).

About multiporosity models, Barenblatt *et al.* (1960) introduced the concept of dual porosity model, which consists of a matrix of high porosity and low permeability fractures and low porosity but with high permeability. Fluid flow takes place through the two systems separately, and then can exchange fluids between its interface systems.

A variety of implementations of numerical models in karstic media have been implemented over time by several researchers in the study of the influence of coal mining in karst springs (Wu *et al.* 2011), predicting flood flows (Liu 2005), studies of groundwater flow behavior (González-Herrera *et al.* 2002) and contaminant transport (Trček 2008), integration of models of linear/non-linear flow (Cheng & Chen 2005) and flow models of geothermal water (Li *et al.* 2007).

In México, the National Water Commission (Conagua in Spanish), is the administrative, regulatory, technical and advisory institution which is responsible for the management and preservation of national waters (based on law) and property inherent to achieve its sustainable use in co-responsibility with the three levels of government and society in general (Conagua 2011).

Water resources in México, are constituted by ocean masses, surface waters (streams, rivers, lakes, lagoons) and underground storage. The distribution of water resources and human activities, doesn't have a direct relationship with each other, as has occurred that areas of less water availability are those that have a concentrated population and economic growth, with a strong productive and social infrastructure (Conagua 2006).

Every year, the average rainfall in the country is about 1489 km^3; of which an estimated about 73.1% (1088.46 km^3) evapotranspires, 22.1% (329.07 km^3) is part of the surface runoff and 4.8% groundwater recharge (71.47 km^3). Taking into account exports and imports of water with neighboring countries, plus incidental recharge, the country has about 460 km^3 annual renewable freshwater (Conagua 2011). As mentioned above the importance of groundwater, it is evidenced by the volume used.

The country is divided administratively into 653 aquifers, 100 which are currently subject to intensive extraction, 16 present seawater intrusion and other 32 are exposed to soil salinization and brackish groundwater phenomena. The volume of water for consumptive use is 30.11 km^3 per year, representing approximately 42% of annual average recharge (Conagua 2011).

The intensive extraction of groundwater has increased since the 1970s, given that in 1975 the total of aquifers in intensive exploitation regime amounted to 32, a figure that has reached 100 today. Of these 100 aquifers nearly 54% of underground water for all uses (Conagua 2011) is removed. It is noteworthy that the term "exploitation" is just a term of administrative nature, indicating that a given aquifer, the amount of water extracted is higher than the estimated recharge calculated by NOM-011-CNA-2000, so it is considered more appropriate to use the term: intensive use or intensive extraction.

In México, more than 75% of the water resource for urban use is groundwater, although in some regions is 100%. Similarly, 75% of the water used in industrial processes comes from the same origin as well as more than 30% of the water used for irrigation (Conagua 2006). These statistics indicate the vital dependence of the country with respect to groundwater.

1.2.9. Groundwater management

Integrated Management of Water Resources seeks sustainable water management through the conjunct use management proposal, with which can determine the distribution in space and time that is convenient to use of different supply sources, to satisfy the current demands (consumptive and non-consumptive) under conditions of maximum guarantee and other hydrological and climate patterns, trying to achieve a comprehensive water management by defining and quantifying the available supply sources and demands, guaranteeing the water supply depending on the capacity regulation of the system(s), with economic, administrative and environmental restrictions (MCI, IGME & DA 2010).

Mérida-Progreso region is within the administrative limits of the aquifer 3105 called “Península de Yucatán”, Yucatán State (Figure 4). The Watershed Council in this region is 25 “Península de Yucatán”, which corresponds to the Administrative Region XII of the same name.

With respect to the administrative groundwater balance there is an annual amount of affordable water of 5 759 221.03 $m^3 \cdot year^{-1}$ and the authorized volume is 1 511 978.97 $m^3 \cdot year^{-1}$ (Conagua 2009). This means that supply exceeds the demand almost four times. In fact, there are no studies that show the seasonal variability of affordable groundwater quantities and the demands of human needs and ecosystems involved.

The “Junta de Agua Potable y Alcantarillado de Yucatán” (JAPAY) is the agency responsible of the water resources management in the Mérida-Progreso region. The supply sources are four well fields located at the periphery of the Mérida city (named Mérida I, Mérida II, Mérida III and Mérida IV) which provide about two-thirds of the average total daily demand of about 242 000 $m^3 \cdot day^{-1}$, while the intraurban wells provide the remaining third (Figure 5). In the last years, the intraurban wells has been eliminated gradually by the JAPAY (Graniel *et al.* 1999). According to BGS, FIUADY and Conagua (1995) from Mérida I, are extracted 42.3 million $m^3 \cdot year^{-1}$, which representing 47.8% of total extraction.

In México exist the Groundwater Technical Committees (COTAS in Spanish) which are associations for groundwater management formed by users from different areas of the society (industrial, agricultural, urban) in a region to participate in making-decision related to groundwater management.

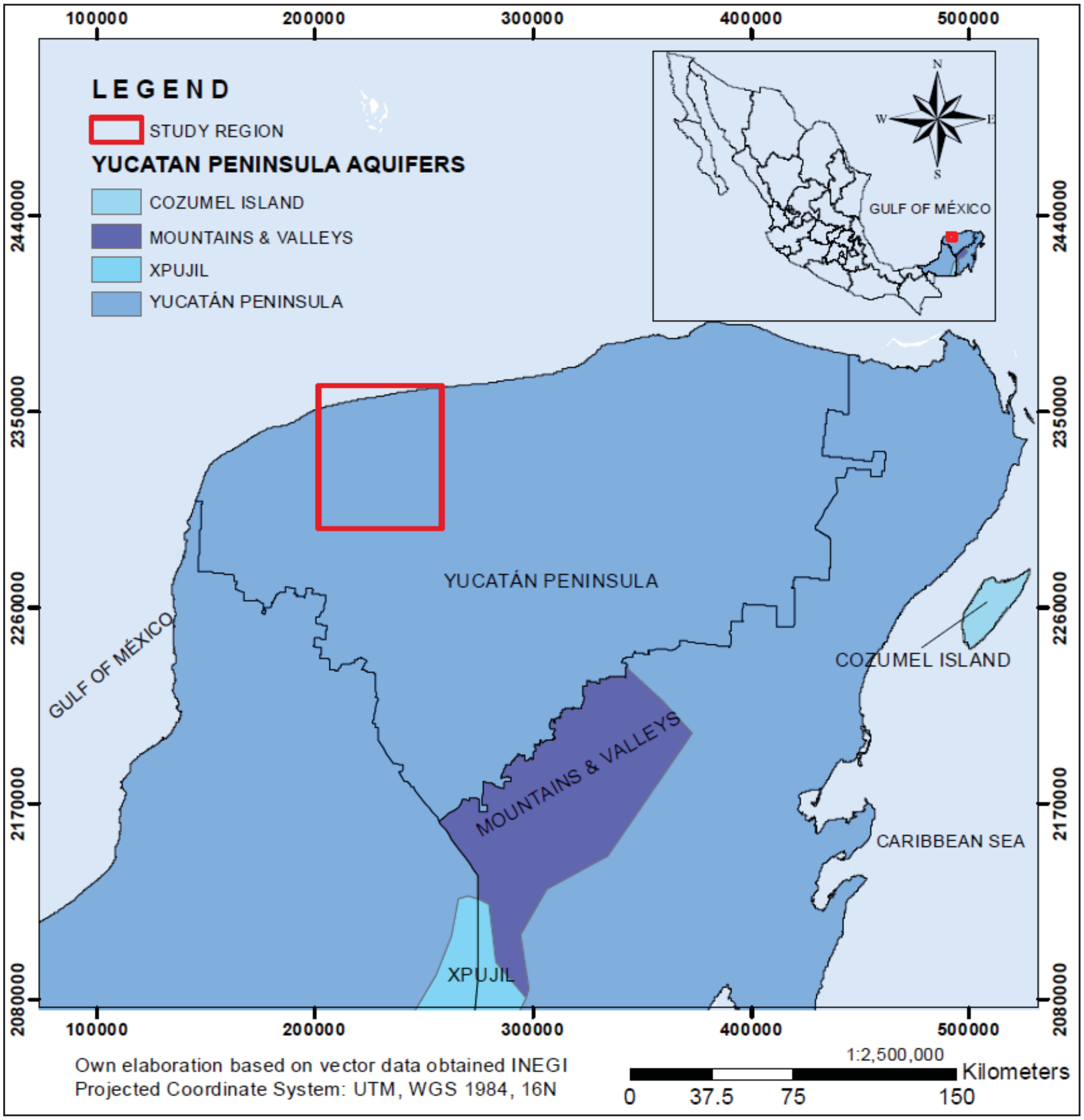


Figure 4. Yucatán Peninsula Aquifers.

On June 26th, 2012 the proposal for the establishment of the Technical Groundwater Committee Association for the Metropolitan area of Mérida (COTASMEY in Spanish) was presented (SEDUMA 2012). The installation of this agency was on January 18th, 2013, so in practical terms, this is very recent (SEDUMA 2013).

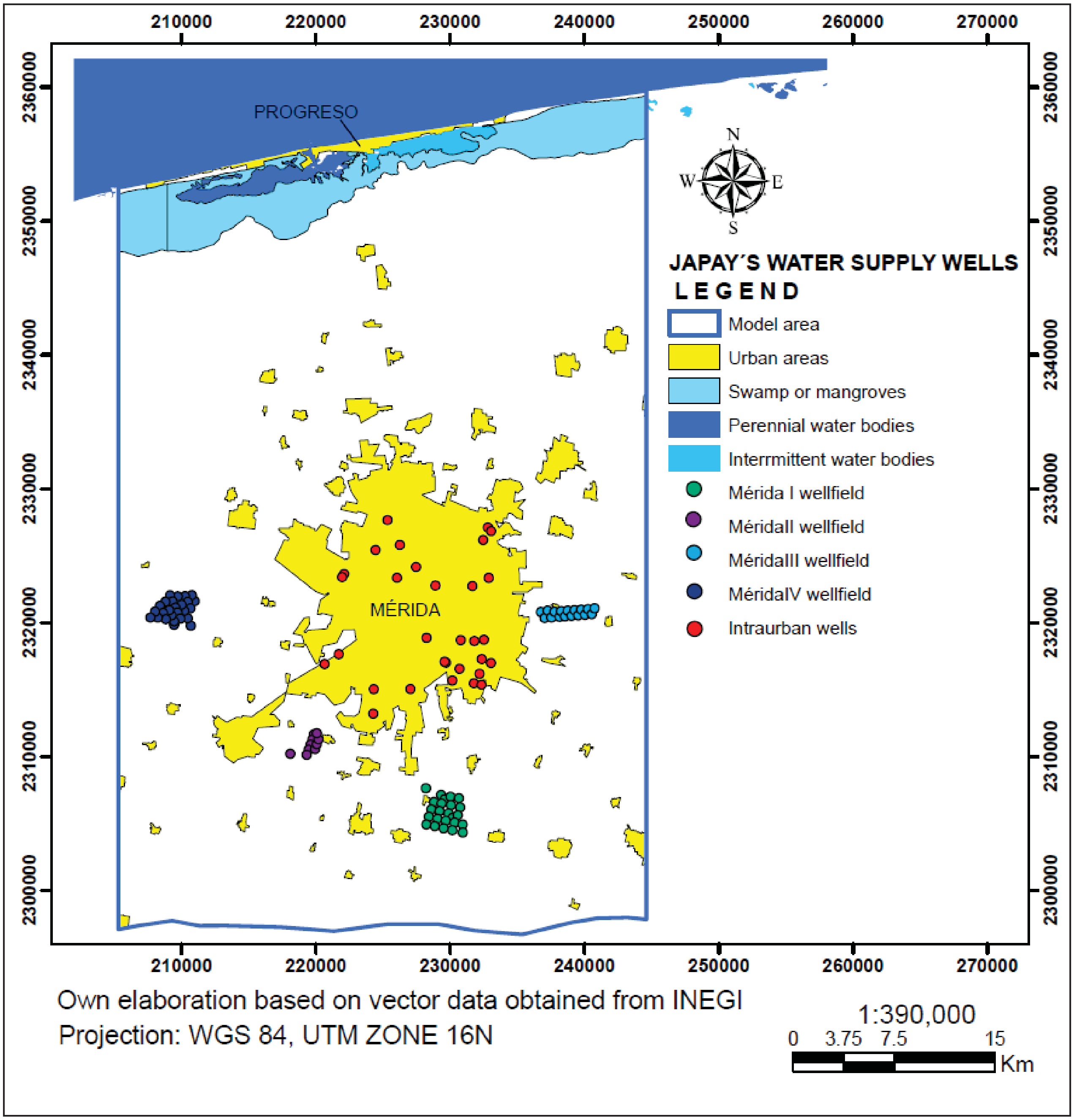


Figure 5. JAPAY's water supply wells.

According to SEDUMA (2013), the aim of COSTAMEY is to improve and develop new mechanisms of municipality coordination, in conjunction with other levels of government for water management in the metropolitan area of Mérida, encouraging the participation of different sectors of society.

The shallow depth of the groundwater level, the absence of soil and extensive karstic conditions of the unconfined aquifer in the region Mérida-Progreso, Yucatán (and generally most of the YP), produces that the groundwater resources are particularly vulnerable to contamination. Mérida lacks of a wastewater drainage system, which causes wastewater to be disposed in septic tanks, injection wells and cesspools to a depth of 4 m to 7 m, and in very few cases it is disposed through deep wells (60-80 m). The volume of wastewater produced by the city inhabitants has augmented the last 10 years with the urbanization increase (people from rural areas moving to urban regions) and the rise of tourism development (Graniel *et al.* 1999; Bauer-Gottwein *et al.* 2011).

This underground injection of wastewater and solid waste disposal has polluted the upper 20 m of the karstic aquifer below Mérida (Bauer-Gottwein *et al.* 2011). However, although several studies have included groundwater chemistry, comparison in time and space of the quality of the process has not defined any contaminant that might have affected the water quality of the aquifer along the horizontal and vertical planes (Graniel *et al.* 1999), and the implications in terms of quality and quantity that could be in the coastal zone due to natural discharge of groundwater and interaction with seawater.

1.3. Justification

Based on the panorama above, it shows the great importance of groundwater for human consumption and development of human activities, more specifically, in the study region where 100% of the population depends on groundwater.

In addition, Mérida-Progreso region, and in general all the urban areas in the YP do not have a municipal sewage system, so wastewater is deposited through several forms to underground. The shallow depth of the groundwater level, the almost total absence of soils and the wide area of the unconfined karstic aquifer in the region, has caused groundwater resources in Yucatán are particularly vulnerable to pollution, being in constant interaction with the seawater of the coastal zone, which it is representing the possibility of damages to the coastal ecosystems areas as the mangrove zones (Figure 6). In addition, there are agricultural, industrial and livestock (swine production, which is very important in the region) wastewaters discharges, of which unfortunately there is no information on a census that mentions an estimate of the magnitude of these sources.

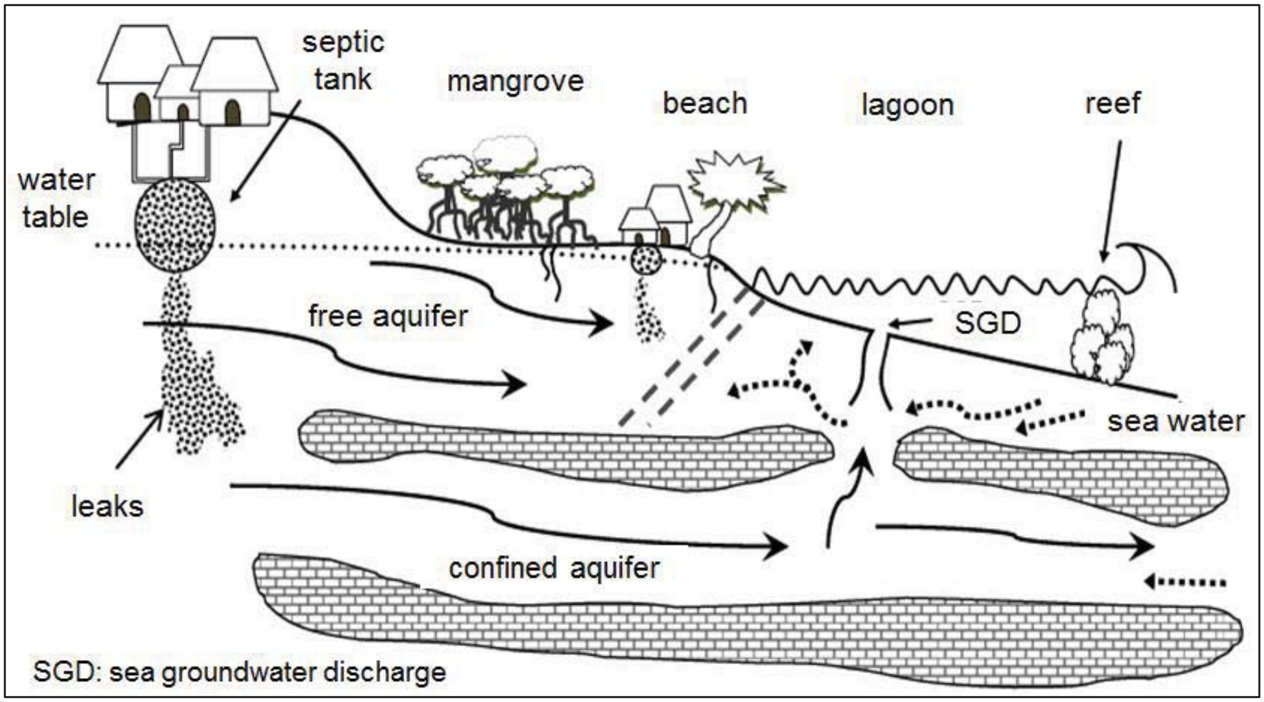


Figure 6. Groundwater pollution problem in the study region (Hernández-Terrones *et al*. 2011).

This is the key point of motivation of this research. In recent years the study of groundwater dependent terrestrial ecosystems has received increased attention due to the recognition that water should be available to the ecosystems and population. The study region has important features with respect to groundwater diffuse contamination from septic tanks and the sewage system and the interaction with the ocean. These interactions must be analyzed and understood through the definition of the spatiotemporal variables that influence the groundwater balance and groundwater flow in terms of quality and quantity. The implementation of a numerical model for the simulation of such a system can be used as a technical-scientific tool of management to generate appropriate management strategies that allow for the use of groundwater and discharge of wastewater with a sustainability perspective.

1.4. Research objectives

1.4.1. General objective

The general objective of this research was to analyze and understanding the hydrogeological behavior in the coastal karstic aquifer and groundwater use in the Mérida-Progreso region, Yucatán, and its implications in the coastal area ecosystems requirements in terms of water quantity and quality.

To achieve the main objective of the thesis, the following seven specific objectives were established:

a) Generate a geodatabase with geological, hydrological, hydrogeological and hydrogeochemical information
b) Analyze the actual water use and management in the study region
c) Develop a conceptual model of groundwater hydrodynamic functioning of the aquifer.
    - Fresh/Brackish water interfaces in the Mérida-Progreso region, Yucatán.
    - Water balance in the model area
d) Implement a numerical model of flow and transport of solutes of the aquifer
e) Assess the implications, in terms of quality and quantity of water, between groundwater and mangrove zone
f) Generate strategies for groundwater usage and sewage disposal with a sustainability perspective

1.5. Hypothesis

The contributions of $N\text{-}NO_3$ derived from the human being under urban areas in the Mérida-Progreso region move and go to coastal ecosystems through groundwater can cause negative implications in terms of environmental quality.

2. Methodology

In this study this proposal discloses a methodology for characterizing groundwater level fluctuations produced by natural and induced recharges and the groundwater quality alterations in the study region. It also includes the characterization of the freshwater/saltwater interface phenomena, the water balance with what was proposed the conceptual hydrogeological model which was implemented in a numerical model of flow and transport of solutes.

For the research project various methods were applied in situ and ex situ to obtain information about the aquifer characteristics, its hydrodynamic conditions and water quality. A groundwater monitoring network has been established within the framework of the primary research project, which includes 29 observation wells (10 - 60 m deep). Most of the deep wells were drilled within the project and some are previously perforated wells of CONAGUA. The observation wells were drilled with a diameter of 10 inches and the upper 6 m consist of a PVC tube of 8 inch diameter that is enclosed with cement to avoid water infiltration from the surface.

Worldwide groundwater converges towards the coastal areas, therefore the sea level (masl) is the benchmark analyzing the water movement along hydraulic gradients towards the coast. Within the project period all the observation wells that form part of the piezometric monitoring network were geopositioned and leveled with a Receptor GPS Trimple 5 700 using a geodetic reference point of the National Institute of Statistics, Geography and Informatics (INEGI) using up to eleven satellites to obtain the exact location of the measuring points.

For the climatological assessment, reliable data were obtained from meteorological stations of CONAGUA for the study region.

The measurement campaigns for this thesis include hydrodynamic, hydrochemical and physicochemical investigations and started with a preliminary phase in April 2012 and includes part of the information generated until December 2013. The procedure of the measurements was of different temporal dynamics according to the specific methods of obtaining the required data and is described in the following section.

In order to accomplish the general objective, was developed a methodology to achieve each of the specific objectives and consequently to reach the general objective. This methodology is detailed below.

Specific objective: Analyze the actual water use and management in the study region.
Water management programs for the study region were collected and analyzed. The information analyzed consisted of government documents, operating and water management regulations and research in technical and social aspects.

Specific objective: Develop a conceptual model of groundwater hydrodynamic functioning of the aquifer.

- Fresh/Brackish water interfaces in the Mérida-Progreso region, Yucatán.

Field data were obtained from a monitoring network of 26 observation wells (of the 29 ones mentioned above) (Figure 7) in which they were installed 20 automated meters for recording levels, and 19 automated meters for recording EC. The location of the EC meters was defined based on the depth at the beginning of the brackish water interface; in order to identify different types of responses, some were placed in the freshwater interface, others one in the brackish water zone and others one in the boundary between these two interfaces. All measuring instruments recorded four registers per day from June 17th, 2012 to November 23rd, 2013 at the following times: 00:00, 06:00 12:00 and 18:00 hours. Four measuring campaigns of EC profiles were done in the months of August and November, 2012, and January and March, 2013 in all observation wells. These profiles were measured slowly (1 m/2 minutes) to each meter of the water column of each observation well. In each measurement the sensor was left two minutes before recording to allow to stabilize the reading. Before each measurement and after the change of batteries of the device for the characterization of profiles, was performed the calibration of measuring sensors with EC standard solutions of 1 413 $\mu S \cdot cm^{-1}$ and 5 000 $\mu S \cdot cm^{-1}$. To obtain atmospheric pressure that would make corrections to define the variations of the water level in the observation wells, two automatic meters of atmospheric pressure (with which the study region was covered) were installed. Daily rainfall and daily mean temperature information of the 5 monitoring weather stations: “Progreso Obervatorio”, “Chicxulub Puerto”, “Mocochá” and “Mérida Observatorio” were obtained from the National Water Commission (Conagua). In addition, information from the monitoring weather station FIUADY (located in the Engineering Faculty of the Autonomous University of Yucatán) was obtained. All observation wells are located more than 1 km away from deep pumping wells in which more than 10 lps of groundwater are extracted, so for practical purposes it is considered that are not affected by extraction. A comparison of the saline water interface elevation obtained by direct measurement of electrical conductivity (EC) profiles and calculated with the Ghyben-Herberg (GH) principle using the equations 1 and 2 was performed. Through a groundwater sampling and laboratory analysis (gravimetric method), were obtained the densities of water by mass difference with glass pycnometers of 50 ml and analytical scale at ambient temperature in freshwater, brackish water and saline water interfaces.

$$z = \frac{\rho_w}{\rho_s - \rho_w} h \quad \text{(used with density values measured in laboratory)} \qquad (1)$$

$$z = 40\ h \quad \text{(assuming } \rho_w = 1gr \cdot (cm^3)^{-1} \text{ y } \rho_s = 1.025\ gr \cdot (cm^3)^{-1}) \qquad (2)$$

where ρ_w represents the density of the freshwater, $\rho_s$represents the saline water density, z the depth of the saline water interface under sea level and h the hydraulic head of the freshwater above sea level.

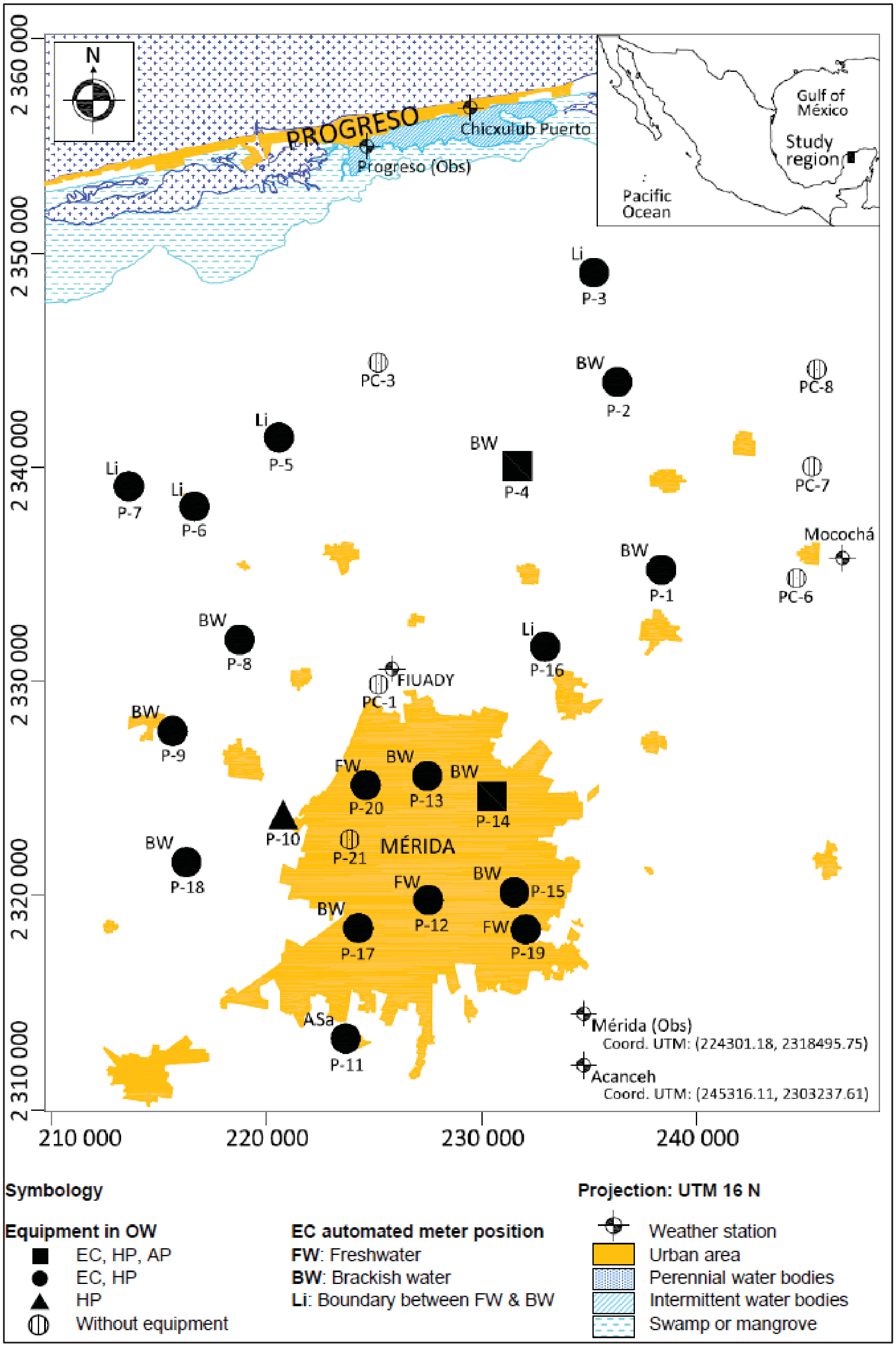


Figure 7. Observation wells and weather stations location used for the study of interfaces freshwater and brackish water.

Specific objective: Develop a conceptual model of groundwater hydrodynamic functioning of the aquifer.

- Water balance in the model area.

A spatiotemporal analysis of the variables that govern the hydrodynamic behavior of the study region was realized. The variables that were subject to analysis for obtaining historical hydrogeological balances are: climatic variables (precipitation, runoff, evapotranspiration, infiltration and temperature), water quality variables (groundwater quality specifically in terms of $N\text{-}NO_3$), hydrogeological variables (groundwater flow) and anthropogenic variables (groundwater extractions, agricultural returns for irrigation and wastewater returns; the techniques used for each variable are explained later).
Develop different temporal conceptual models of hydrodynamics and water quality of the aquifer in the study region.

Specific objective: Implement a numerical model of flow and transport of solutes of the aquifer
With the variables analyzed in the water balance and the geological and hydrogeological components of the study region, was generated a database platform which was used in the implementation of the numerical model of flow and solute transport in 3 dimensions in the software FEFLOW that solves the system of equations by Finite Element Method and it was proposed as a Porous Medium Equivalent approach. The numerical model was calibrated and validated and subjected to a sensitivity analysis and then, three future scenarios were performed consisted of: 1) current conditions (2013), 2) increase of pumping extraction due to population growth and 3) infiltration decreasing by a reduction in precipitation of 50% in combination with scenario 2.

Specific objective: Assess the implications, in terms of quality and quantity of water, between groundwater and mangrove zone
Based on the results of the three scenarios, were analyzed the implications in terms of quantity and quality of water that arrives to the ecosystems of the coastal zone of the study region.

Specific objective: Generate strategies for groundwater usage and sewage disposal with a sustainability perspective

Based on the conclusions analyzed about the implications in terms of quantity and quality of water that arrives to the ecosystems of the coastal zone, were integrated the management proposals of groundwater usage and wastewater disposal of the study region, that can be used in a joint-use project, to meet the present demands, consumptive and non-consumptive, in maximum security conditions (in environmental, social and economic terms), trying to achieve and integral water management.

Specific objective: Generate a geodatabase with geological, hydrological, hydrogeological and hydrogeochemical information.

With all the information analyzed and treated during this study, it was formed a georeferenced database (with current available information and subject to be constantly updated) that condenses all the information of this thesis of the study region which can function as part of a management tool together with the groundwater numerical model implemented.

3. Study region

In this chapter the physical, geological, hydrogeological and the historical behavior of meteorological phenomena of the study region are shown. Based on the structure of this chapter the model groundwater model of flow and solute transport was implemented as is explained in Chapter 4.

3.1. Geographic settings

3.1.1. Location

Mérida-Progreso region is located in the east of México, specifically in the northwestern of the Yucatán state. The main municipalities and urban areas in the study region are Mérida and Progreso. Mérida is located between parallels 20°41' and 21°12' north latitude and between meridians 89°27' and 88°49' west longitude with altitudes between 7 and 10 meters above sea level (masl), and has a population of 830 732 inhabitants (INEGI 2009a). The municipality of Progreso is located between parallels 21°07' and 21°20' north latitude, and between meridians 89°29' and 89°52' west longitude with altitudes between 0 and 10 masl, and has a population of 53 958 inhabitants (INEGI 2009b).

3.1.2. Study region and model area

In order to realize the geological, hydrological and hydrogeological analysis and to propose the appropriate border conditions in the model implementation, two areas for the realization of annual water balances were defined. These areas were designated as (i) study region with 3 434.97 km^2 and (ii) model area with 2 319.49 km^2 (Figure 8). In addition it was estimated a water balance for the southern region adjacent to the study region in order to obtain an approach about the volume of water which is entering as groundwater flow. Water balances were calculated annually for the period 1995-2013.

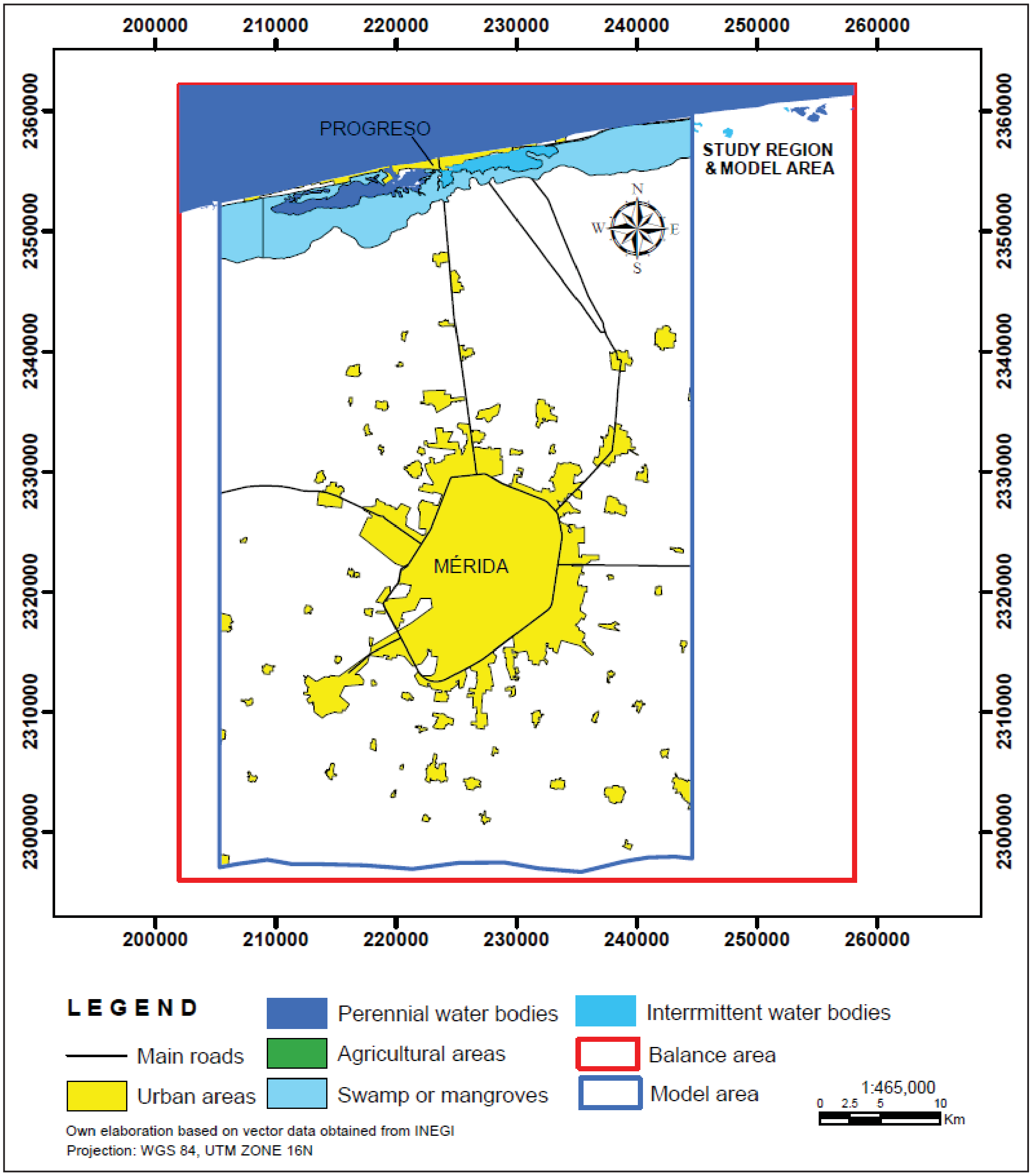


Figure 8. Study region and model area.

3.1.3. Climate

According to INEGI (2009a, 2009b), the weather in Mérida city is warm humid with summer rains, average annual rainfall between 500 mm and 1100 mm, and an average annual temperature range between 24 °C and 28 °C is presented. In Progreso city, the climate is warm dry and warm semi-dry, average annual rainfall of 700 mm and average annual temperature of 25 °C is presented (Figure 9).

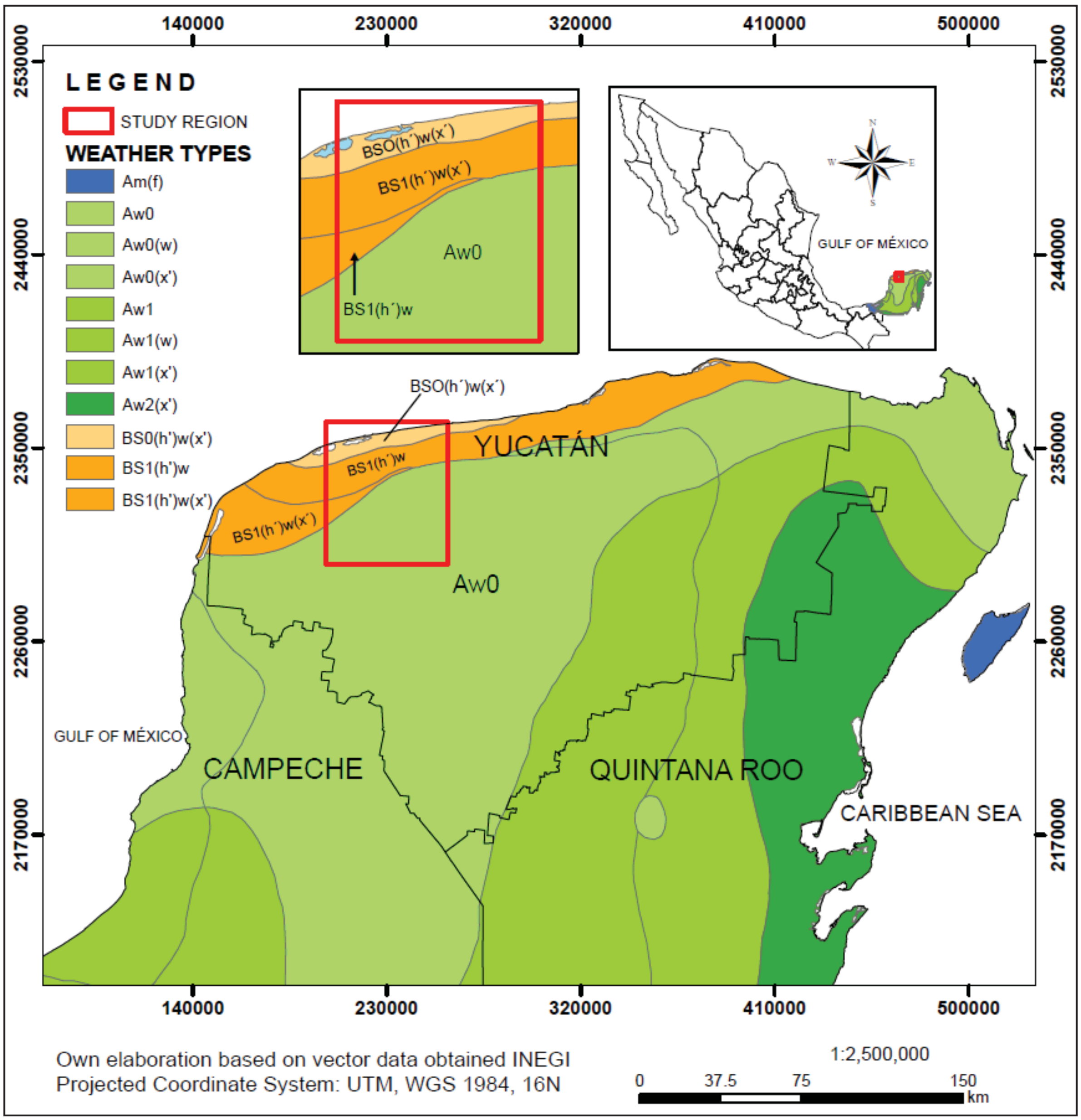


Figure 9. Climate context of the study region.

3.1.4. Hydrology

The only permanent rivers that reach the Mexican part of the YP are the Champeton River and the Candelaria River in the southwestern part of Campeche that open to the Gulf of México and the Hondo River in the state of Quintana Roo (Kauffer-Michel & Villanueva-Aguilar 2011) belonging to the border between México and Belice. In Yucatán state no permanent surface streams are present and most of the intermittent rivers coming from the southern part of the YP disappear in the subsoil forming the karst aquifer.

In the northern coastal part of the study area shallow intermittent to perennial water bodies, mostly originated due to extreme flooding during hurricane events can be found. Due to road construction the natural water between lagoons and wetlands has been modified and interrupted. The coastal lagoons are recharged by groundwater from artesian springs and their water is extremely saline (Heise 2013).

The calculations concerning to the hydrological study are explained to obtain the water balance of the study region.

Precipitation and Temperature

For precipitation and temperature analysis, the Thiessen polygons method was used, considering the information of weather stations located in the study region (Figure 10) and southern region (Figure 11). Monthly precipitation, monthly average temperature and monthly average evaporation data were obtained directly from “Organismo de Cuenca Península de Yucatán” of Conagua in 2014. Weather stations named Mérida (Obs) and Progreso (Obs) contained more information such as atmospheric pressure, relative humidity, wind speed, solar radiation and daylight hours, information were also obtained from FIUADY weather station belonging to the Engineering Faculty of the Autonomous University of Yucatán; these data were used to calculate potential and actual evapotranspiration. The precipitation and temperature of the study region and the southern region (Table 1, see calculations in Appendix 1) was calculated in terms of $mm \cdot year^{-1}$ to use the information in subsequent calculations.

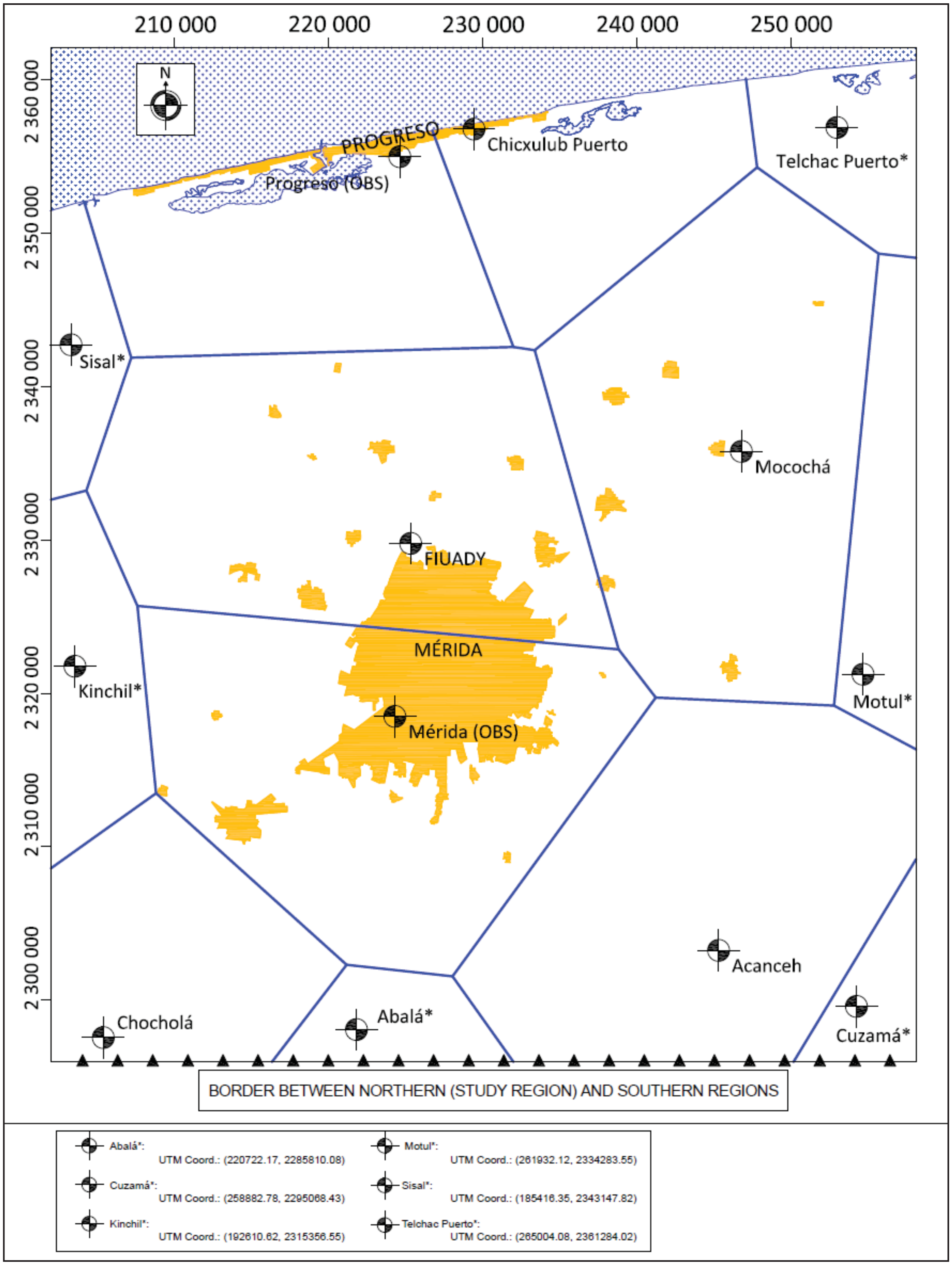


Figure 10. Thiessen polygons and weather stations located in the study region.

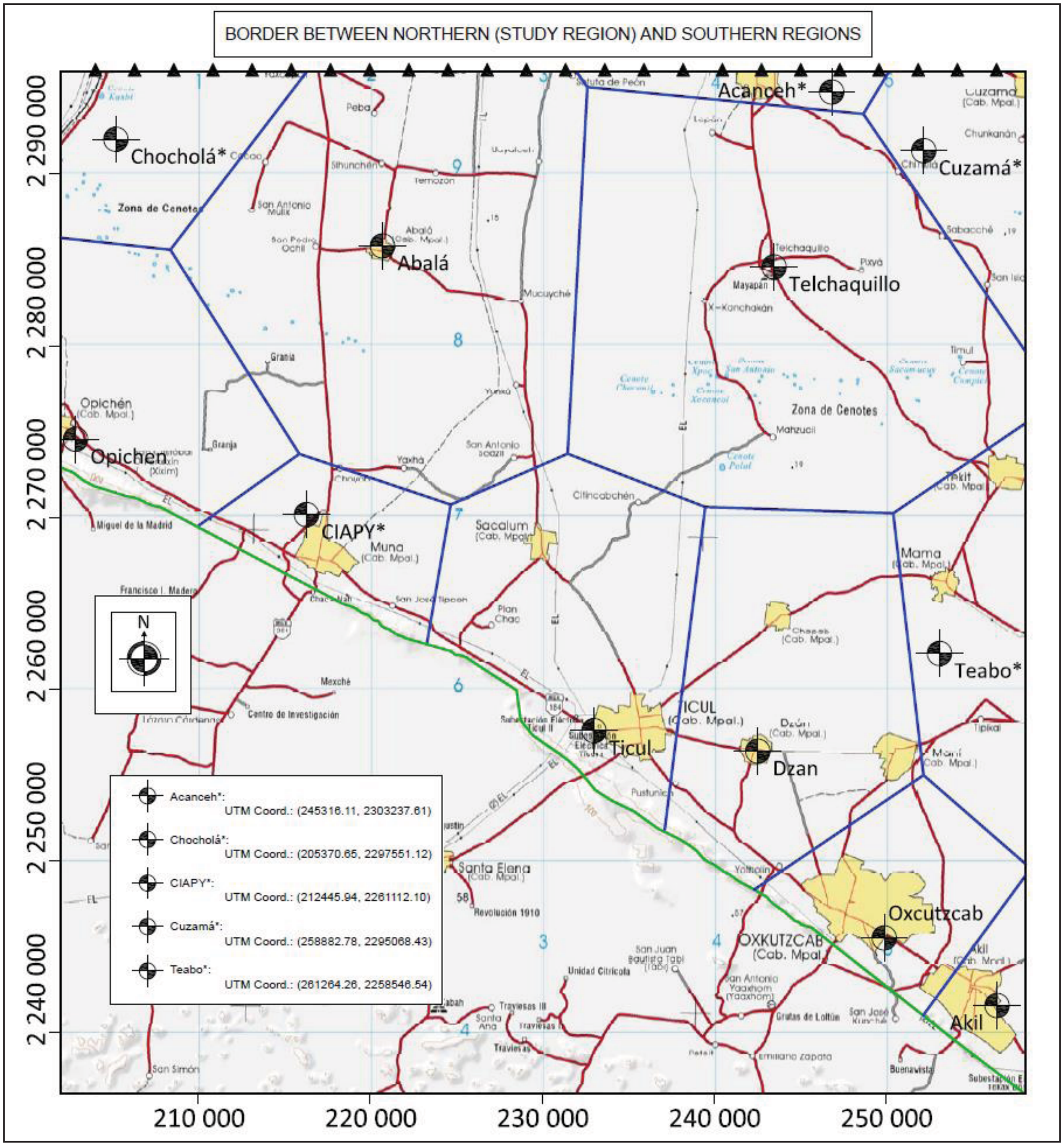


Figure 11. Thiessen polygons and weather stations in the southern region.

AÑO	Study region		Southern region	
	Annual Precipitation	Average Annual Temperature	Annual Precipitation	Average Annual Temperature
	(mm·year^{-1})	°C	(mm·year^{-1})	°C
1995	942.97	28.02	1290.56	27.78
1996	859.49	27.23	969.33	28.71
1997	944.80	27.41	1087.42	28.17
1998	980.93	27.50	961.56	28.25
1999	1237.04	26.88	1182.41	27.92
2000	868.73	26.60	1033.71	27.42
2001	842.47	26.17	997.28	26.63
2002	1237.30	26.48	1508.17	26.39
2003	911.26	26.58	1095.81	26.36
2004	982.71	26.41	984.78	25.41
2005	1002.46	26.58	1161.00	26.31
2006	988.79	26.86	1073.01	26.89
2007	1155.32	27.03	1282.82	26.67
2008	919.04	26.89	1124.32	26.35
2009	812.06	27.37	1044.28	26.58
2010	1085.33	25.94	1040.55	25.46
2011	917.91	26.89	1042.77	26.20
2012	853.37	26.64	984.82	25.69
2013	1209.61	27.05	1424.98	26.22

Table 1. Annual precipitation and average annual temperature in study and southern regions (see calculations in Appendix 1).

Evapotranspiration (potential and actual)

For calculating evapotranspiration (Figure 12) were used three potential evapotranspiration methods: Penman-Monteith, Hargreaves and Thorntwaite; and two actual evapotranspiration methods: Coutagne and Turc which they were used in the water balance.

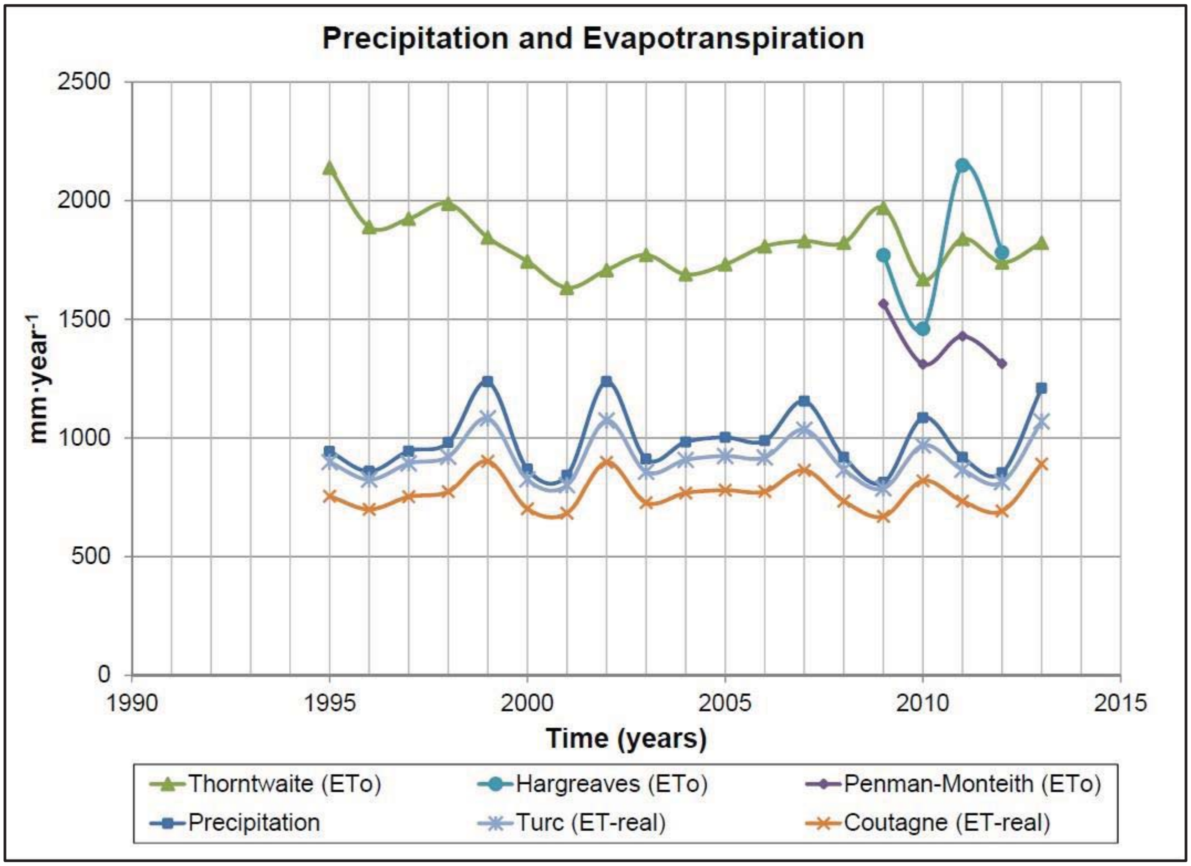
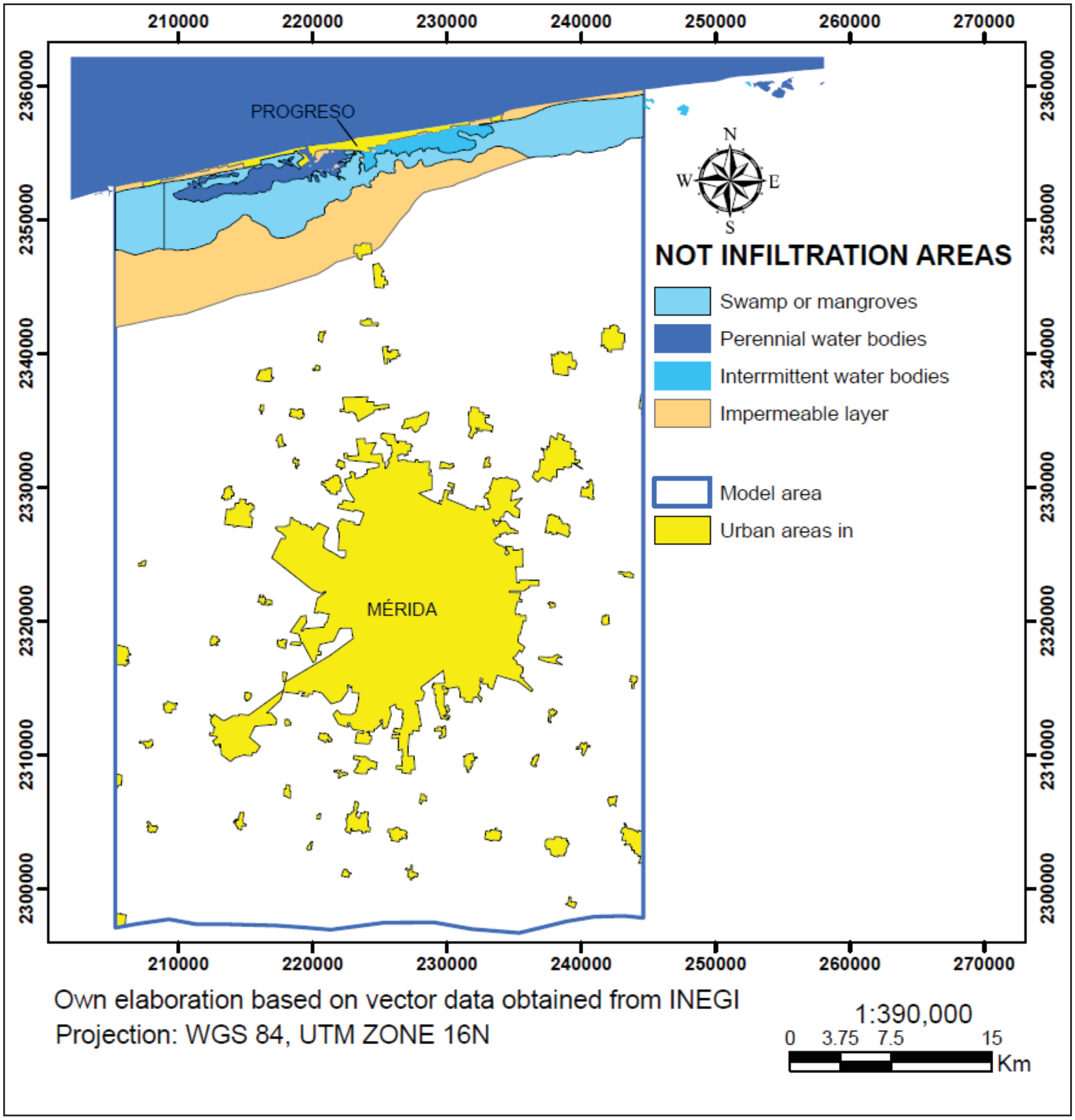


Figure 12. Evapotranspiration methods comparison.

Runoff

Due to karst features of the study region and the non-presence of surface runoff, this variable was considered as 0 (zero). In the northern area of the study region, there are depressions that collect water from rainfall in the rainy season, plus as mentioned above, that area constitutes an impermeable region of about 20.16 km^2 that does not allow infiltration (Figure 13). For these reasons, it is considered that water, which precipitates in the region, returns to the atmosphere by evaporation.



Note: Water volumes which precipitate on the surface water bodies and impermeable area

Figure 13. Surface water bodies and impermeable area.

Infiltration

For calculating annual infiltration in the model area was used the water balance equation (3):

$$P - (R_{out} - R_{in}) - (G_{out} - G_{in}) - (ETr_s + ETr_g) = \Delta (S_s + S_g) \qquad (3)$$

Where

P = Precipitation

R_{out} = Runoff outflow

R_{in} =Runoff inflow

G_{in} = Groundwater inflow

G_{out} = Groundwater outflow

ETr_s = Surface evapotranspiration

ETr_g = Groundater evapotranspiration

S_s = Change in surface storage

S_g = Change in groundwater storage

Runoff corresponds to the water that precipitates over water bodies and impermeable area.

3.1.5. Vegetation

Along the shoreline a lot of marshlands and lagoons can be found with aquatic vegetation (INEGI 2012). The vegetation of the wetlands along the northern Yucatán coastline is characterized by various species of mangrove with evergreen leaves (CONABIO 2012). The adjacent regions in the central northern part of the study area are dominated by tropical and subtropical deciduous forest and agricultural terrain while in the central and southern part and the east coast evergreen tropical and subtropical forest is prevalent (Figure 14). According to INEGI (2012) almost 25 % of the Yucatán state surface is used for agricultural practices.

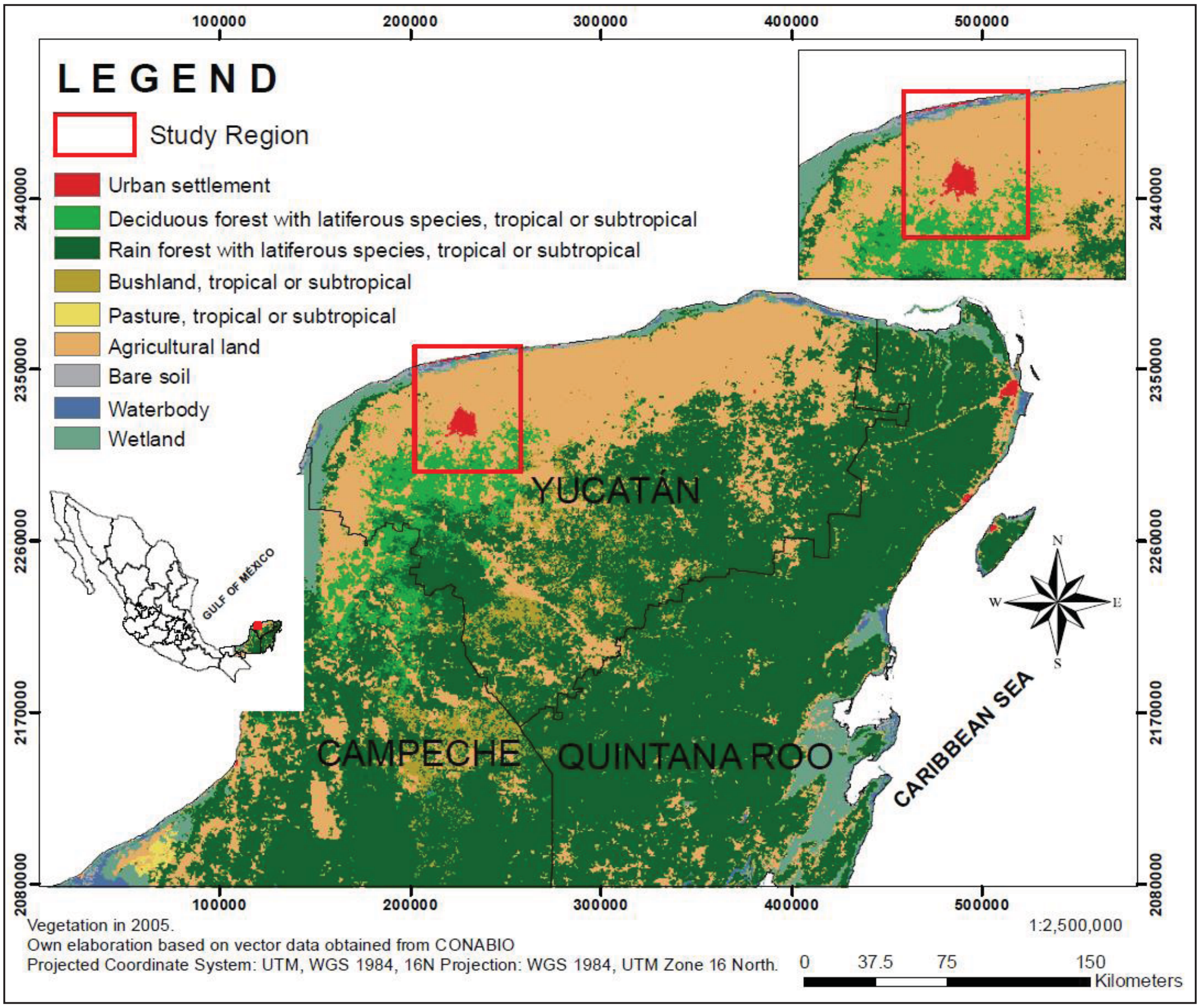


Figure 14. Vegetation.

The mangrove wetlands at the northern coastline in the study area, formed of clay, sand and calcareous mud are subjected to flooding and tidal fluctuations (Villasuso-Pino *et al.* 2011), they are connected to the sea and to the aquifer. The YP provides more than 50 % of the total mangrove area in México nevertheless there were reported great losses due to industrial activities, harbours, urban and tourism development and passing hurricanes in the valuable ecosystems (Herrera-Silveira *et al.* 2012). Worldwide, at least 35 % of mangrove forest areas has been lost in the past two decades (Valiela *et al.* 2001).

Contributions of groundwater discharge and ocean water are responsible for the particular ecosystem characteristics and its water balance. The coastal wetlands and particularly the mangrove forests provide a huge variety of environmental services as they act like natural control systems, barriers against hurricanes, biological water filters, animal refuge and control coastal erosion, among other benefits (CONABIO 2012).

3.1.6. Land use

In the study area the land use can be divided into three main types: urban areas with settlements, agricultural and rural areas and natural forest with nearly no settlements:

There are urban areas with settlements, commercial and industrial zones. The urban area of Mérida, where the main part of the population is currently living, has a total surface area of about 390 km^2. It is important to know, that the area used for urban environments is rather huge in comparison to other cities with a similar population. The majority of the private homes are houses with only one to two storeys, which need more space per person than higher buildings. Even though the industry is not very distinctive in Mérida City, the city can be considered as a regional center of economics: particularly food processing and agro industrial businesses are thoroughly represented. The industrial zone is mainly located in the southeast of the city, where larger companies are situated. In contrast to that, smaller businesses are distributed all over the city (Graniel *et al.* 1999).

In the agricultural and rural areas, on the fields and on farms, crops and animals are produced. In the villages the population density is rather low.

The natural forest with nearly no settlements contain of typical subtropical vegetation and caducifolius forests (Pacheco & Cabrera 1997). Towards the coastline and along this, mangrove forests dominate the landscape (INEGI 2011).

3.2. Geological framework

3.2.1. Topography and physiography

The north of Yucatán is a karst plain with an elevation from 0 masl to about 30 masl (Back & Lesser 1981). Mérida is only about 9 masl. The heights in the south of the study region are about 9-10 masl and steadily become lower to the north, to reach 0 masl at the mangrove area and the coast. Remarkable are elevations in the northeastern part of the study area, with heights around 20 masl. As can be seen, the study region is practically flat.

3.2.2. General Geology

The karst of the YP is considered as an example of a common karst, although many of its features make it very special, with lesser similarities with other karst in the world (Espinaza 1990).

Butterlin & Bonet (1963) mentioned that the northern coast of the YP is composed of Pleistocene and Holocene deposits while the rest is practically composed of Miocene and Eocene deposits. All the rocks are calcareous but its composition is variable: some are compact, dolomitized and/or silicified and recrystallized, with strata thick and massive thicknesses; others are less compact, interspersed with gypsum, in thin and very thin layers, sometimes with caliche. In general, the stratification in the northwestern portion is horizontal and in the northeast region is tilted to the northwest, as a result of a regional uprising occurred in the Late Tertiary. The eastern region is a staggered fractured plain, while the central and southern consists of a series of fractured blocks slightly folded, probably as a result of the deformations occurred since the Oligocene (Espinasa 1990).

Espinoza (1990) mentions a subdivision of the YP in two regions: a) the **Northern plains** (4 zones) and b) **Southern plains and low hills** (2 zones), according to the karstic manifestations.

The **Northern plains** is a plateau platform karst where all the caves have had a phreatic origin. There are fossil cavities above the current water table also formed similarly. The aeration or vadose zones and absorption zone, are practically undeveloped. The zones in which it is divided are: ***Coastal marshes*** with many springs and resurgences located on the coast or at sea, flooded cavities (mostly narrow and small); the ***Northwestern coastal plain*** with little surface evidence of karstic relief, is observed some lapiaz and wide cenotes but shallow, has small caves of phreatic origin, which normally ends up in siphons located 10 m depth; the ***Northeastern coastal plain*** is characterized by an abundance of karstic forms, mainly deep cenotes (some of them with depths greater than 100 m) with deeper water level, also there are some fossils cavities of phreatic origin and horizontal development; in the ***Eastern portion*** there are a lot of closed basins stuffed of saline soils (poljes), mostly flooded with predominantly horizontal development of phreatic and vadose origin with strongly marked influences on the change in the water table (fossilized phreatic caves, flooded vadose galleries and drowned stalagmite formations) (Espinasa 1990).

The **Southern plains and low hills** region, presents a karst folded and/or fractured with lower elevations. It is possible to distinguish two different zones with different origin, physiography and stratigraphy: the "***Sierrita de Ticul"*** zone consists of two parallel ridges ranging from Maxcanú to Lake Chankanab. The relief is higher than in the coastal plain and the karst development is limited to caves, underground drains only exist without contributions from surface runoff; caves are abundant and many types, from small vertical depth with narrow galleries to large rooms of more than 30 m in diameter, commonly groundwater oval fossils rooms, more than 50 m in diameter and 20 m depth interconnected by narrow galleries or large horizontal tunnels; "***Sierra de Bolonchén"***, south of the previous one, is formed by many rounded small hills, with elevations between 100 and 300 masl, flat-bottomed valleys up to 5 km wide, closed, dry and filled by soil up 10 m thick, is the only karst area in the YP which presents all the well-developed hydrodynamic areas. The relief, is much higher than elsewhere in the peninsula. Most entries are receiving surface drainage and are sump type. Some caves are very active during the rainy season. Almost all cavities down to the water table. The horizontal development can also be important, but the caves are mainly vadose, except for the deepest parts, which belonging to the area of seasonal fluctuation hydrodynamics (Espinasa 1990).

The karstic aquifer of the YP is one of the largest in the world with an area of approximately 165 000 km^2 in México (115 000 km^2), Guatemala and Belize (Gunn 2004). Large amounts of groundwater maintain a great diversity of ecosystems, however, there are large areas affected by saline intrusion and anthropogenic pollution, which has increased in recent decades because of economic development and population growth (Bauer-Gottwein *et al.* 2011).

Because the YP is practically flat (except in the south region where there are some important rivers), there are not surface runoff. Groundwater storage and flow occurs regionally through large cave systems where there is a turbulent flow regime. Preferential flow paths are variable on the YP and occur at a range of different scales classified as: regional-scale cones fractures (10-100 km), large dissolution ducts (1-10 km) and small-scale fractures and cavities of dissolution (tens of meters) (Bauer-Gottwein *et al.* 2011).

Several studies have established that the subsoil below of Mérida city, is constituted by Pleistocene-Holocene calcareous rocks, which includes coquinoidal limestones, clayey, microcrystalline, plus sandstones and shales. The coquiniferas limestones reach a maximum thickness of 50 m and overlie the fossiliferous limestones of the Carrillo Puerto Formation; underlying this Formation, there are compact limestones and sandstones of the Oligocene (Graniel *et al.* 1999).

The geology of the study region consists of marine carbonate rocks of Tertiary age and marine rocks and continental deposits of Quaternary age (Butterlin & Bonet 1963; López 1973; Brewerton 1993; Herrera-Rendón, Cardona-Benavides & Graniel-Castro 2014).

The Tertiary age is represented by the Carrillo Puerto Formation (upper Oligocene, Miocene-Pliocene); based on studies of rock samples from wells up to 55 m deep (Rivera-Armendariz 2014) the study area is represented by: (a) deposits of restricted platform, characterized by wackestone-grainstone of pellets and grainstone of ostracods, associated with benthic foraminifera, pelecypods and green and blue algae; (b) oolitic banks systems/behind reef, formed by ooids and oncoids grainstone associated with tubular fragments of corals, bryozoans and red algae, benthic foraminifera and iron minerals; (c) reef patch systems, formed by framestone red algae and tubular corals, where allochems constituents associated are benthic and planktonic foraminifera, bivalves, brachiopods, red algae, pellets, ooids, dolomite and iron minerals; (d) open platform deposits, formed by wackestone of cyanobacteria, bivalves, foraminifera (*Nummulites* sp.) and gastropods, packstone of bivalves and graisntone of *Nummulites* sp., with bryozoans and some iron minerals. The Quaternary age near to Puerto Progreso area is represented by an alternation of fossiliferous limestone(grainstone-packstone), clams (boundstone) and clayey limestones (mudstone-wackestone), all of whitish to yellowish color, porous and fairly cemented because the textural change induced by mixing zones in the freshwater/saltwater interface (Herrera-Rendón *et al.* 2014).

3.2.3. Stratigraphy

In the YP mostly a Cenozoic sequence emerges, mainly calcareous sequence, and is formed by layers in a horizontal arrangement. The oldest outcrops, located in the southern region, consist of limestones and evaporate rocks of Paleocene, surrounded by more recent calcareous deposits (Butterlin & Bonet 1960; Figure 15).

During the Cretaceous age basins of restricted circulation were formed, which created favorable conditions for the development of evaporitic sedimentation. In the Upper Cretaceous changes occurred in sedimentation process; the central portion began to emerge until to be well exposed which is associated with materials like marls and bentonite horizons in remote areas of ancient coastlines, and dolomites, sandstones and andesitic spill in shallow areas (Conagua 1997).

The subsoil of Yucatán State is constituted by a sequence of calcareous sediments of marine origin of Tertiary and has been under slow continuous subsidence. Quaternary rocks outcrop in the coastal areas and corresponds to calcareous deposits exposed after a light emersion of the peninsula (Butterlin & Bonet 1960).

Tertiary Stratigraphy

The study region consists of Cenozoic deposits. These deposits consist mainly of layered calcareous sediments, which were mostly horizontally deposited during the evolution of the Yucatán platform (Viniegraf 1981).

The Differentiated non Oligocene Unit presents an irregular distribution and therefore has not received a formal name. Lesser *et al.* (1980) described these unit at south of Mérida city, to approximately 130 m of the surface and mentioned it consists of calcareous shales with interbedded calcarenite, marl and shale. These deposits are of batial type, while outcrops in south of Mérida city are neritic type (García & Graniel 2010). For Zárate *et al*. (2005), it consists of Mudstone, Grainstone and Boundstone. The Differentiated non Oligocene Unit overlies Chichén Itzá Formation and underlies Carrillo Puerto Formation in a transitional and a concordant manner (Herrera 2013).

The Coquinoidal limestones unit (Carrillo Puerto Formation (TmplCz-Cq)) is the oldest one of the study region (late Miocene-Pliocene). Butterlin & Bonet (1963) describe it as a gray sedimentary rock with light yellow tonalities which, according to Dunham (1962) is classified as a Wackestones-Grainstone. Microscopically its different components are bioclasts, grains, aggregates and organic matter. Its components are angular and poor to moderately sorted, with grain sizes from 0.10 to 15 mm and brown and light yellow tonalities. The matrix is represented by variations esparitic cement and microcrystalline calcite, with oxidation zones due to the presence of minerals rich in Fe. A sedimentary package overlies it in a concordantly form, composed of fine limestone crystals and poorly consolidated shells horizons (Qc) of Pleistocene age (1) (Rivera-Armendáriz 2014).

Quaternary stratigraphy

The molluscs limestones unit (QptCq-Cz, Qpt (?)Cq-Ar, Qpt(?)Ar, QptAr-Cz) of Pleistocene-Holocene in the coastal zone consists of mollusk coquiníferas massive limestone mollusk, hardened caliche material, calcareous mud and coastal sands with white and light yellow tonalities; these sediments include limestones, sandstones and shales associated with marshy lagoons and coastal areas, as well as a series of shallow bays (Virgen-Magada 1988; Miranda-Huerta 2005, Garcia & Graniel 2010). Its outcrops form a wide fringe along the north and west coast of the Yucatán state. This unit overlies in a concordant form on the limestones of the Carrillo Puerto Formation of Superior Miocene-Pliocene. These rocks maintain a high permeability and porosity due to fractures and dissolution cavities. However, groundwater use is limited in this area by the shallow depth of the saltwater interface (García & Graniel 2010).

Almost all the rocks of northern Yucatán are overlain by a Caliche layer, a few meters thick layer of recrystallized hard limestone hard limestone crusts. Due to evaporation processes, minerals accumulate in the upper horizon. Assumed this process dominates dissolution by water infiltration, those minerals, especially calcite agglutinate the porous medium and thus an impermeable horizon develops (Gerstenhauer 1987).

Due to the precipitation distribution in YP, there are two main types of caliche. In the north, where the annual precipitation is about 500 $mm \cdot year^{-1}$ recent caliche is formed. More in the south with higher precipitation rates, about 1000 $mm \cdot year^{-1}$ the fossil caliche is dissolved. Villasuso *et al.* (2011) mentioned the boundary is about 8 km inland in the south of the coastline. Therefore the aquifer near to the coast under the recent caliche layer is confined (Perry *et al*. 2003).

Covering partially these units, there are alluvial deposits consist of silt, clay, sand, calcareous gravels and consolidated limestone sands (Qa) which consist of reworked lithic and shell fragments. There are also marshy deposits (Qs) consisting of fine sediments, calcareous mud, salts and decaying organic matter deposited in shallow lagoons separated from the sea by a littoral fringe. The carbonated sequence rocks do not show a significant deformation and the strata have a horizontal or subhorizontal position with inclinations of not more than 5 degrees.

Figure 15. Geology of the study region.

3.2.4. Soils

The soils of the YP (Figure 16) formed from Tertiary karst limestone on a flat rock terrain, creating a mosaic of black litosols and red rendzins (Duch 1988). Black and surface soils are given either as a thin layer on the rock or in a deeper way with gravel content without visible horizons and usually occur on mounds and thickness less than 20 cm. The red soils are presented in thicknesses greater than 20 cm with a low content of gravel and are mostly found in depressions. These soils occur in small areas, resulting in a spatial heterogeneity (Ravina & Magier 1984; Terán & Rasmussen 1992). Rendzins is the most abundant soil type typically overlying carbonate material, followed by Litosols and Luvisols. In the coastal area a narrow band covered by Regosols can be found. In many national soil classifications Rendzina and Litosol are subtypes of the Leptosoles used to indicate shallow soils on firm or loose bedrocks (IUSS 2007). Rendzina soils are very typical for karst and mountainous terrain and develop during the solution decomposition and weathering process (Scheffer/Schachtschabel *et al.* 2010). Litosols develop on firm and continues bedrocks and can be found in cemented carbonate layers (caliche) in the study area (INEGI 2013). The Regosol soils predominate on loose rocks and sand with low calcium content and are more than 30 m thick (Scheffer/Schachtschabel *et al.* 2010).

The surface limestones are forming a calcareous coating (“laja” or “chaltún”) or softened (“sahkab”).

Water erosion is minimal (10 $t \cdot ha^{-1} \cdot year^{-1}$) due to the flat terrain, unlike wind erosion, which is classified as severe (> 50, < 200 $t \cdot ha^{-1} \cdot year^{-1}$) and extreme (> 200 $t \cdot ha^{-1} \cdot year^{-1}$; Conagua 1997).

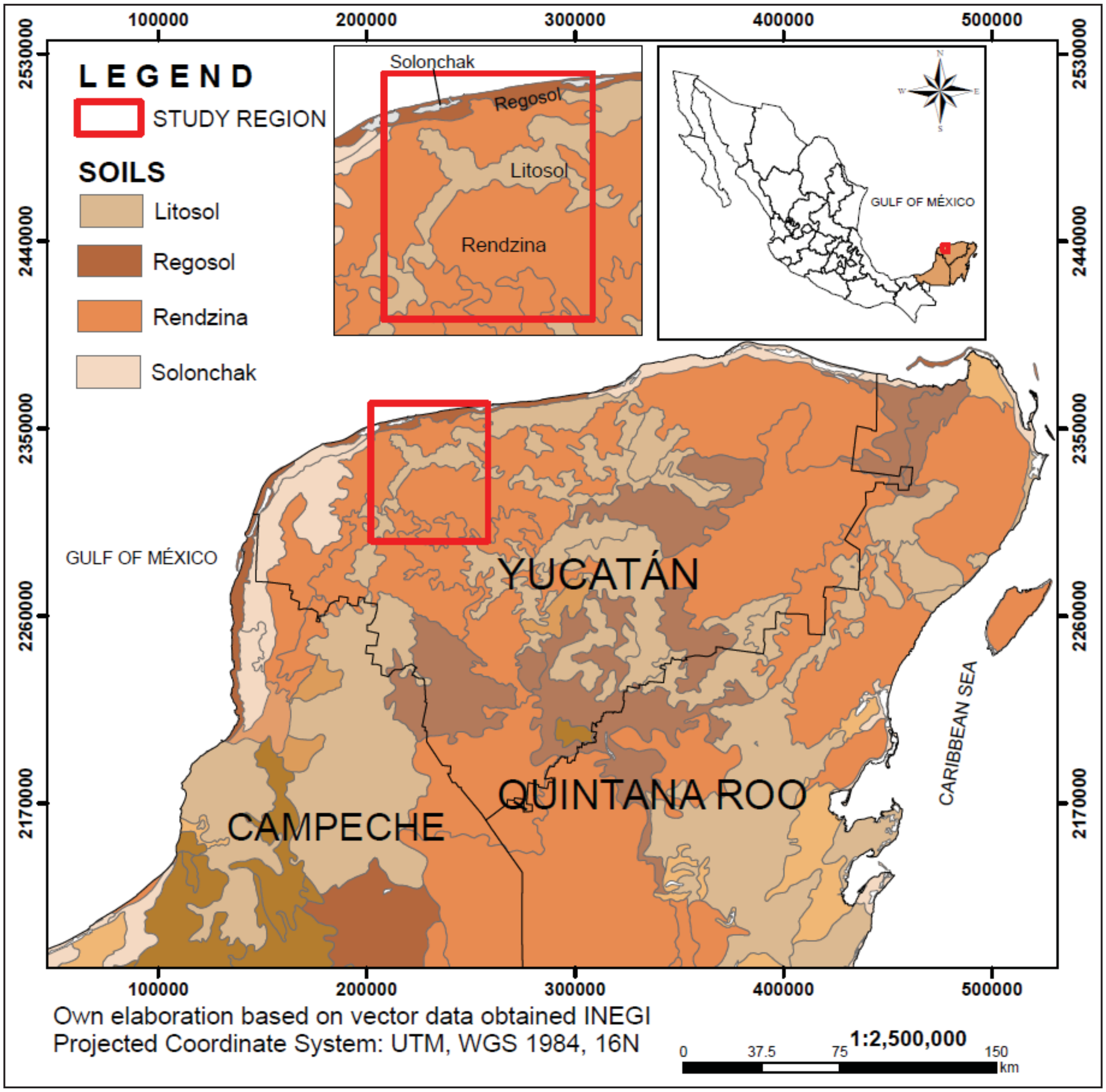


Figure 16. Soils.

3.3. Hydrogeological framework

3.3.1. Hydrogeological units

Because YP is practically flat with a karstic landscape, there are not surface runoff. Groundwater storage and flow occurs regionally in large cave systems where there is a turbulent flow regime. Preferential flow paths are variable and presented in a range of different scales classified as regional fractures (10-100 km), large dissolution ducts (1-10 km) and small scale fractures and dissolution cavities (dozen of meters) (Bauer-Gottwein *et al.* 2011).

Also, the groundwater distribution is conceptualized as the existence freshwater lens with thickness between 1 and 40 m, which is located above a brackish water lens between 2 to 20 m thickness that overlies the saltwater, there is constant interaction with the coastal area where saltwater penetrates more than 40 km inland (Graniel *et al.* 1999; Gonzalez-Herrera *et al*. 2002).

3.3.2. Census of wells

According with Escolero *et al.* (2002) in Mérida are extracted by pumping wells about 3.8 $m^3 \cdot s^{-1}$ and CONAGUA (2010) reports that in all administrative aquifer, the extraction is about 1.4% of the annual average precipitation. In the study region, it has a free karst aquifer type; based on the information generated in this study it was determined that the depth to the water level varies from 6.50 to 9.50 m in the south and from 2.50 to 4.00 m in the north; water table elevations vary between 0.50 and 2.00 m to the south in the vicinity of Mérida and between -0.10 and 1.50 m in the north to 11 km of the coastline; the general groundwater flow direction is from south to north and the average hydraulic gradient is 0.022 $m \cdot km^{-1}$. The hydraulic conductivity values defined and reported for the study region are: $9x10^{-4}$ - $1x10^{-2}$ $m \cdot s^{-1}$ in the wellfield Mérida I (Andrade-Briceño 1984), $1.75x10^{-2}$ - $4.37x10^{-2}$ $m \cdot s^{-1}$ in the wellfield FIUADY (Schmidt 2012), and $3x10^{-4}$ - $5x10^{-2}$ $m \cdot s^{-1}$ in the coastal area at west of Progreso (Reeve & Perry 1990).

Census of pumping wells data was obtained firectly from the “Organismo de Cuenca Península de Yucatán” of Conagua in 2014. According to this information was possible determine that in the study region there are about 5 297 pumping wells with a total annual extraction about 373.01 $Mm^3 \cdot year^{-1}$ (Table 2); while in the model area there are 3 956 pumping wells with a total annual extraction about 311.21 $Mm^3 \cdot year^{-1}$.

Study region			Model area		
Use	$Mm^3 \cdot year^{-1}$	Number of wells	Use	$Mm^3 \cdot year^{-1}$	Number of wells
Agricultural	47.12	5297	Agricultural	27.25	3956
Industrial	42.37		Industrial	40.47	
Multiple	75.98		Multiple	44.64	
Livestock	7.58		Pecuario	4.91	
Urba-Public	182.45		Urban-Public	176.92	
Services	17.52		Services	17.03	
Total	**373.01**		**Total**	**311.21**	

Table 2. Census of wells of the study region and model area.

3.3.3. Groundwater use

The distribution of the groundwater use in the study region is (Figure 17):

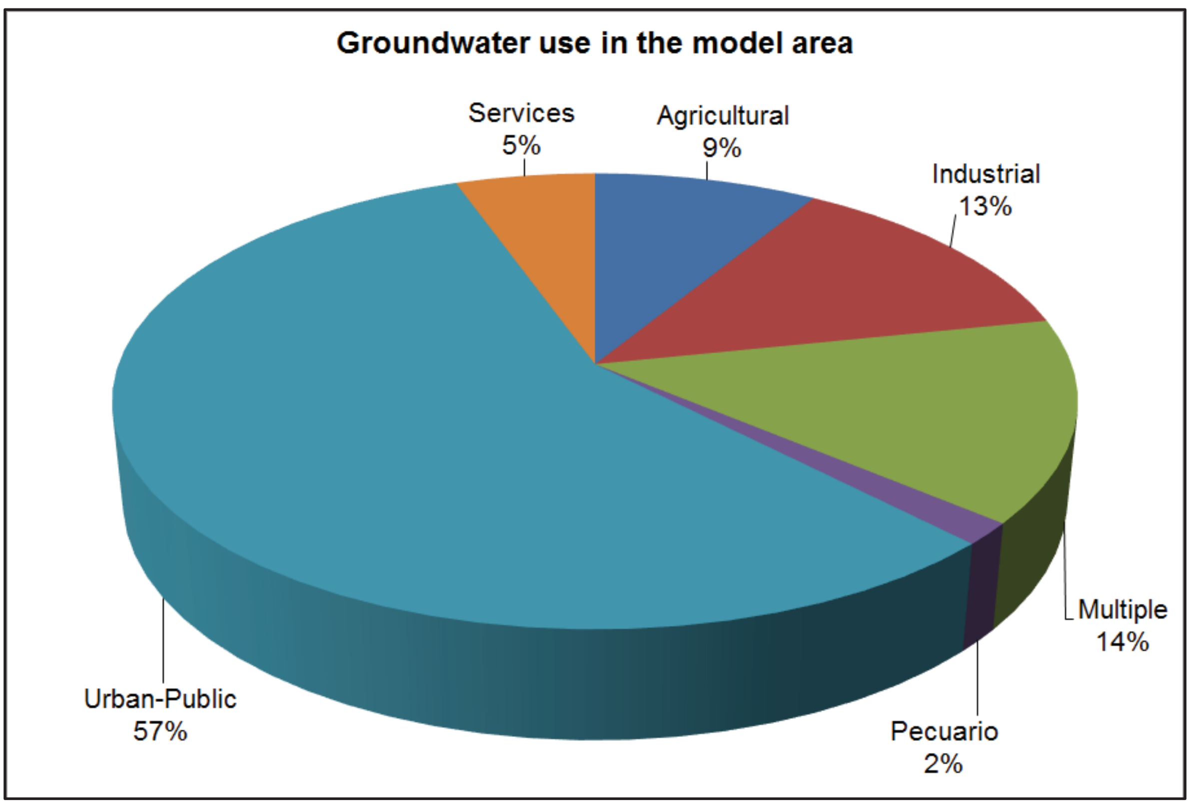


Figure 17. Groundwater use in the study region.

The distribution of the groundwater use in the model area is (Figure 18):

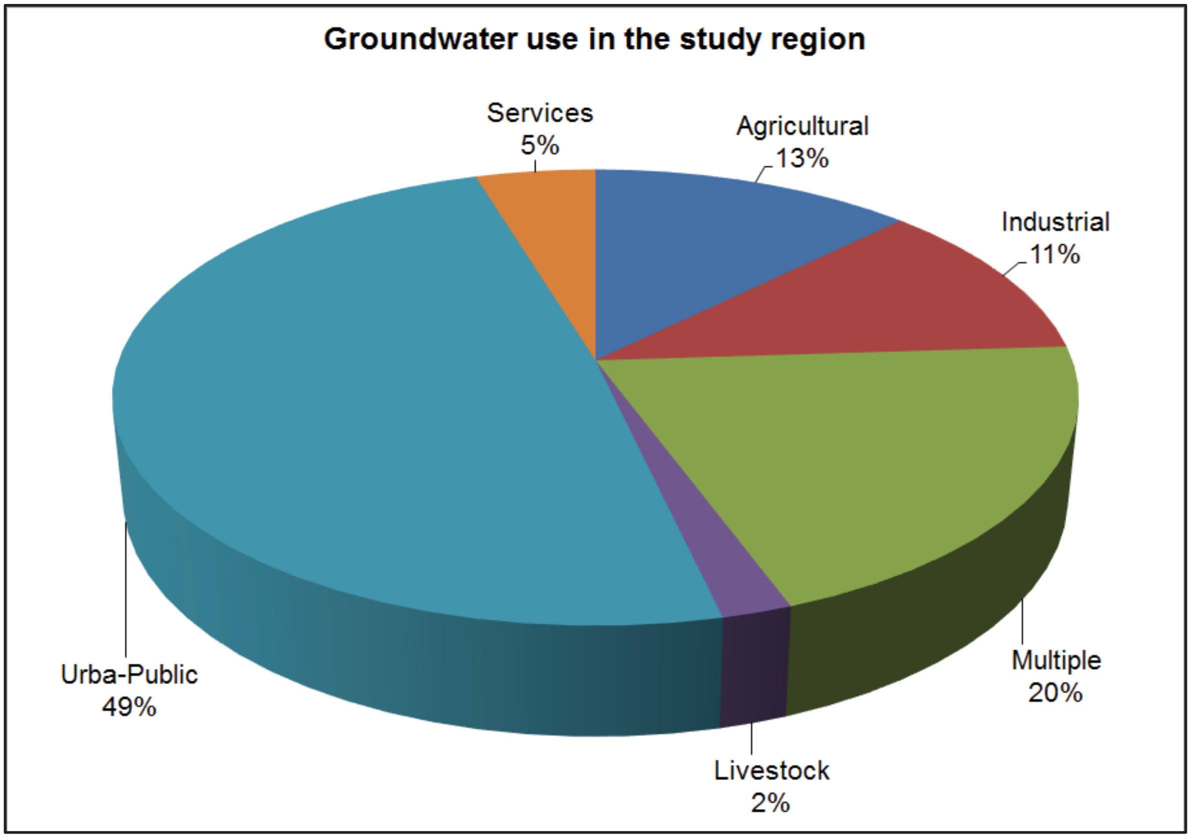


Figure 18. Groundwater use in the model area.

3.3.4. Monitoring wells and hydraulic heads

For the monitoring of water level and some physicochemical characteristics of groundwater were defined spatiotemporal variations of water level and changes in the thickness of freshwater by the variations of the EC in an automated network of monitoring wells. The monitoring network was formed by 26 observation wells (Figure 19) where were installed 20 automated meters for recording hydrostatic pressure (HP), 19 EC automated meters, and 2 automated meters to measure atmospheric pressure (AP) with study region were covered. The EC automated meters were located based on the depth at the beginning of the brackish water interface; in order to identify different types of responses, some of them were placed in the freshwater lens, others in the brackish water lens and others in the boundary between these interfaces. All automated meters recorded four registers per day during the period from June 17th, 2012 to December 31st, 2013 at the following times: 00:00, 06:00, 12:00 and 18:00. Additionally, historical groundwater level records were obtained from “Organismo de Cuenca Península de Yucatán” of Conagua in 2014 (Figure 19, Figure 20, Figure 21, Figure 22 & Table 3).

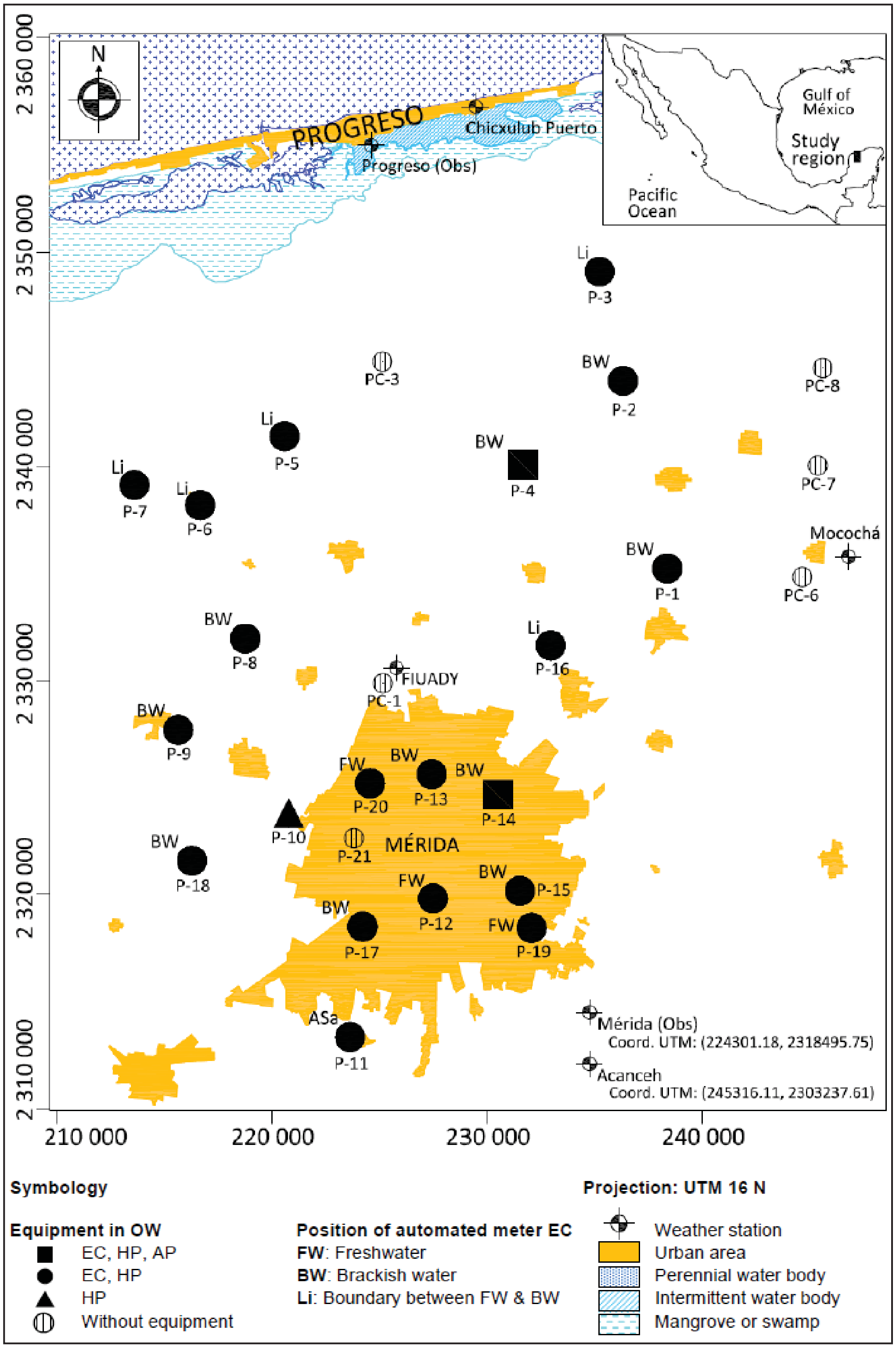


Figure 19. Monitoring wells.

Name	Location (UTM WGS84)		Flow calibration			Validation	Transport calibration
			August 1995	May 2006	June 2012	October 2013	February 2013
	X (m)	Y (m)	(masl)	(masl)	(masl)	(masl)	$mg \cdot L^{-1}$
Km 17-Chuburná Puerto	206600.21	2347687.29	0.45	0.39	0.39		
Km 19 a Chicx. Puerto	233735.48	2349864.09			0.34		
Chichí Suárez	234290.33	2324037.72	1.48	1.39	1.32		
Kanasín	233999.28	2317088.51			1.57		
San Pedro Chimay	231554.27	2309696.30	2.07	2.17			
Dzununcán	223850.91	2309641.14	2.03	1.96			
Tanil	218230.33	2312337.48	1.98	1.80	1.83		
Dzibikak	209761.13	2313797.72	1.92	1.83			
Caucel	218680.77	2326356.69			1.11		
Susulá	219610.56	2321285.33	1.60	1.44	1.38		
Vivero Forestal	222204.63	2317216.69	1.73	1.48	1.40		
Camioneros Aliados	230384.20	2317835.70			1.58		
Megalita	238350.97	2335222.11					5.40
Crio	236296.58	2343980.27				0.79	5.90
BAAG	235198.28	2349086.98				0.15	
Sac-Nicté	231623.29	2340055.10				0.69	5.20
Dzidzilché	220586.33	2341397.61				0.36	3.70
Papacal	216653.95	2338173.18				0.54	4.50
San Miguel	213592.81	2339115.08				0.51	
Cheuman	218755.19	2331956.31				0.94	5.00
Ucú	215633.11	2327693.01				1.01	
Anicabil	220785.55	2323798.18				1.43	7.20
UDS	223635.87	2313336.39				1.47	5.70
Tecnológico	227441.05	2325618.01				1.03	3.80
SAGARPA	230459.10	2324656.82				1.00	
Pacabtún	231492.37	2320171.32				1.09	11.20
Chalmuch	216274.63	2321580.45				1.01	4.20
Acuapaque	232033.30	2318438.63				1.09	4.90

Table 3. Historical groundwater levels used for calibration and validation processes.

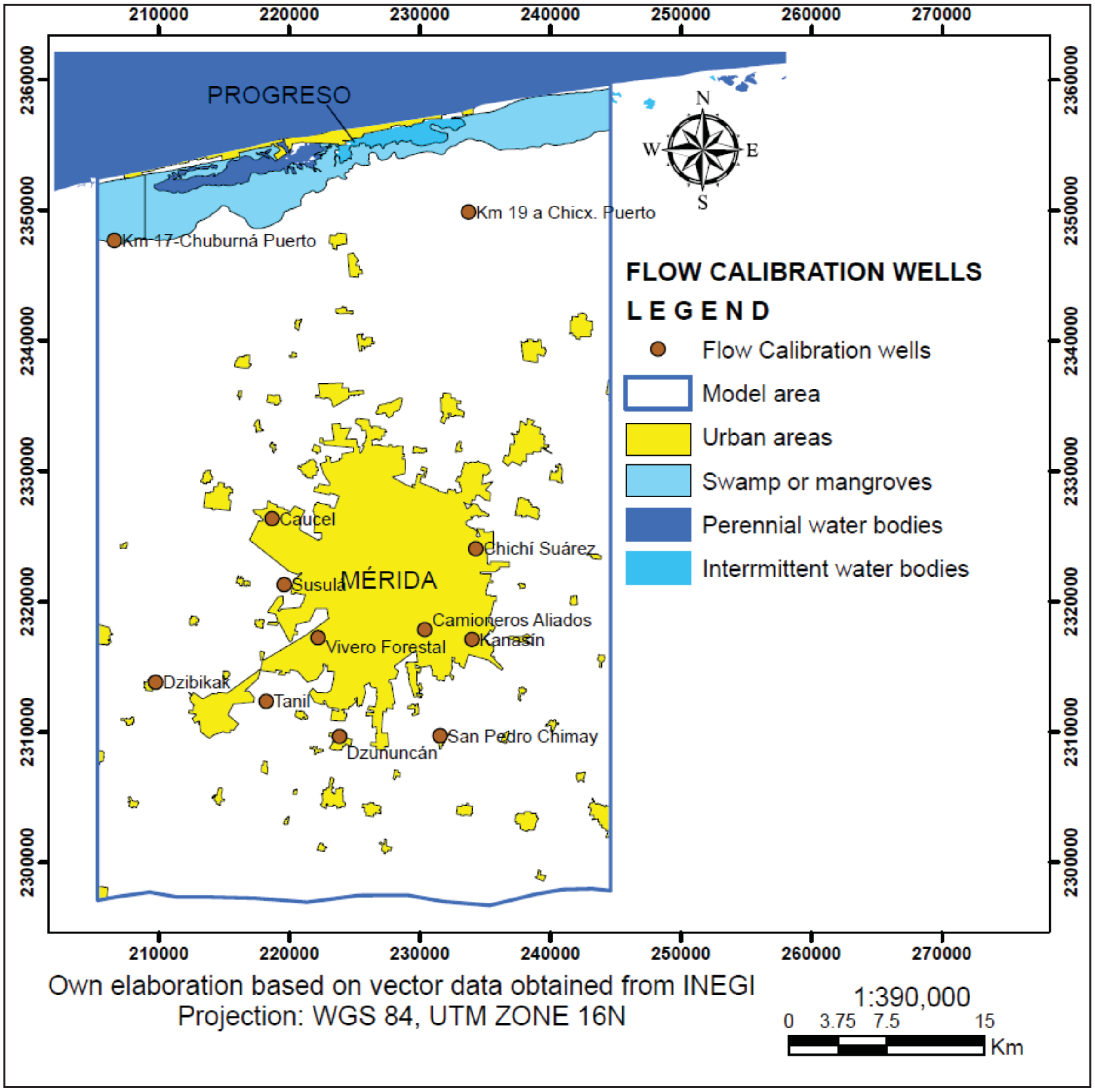


Figure 20. Flow calibration wells location.

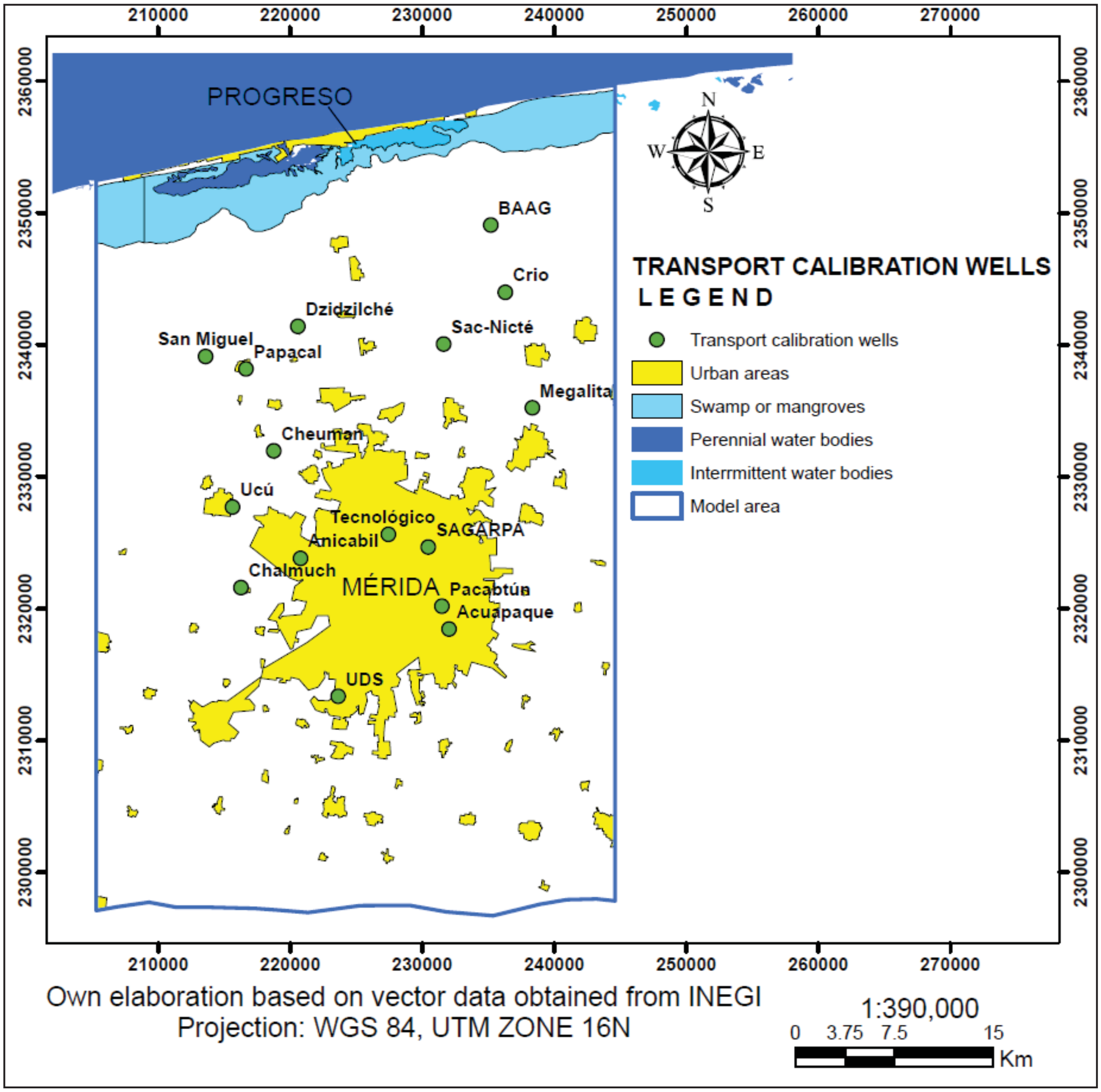


Figure 21. Transport calibration wells location.

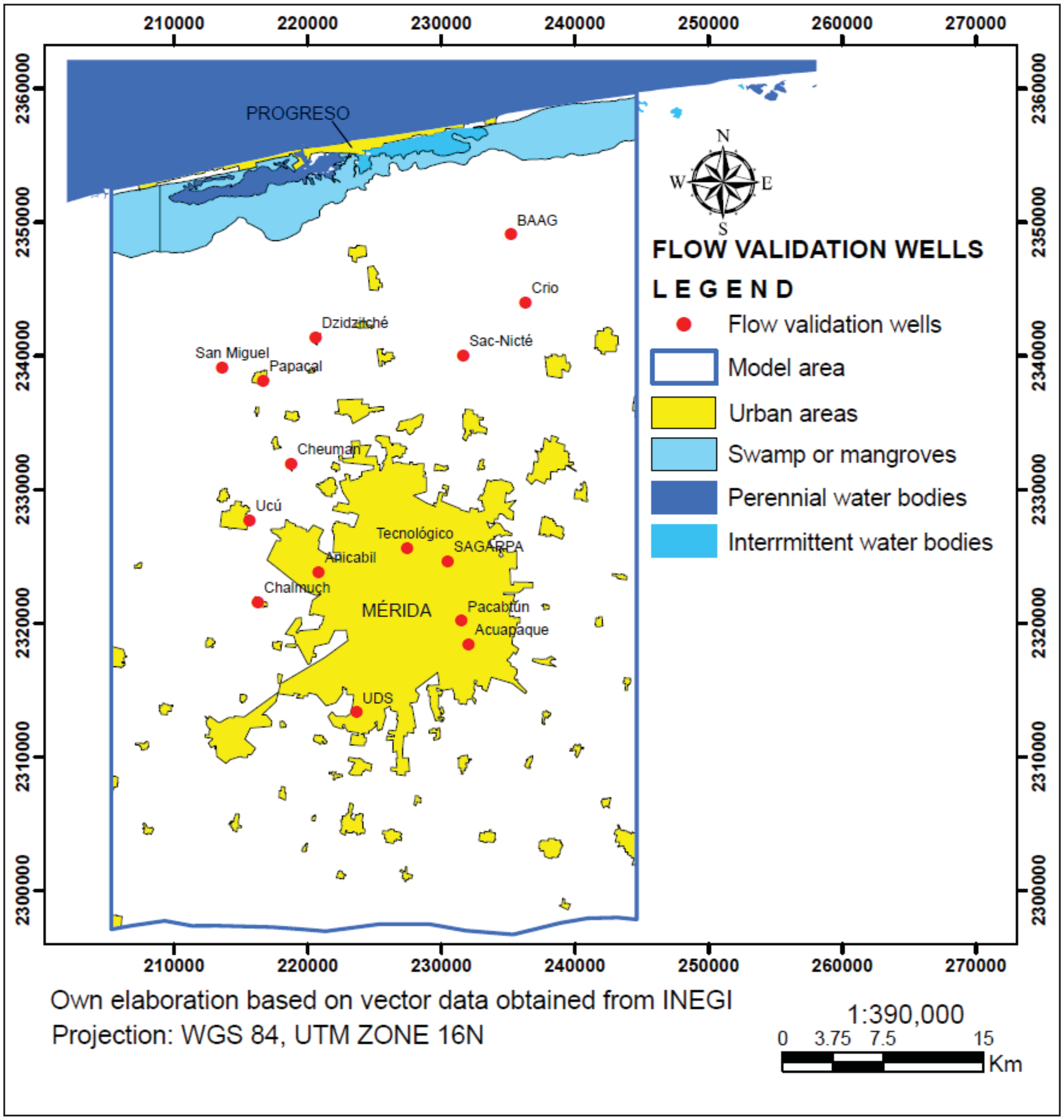


Figure 22. Flow validation wells location.

3.3.6. Tidal effects

The discharge at the coast varies with the tidal cycle. The range of tide on the coast is with up to 60 cm relatively low. The influence is reflected up to 13 km inland; the sea changes the piezometric head in this area (Villasuso *et al.* 2011). These authors measured 1.5 km inland a difference in piezometric head of 40 cm following the tidal cycle reference at the ocean. Because the analysis time is long-term, sea level can be considered as zero and not take into consideration the daily hourly variation of the tidal effects.

3.3.7. Fresh/brackish water interfaces

As part of the project, which is part of this research Rocha *et al.* (2015) (see Appendix 2) investigated fresh/brackish water interface changes linked to precipitation events and correlated with the principle. Water level elevations and EC values were manual and automatic recorded in a 26 wells monitoring network. Results indicate a fast water level increase (hours) to precipitation events, for example a 19 cm water level increase and 570 $\mu mhos \cdot cm^{-1}$ decrease measured at the fresh/brackish water interface was recorded in an observation well located west of Mérida city less than 24 hours after a 60 mm rainfall. They detected that using the measured density values in water sample it was identified that the principle of Ghyben-Herzberg is not valid to determine the thickness of freshwater, similar condition identified by Moore *et al.* (1992) and Escolero *et al.* (2007) in other areas of the YP.

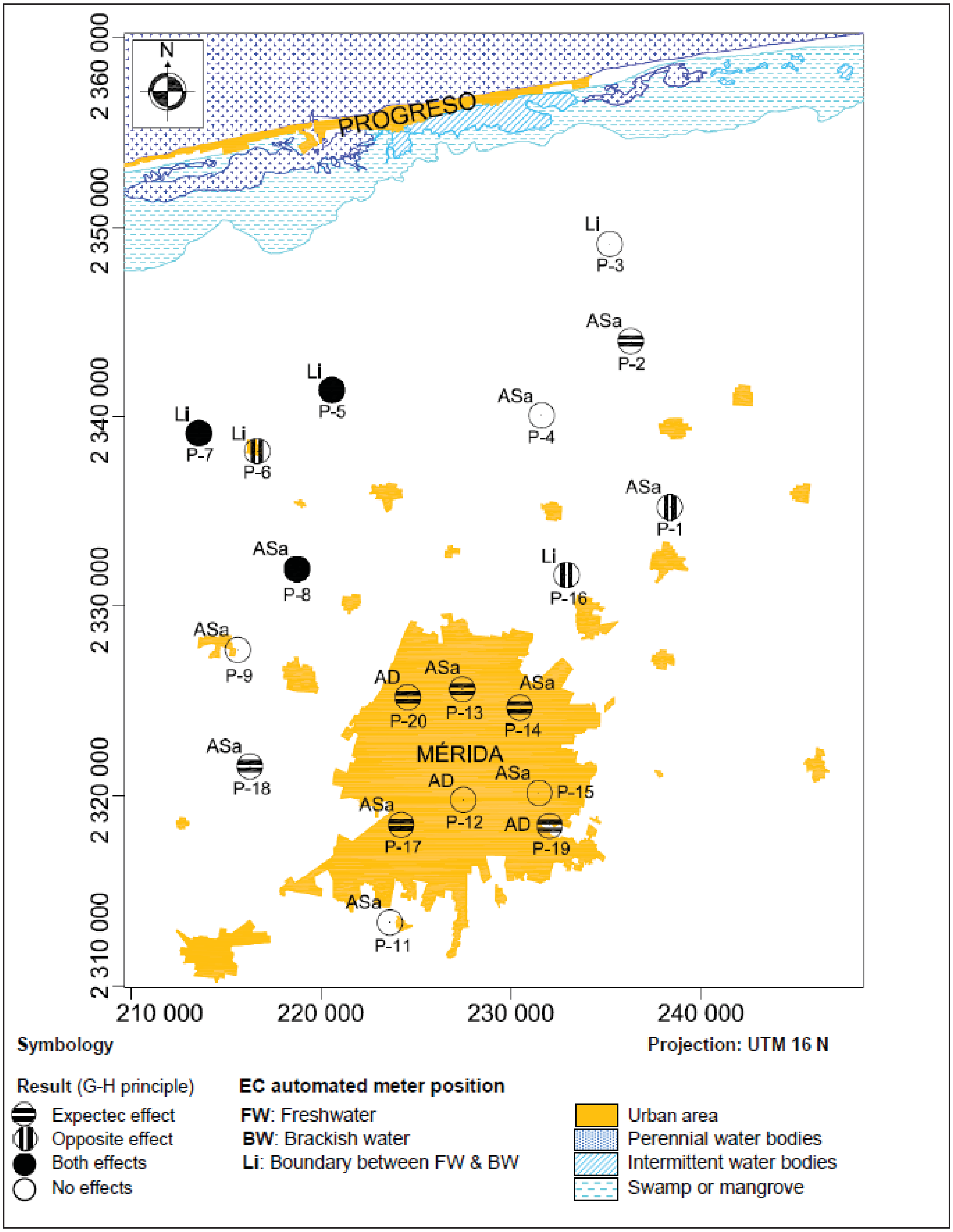


Figure 23. Brackish water interface/precipitation and its relationship with the principle of Ghyben-Herzberg.

Definition of the freshwater lens thickness

Based on the EC records measured in the observation wells for different dates, was possible to produce various types of configurations with respect elevation and time. This information was useful to represent space vertical changes of the overall composition of groundwater associated with the rainy season (November 2012) and dry season (March 2013), which determine the geometry of the freshwater lens in the analyzed region.

Comparing developed for conditions different configurations, indicates that there are spatial changes of the global chemical composition of groundwater for selected depths and that the temporary effects of water infiltration that increase the water table elevation in the rainy season, no generate a significant change in the global chemical composition of groundwater when compared to the dry season. According to the geophysical exploration by Kind (2014), the increase in the EC in the W-NW portion may be associated with well-developed dissolution ducts in Tertiary sediments forming ad hoc networks that facilitate direct interaction between freshwater, brackish water and saltwater interfaces; in addition to this, because concentrations of sulfates in the observation wells P-5, P-6 and P-7 (130 $mg \cdot L^{-1}$ on average; Salazar, 2014) are higher than in the observation wells P-2, P- 3 and P-4 (35 $mg \cdot L^{-1}$ on average) located at similar distances to the coast, it follows that the increase in salinity may be associated with the dissolution of gypsum ($CaSO_4 \cdot 2H_2O$) present in the Carrillo Puerto Formation.

The effect of infiltration of water derived from the precipitation and the displacement of groundwater flow in the karstic aquifer is most noticeable when the water table elevations and the spatial configuration of the precipitation (Figure 24) are analyzed. The rainy period analyzed, where mean precipitation was obtained with the arithmetic method with the information of the weather stations analyzed, initiated in August 2013 (mean precipitation = 125.9 mm) and ended in mid-October 2012, so the November 2012 configuration (mean precipitation = 12.7 mm) represents the effect of the infiltration procedure after that season; while January 2013 (mean precipitation = 56.2) and March 2013 (mean precipitation = 6.2 mm) configurations represent the beginning and ending of the dry season respectively (with an increase in the average precipitation from November 2012 to January 2013 due to scattered rains in the last month), as considering meteorological records available, the rains began again in mid-May 2013. Following that period there were sporadic rains, but according to the records, do not influence significantly in increasing of water table elevation.

According to the general pattern of distribution of groundwater flow, recorded the highest elevations in the southern part of the study area, specifically in the vicinity of the urban area of Mérida city; the effects of infiltration resulting from precipitation and the planned and unplanned induced recharge associated with urban infrastructure, create a sort of dome with maximum elevations of the order of 1.3-1.0 masl, which also has been reported by Graniel *et al*. (1999) and Marín *et al*. (2000). Lower elevations were recorded in the north of the study area, which is consistent with the direction of groundwater flow to the coastline, in the rainy season elevations were of the order of from 0.05 to 0.0 masl to 6 km south of the coastline. In the dry season elevations near to the coastline zone were much higher (between 0.25-0.30 meters) than in the rainy season, which is a reflection of the dynamics of groundwater flow when moving through the karstic environment, the arrival in the coastal area of groundwater infiltrated in the south increased the water level rises also creating an interesting dynamic in coastal ecosystems and the natural groundwater discharge increases during the dry season. Additionally, changes in the patterns of the equipotential lines suggest changes in the directions of groundwater flow. As a heterogeneous and anisotropic medium, the flow lines are not necessarily perpendicular to equipotential lines; anyway it can be seen that the configurations presented undoubtedly reflect changes in flow directions are modified throughout the year, especially in the dry season. The main changes in the flow directions are observed in the urban area of Mérida, which may be due to continuous extraction and artificial recharge. Between Mérida and Progreso changes in the flow direction is observed, especially in March 2013 where the flow direction is mainly towards the NW, presenting in previous months flow directions to the N, NE and NW.

The dynamics of the freshwater lens were analyzed with the EC records obtained, which jointly is presented in the plans which showing changes in elevation of groundwater level are not reflected proportionally with changes in the thickness of the freshwater lens. In Figure 25 the upper limit of the elevation of the brackish water interface (considering that border on the first abrupt change in EC graph) is presented. It is noted that the upper limit of the elevation of brackish water interface in the northern zone is maintained between -20 and -10 masl throughout the year; water level elevation increased of in the dry season does not generate the notorious deepening in the upper limit of the elevation of the brackish water interface. In the south, the upper limit of the elevation of brackish water interface lies from -36 to -30 m in the dry season; on the other hand is notorious depression of the upper limit of the elevation of brackish water interface in the north of Mérida indicated by the -32 and -40 masl, taking into account, for example, the elevation of -16 meters.

In Figure 26 the freshwater thickness (considering its lower limit in the first abrupt change graph CE) for 4 months analyzed are presented. Moreover, the area where the upper limit of the elevation of the brackish water interface (first abrupt change in EC graph) has an EC > 2500 $\mu S \cdot cm^{-1}$ is zoned. This limit has a spatial increase (which may be due to a combination of decreased in precipitation in combination with saline intrusion) to the north of the urban area of Mérida in January 2013 with respect to the other three months monitored. No important changes are observed in freshwater thicknesses, except in March 2013, where some areas of the E and SE of the study area there are decrements of between 6 and 8 m of thickness relative to the other months. This decrease in the thickness of freshwater interface may be due to the lack of groundwater recharge as a result of precipitation because it is notoriously an important decrease in precipitation from mid-October 2012. The average freshwater thickness was also estimated in a selected area, including the urban area of Mérida where it is possible to note an increase of 0.5 m from August to November 2012 and 0.7 m from November 2012 to January 2013 (increase as a result of rains in the last month); Also, it is possible to notice a decrease of 3 m of freshwater average thickness from January to March 2013 which is the dry season.

The actual thickness of the freshwater lens change from rainy (33 m) to dry (31.5 m) (Figure 26) season below Mérida city, minor thickness changes along the year were identified at north of the Mérida city (26 m freshwater lens thickness), coupled with the directions of groundwater flow reflect changes mainly in this area, which may be due to continuous extraction and natural and artificial recharge (planned and unplanned).

The arrival in the coastal area of groundwater infiltrated in the south generates an interesting dynamic by showing an increase and change in the direction of the flow of natural discharge in the dry season. The response of water table levels to precipitation events is immediate and generates contrasting phenomena in the brackish water interface where, after a precipitation event, water table elevation can increase, decrease, or none of them, which shows a great heterogeneity characterized by the karst environment of the region.

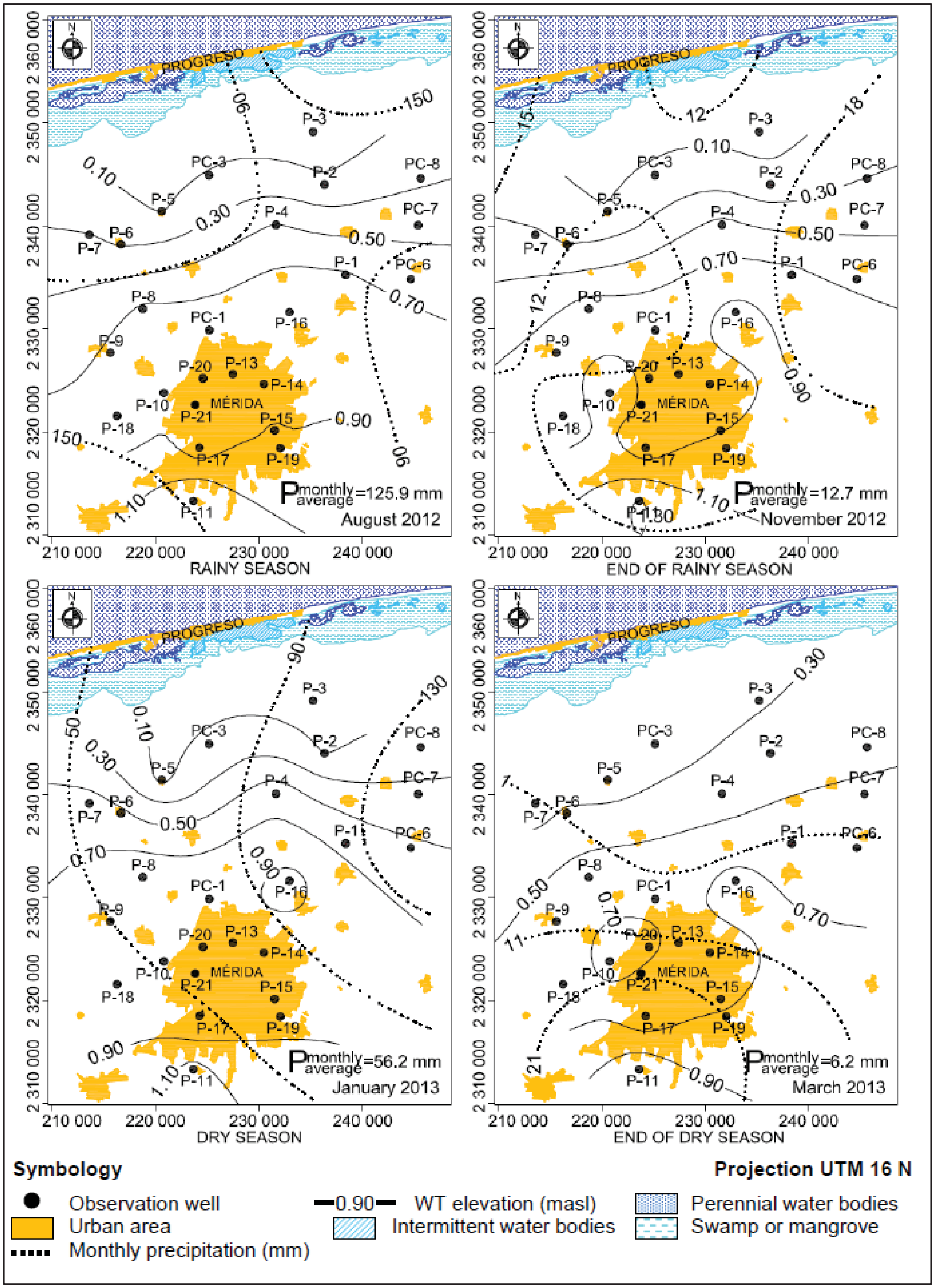


Figure 24. Water table elevations.

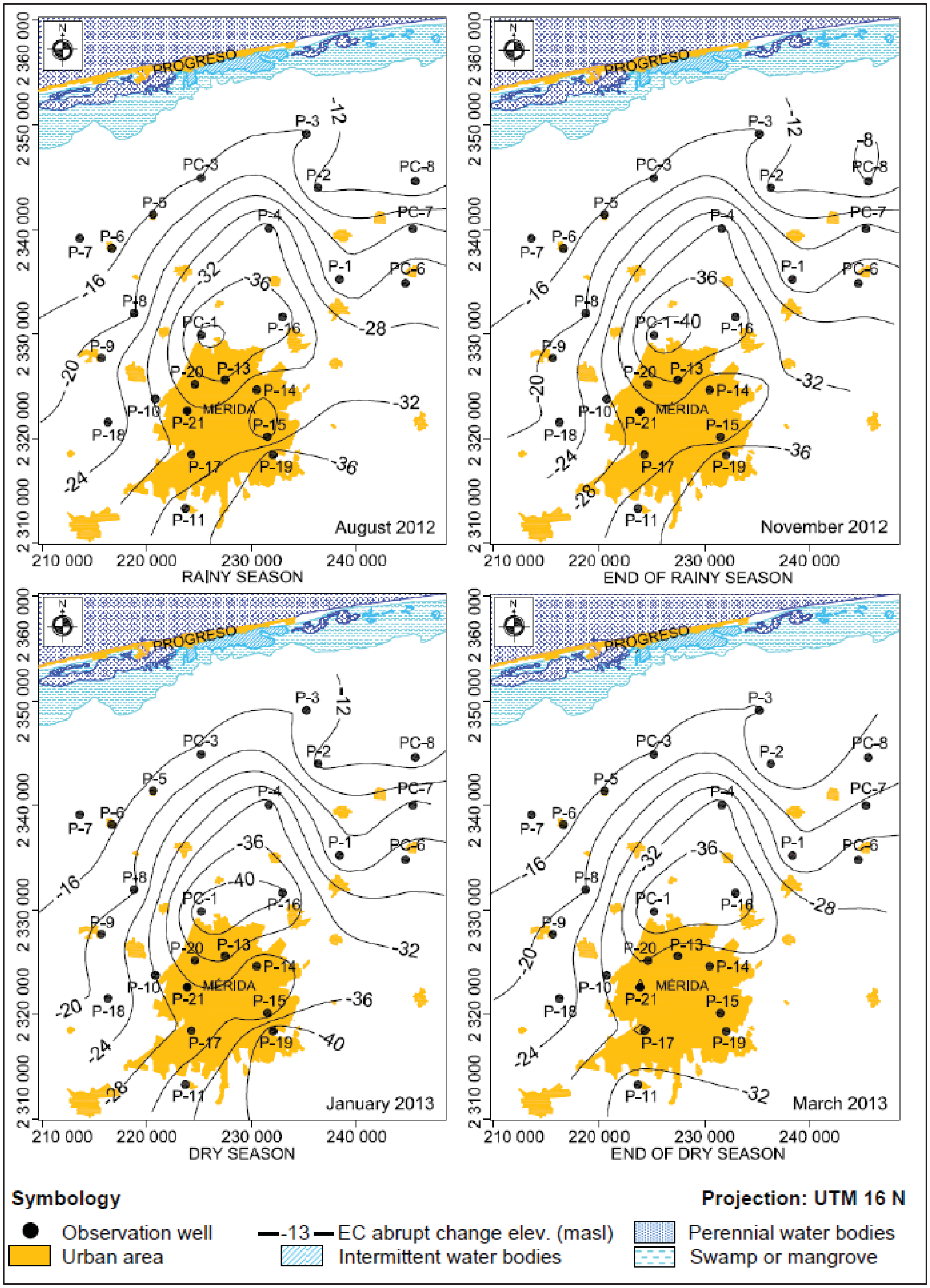


Figure 25. Brackish water interface elevations (first abrupt change in the electrical conductivity profile).

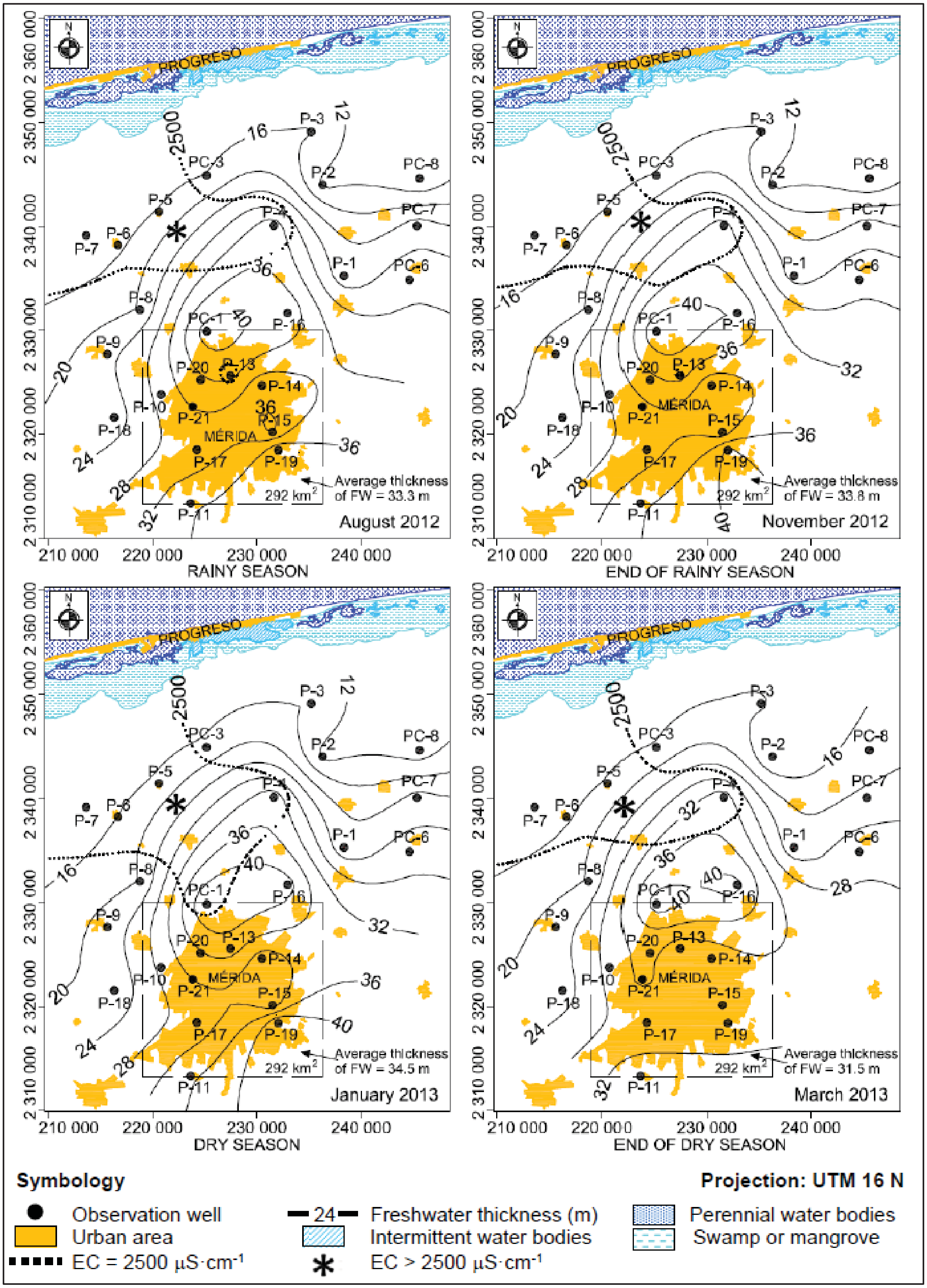


Figure 26. Freshwater thickness.

3.3.8. Nitrate sources and amounts

Groundwater quality in the city of Mérida, Yucatán, México, where dependence on groundwater supply is 100%, is affected by urbanization (Graniel *et al.* 1999).

The main factors which modify recharge quantities and quality of water in the particular case of Mérida are: surface impermeabilization, stormwater soakaways, imported water supply, unsewered sanitation, storage/disposal of effluents and residues (like private extraction, the volume of industrial and non-domestic effluent which reach the aquifer is not known) and agricultural irrigation (the impact from different quantities of groundwater recharge are substantial and includes volumes that are deteriorating the original chemical and bacteriological characteristics of the local groundwater) (Graniel *et al.* 1999).

Municipal and industrial wastewater discharges are concentrated sources of nitrogen compounds, largely, deposited directly into surface water bodies. Differentiation of contamination between easily identifiable point sources and diffuse pollution is essential. The main concern is the subsoil contaminant load associated with sanitation without a sewage system in suburbia, tanks or septic tanks and latrines. The potential risk of nitrate pollution comes from in situ decomposition of excreta (Pacheco & Cabrera 2003).

In Mérida, ambient dissolved oxygen in the upper aquifer is sufficient to make nitrification to nitrate the predominant process except in the city center, where mineralization of organic nitrogen to ammonium is occurring. If all the nitrogen produced from human excreta were nitrified and dissolved in about 675 $mm \cdot year^{-1}$ (rainfall and leakage sources) the resultant nitrogen concentration results 30 $mg \cdot L^{-1}$ (this calculation takes into account background nitrate concentrations in groundwater supplies from the periurban boreholefields which are generally below 5 $mg \cdot L^{-1}$ $N\text{-}NO_3$. Although this is still higher than the levels of 15–25 $mg \cdot L^{-1}$ $N\text{-}NO_3$ observed in the April 1991 sampling, of the upper part of the aquifer in the most densely populated suburbs, it is reasonable, as the dilution effects of the mixing with throughflow water are not included (Graniel *et al.* 1999).

Based on the same procedure of Graniel *et al.* 1999 calculations for estimating concentrations of $N\text{-}NO_3$, calculations for estimating concentrations of nitrates for the year 2013, were made in order to have input data for model calibration transport of nitrates.

In 2010 the population of the city of Mérida was 770 615 inhabitants and the urban area of 272.31 km^2 (INEGI 2011). According with the census of wells (Conagua 2014) the pumping extraction were of 283.96 $Mm^3 \cdot year^{-1}$ without agricultural use and only taking account the urban areas in the model area. Distributing extraction within urban areas of the model area the pumping extraction was of 732.38 $mm \cdot year^{-1}$. Therefore the pumping extraction in the Mérida urban area was about 199.44 $Mm^3 \cdot year^{-1}$. Proposing a 20% of evaporation losses, consumptive use and reuse of treated water is obtained which 159.55 $Mm^3 \cdot year^{-1}$ returning to the groundwater.

Groundwater recharge by precipitation was estimated at 193.77 mm for 2013, so that in the urban area of Mérida city the recharge were of 52.77 $Mm^3 \cdot year^{-1}$.

Total recharge by precipitation and wastewater urban returns, are 212.32 $Mm^3 \cdot year^{-1}$ (159.55 $Mm^3 \cdot year^{-1}$+ 52.77 $Mm^3 \cdot year^{-1}$).

The $N\text{-}NO_3$ average human contribution to the wastewater is about 5 $kg \cdot person^{-1} \cdot year^{-1}$ (Lewis *et al.* 1982) in organic forms which are subsequently mineralized to inorganic species during decomposition (in septic tanks or during percolation; Graniel *et al.* 1999). Therefore, in the urban area of Mérida in 2013 with a population about of 770 615 inhabitants, the annual contribution of $N\text{-}NO_3$ was about $38.53E10^5$ kg which resulting in a concentration of 18.15 $mg \cdot L^{-1}$ of $N\text{-}NO_3$.

$N\text{-}NO_3$ concentrations in groundwater below the urban area of Mérida city in the most superficial samples in 2013 were (Table 4):

Monitoring well	Date	Concentration (mg/l)
Chenkú	feb-13	10.70
Pacabtún	feb-13	11.20
Bomberos	may-13	10.80
Conagua	sep-13	10.20
Concentrations measured at 10 m below the water table		

Table 4. $N\text{-}NO_3$ concentrations in groundwater below the urban area of Mérida city.

3.4. Groundwater balance (study region and model area)

Based on the information showed previously the following scheme was proposed for the water balance in the study region.

The groundwater balance comprising recording inputs, outputs and change in storage.

The components that are necessary to know in the study region for defining the water balance include changes in storage, pumping, runoff, recharge, evapotranspiration, groundwater inflows and outflows, among others.

Typically, the procedure used to raise the balance equation is to determine the natural groundwater recharge based on previous parameters and from the difference between inputs and outputs. This equation was initially justified under the condition of continuity which states: Inputs = Outputs. Based on the calculated amounts presented previously about each parameter of the water balance equation, it proposes the next conceptual model (Figure 27) for 2013 and the annual water balance for the study region (Table 5) and the annual water balance for the southern region for establishing the groundwater inflow to the model area (Table 6).

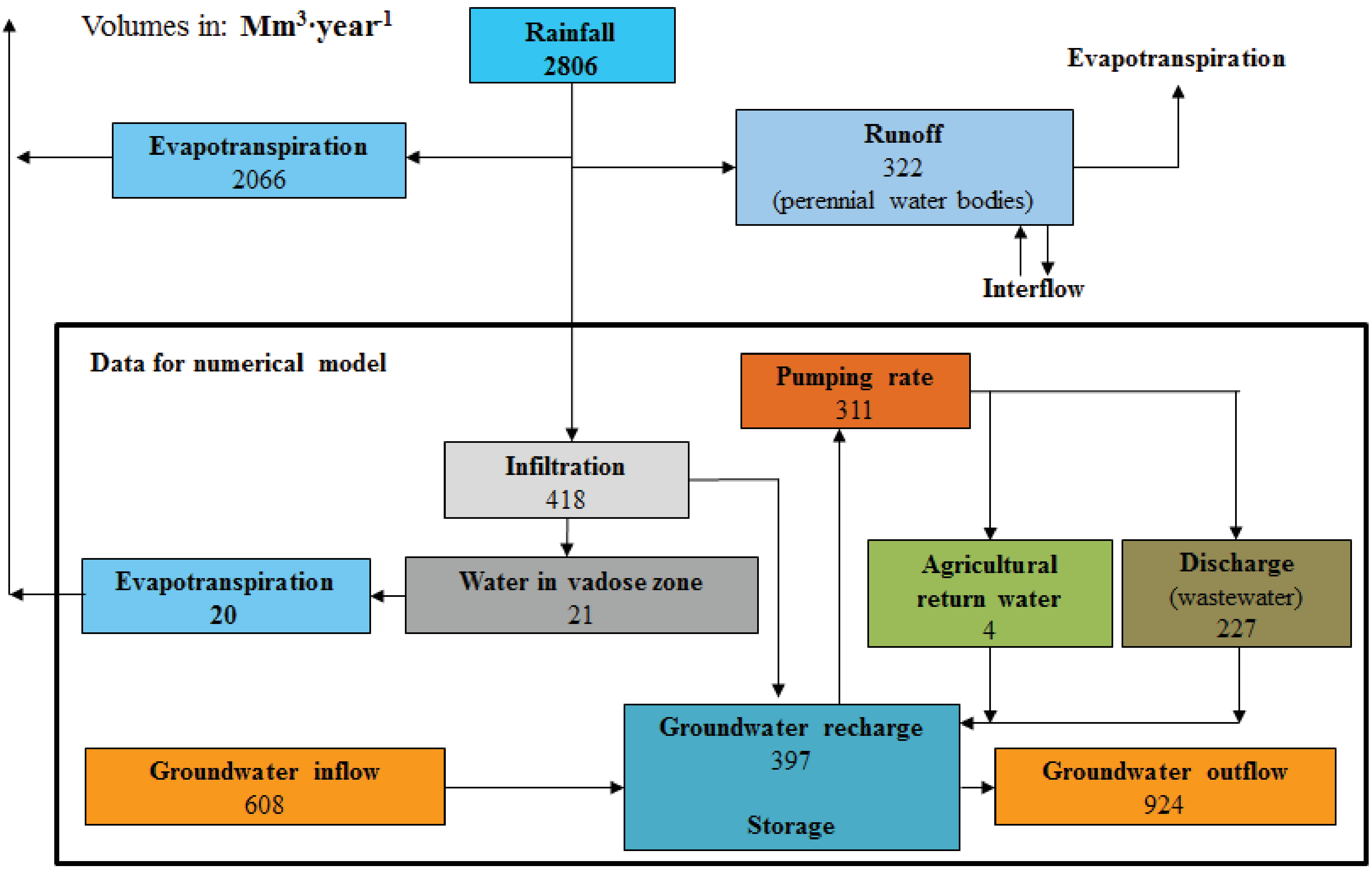


Figure 27. Conceptual model of the model area (water balance 2013 example).

Year	Precipitation ($Mm^3 \cdot año^{-1}$)	Evapotranspiration ($Mm^3 \cdot año^{-1}$)	Runoff ($Mm^3 \cdot año^{-1}$)	Infiltration ($Mm^3 \cdot año^{-1}$) impermeable area 266.38 km^2	Infiltratión ($Mm^3 \cdot año^{-1}$)	Pumping rate ($Mm^3 \cdot año^{-1}$)	Agricultural return ($Mm^3 \cdot año^{-1}$)	Wastewater retunrs ($Mm^3 \cdot año^{-1}$)	Groundwater inflow ($Mm^3 \cdot año^{-1}$) 39.64 km	Groundwater outflow ($Mm^3 \cdot año^{-1}$) 40.10 km
1995	2187	1751	19	251	185	206	2	150	482	605
1996	1994	1622	17	229	143	210	2	153	230	311
1997	2191	1745	19	252	195	215	3	156	314	443
1998	2275	1795	20	261	219	219	3	160	227	377
1999	2869	2091	25	330	448	224	3	163	385	753
2000	2015	1628	18	231	155	229	3	167	280	368
2001	1954	1585	17	224	144	234	3	170	262	338
2002	2870	2082	25	330	458	239	3	174	708	1081
2003	2114	1688	18	243	183	244	3	178	333	444
2004	2279	1781	20	262	236	250	3	182	262	422
2005	2325	1810	20	267	249	255	3	186	382	552
2006	2293	1796	20	263	234	261	3	190	304	459
2007	2680	2004	23	308	368	266	3	194	476	756
2008	2132	1702	19	245	184	272	3	198	347	452
2009	1884	1553	16	216	114	278	4	202	282	318
2010	2517	1901	22	289	327	284	4	207	292	529
2011	2129	1701	19	245	184	290	4	211	282	381
2012	1979	1606	17	227	146	297	4	216	245	307
2013	2806	2066	24	322	418	311	4	227	608	924
			Rained in perennial water bodies							

Table 5. Annual water balance of the model area.

Year	Precipitation (mm·year^{-1})	Evapotranspiration (mm·year-1)	Precipitation (Mm^3·year^{-1})	Evapotranspiration (Mm^3·year^{-1})	Runoff (Mm^3·year^{-1})	Infiltration (Mm^3·year^{-1})	Water in vadose zone (Mm^3·year^{-1})	Evapotranspiration (from vadose zone) (Mm^3·year^{-1}) 95% Turc-PM	Groundwater recharge (Mm^3·year^{-1})	Pumping extraction (Mm^3·year^{-1})	Agricultural returns (Mm^3·year^{-1})	Wastewater returns (Mm^3·year^{-1})	Groundwater outflow (Mm^3·year^{-1}) (inflow to study region) (56.16 km)
1995	1291	935	2999	2174	0	825	41	39	786	168	21	44	683
1996	969	774	2253	1800	0	453	23	22	432	171	21	45	326
1997	1087	838	2527	1948	0	579	29	28	552	175	22	46	444
1998	962	767	2234	1783	0	452	23	21	430	179	23	47	321
1999	1182	885	2748	2058	0	690	34	33	657	183	24	48	546
2000	1034	803	2402	1867	0	535	27	25	510	187	25	49	396
2001	997	778	2318	1807	0	510	26	24	486	191	26	50	371
2002	1508	1002	3505	2329	0	1176	59	56	1120	195	27	51	1003
2003	1096	828	2546	1925	0	622	31	30	592	199	27	52	472
2004	985	762	2288	1771	0	517	26	25	493	204	29	53	371
2005	1161	860	2698	1999	0	699	35	33	665	208	29	55	541
2006	1073	821	2493	1907	0	586	29	28	558	213	30	56	431
2007	1283	920	2981	2138	0	843	42	40	803	217	31	57	674
2008	1124	843	2613	1958	0	654	33	31	623	222	32	58	492
2009	1044	803	2427	1866	0	561	28	27	534	227	33	59	400
2010	1041	792	2418	1842	0	576	29	27	549	232	35	61	413
2011	1043	799	2423	1858	0	565	28	27	539	237	36	62	400
2012	985	764	2289	1776	0	513	26	24	488	242	37	63	347
2013	1425	971	3311	2256	0	1055	53	50	1005	247	38	65	861

Table 6. Annual water balance for the region located in the southern part of the study region.

4. Numerical 3D groundwater model implementation

4.1. Objectives of the model

Normally, when it is possible to express mathematically a set of results are usually to obtain optimal values (maximum or minimum) according to the function or functions analyzed. However, in the case of groundwater modeling it is not like this, because in this kind of analysis is not possible to obtain optimum values. Most commonly is perform simulations on the system where different alternative groundwater uses and/or climatic scenarios are implemented and then choose the most feasible alternative use or management decision(s) in accordance with the goals sought with a solid support.

The aim of this groundwater model is to have a reliable tool that represents the flow and solute transport that works to make future predictions and to know the state of the quantity and quality of groundwater to propose management strategies that help water management in the region with a sustainability perspective.

4.2. Study region and model area

For the purpose of establish the boundary conditions of the groundwater model, a study region was defined, based on the configuration of the hydraulic heads.

4.2.1. Groundwater balance

The groundwater balance showed in the section 3.4. was implemented in a numerical model in the software FEFLOW. In the next topics it is mentioned the process through were implemented the hydrological and hydrogeological variables. FEFLOW 6.2 solves the numerical problem (groundwater flow equation) using a finite element analysis based on several considerations. Turbulent water flow (Reynolds number higher than 10) cannot be considered. The modeling software FEFLOW is working with Darcy's law as a continuum, which could not be applied to such high values. Flow through karstic features like karstic channel flow, and water flow through the matrix of the rock formations (double continuum), cannot be distinguished (Reisinger 2013).

Figure 28 illustrates a general approach in the construction of the groundwater models.

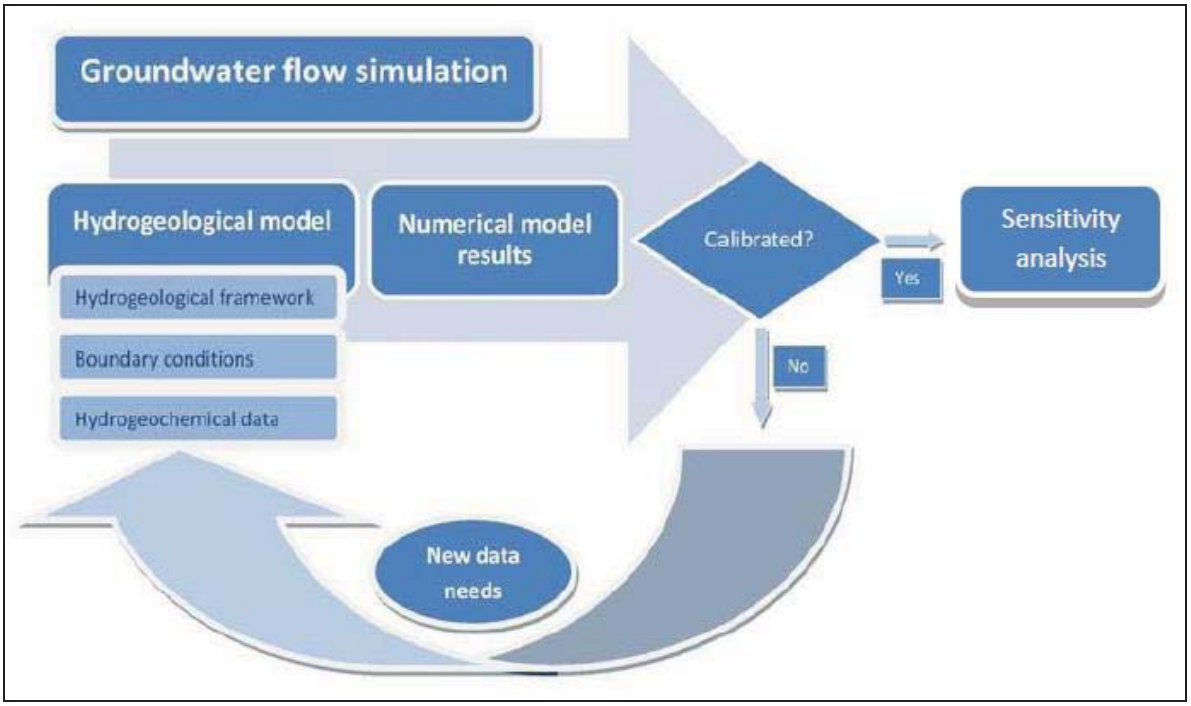


Figure 28. General approach in the construction of a groundwater model (Putranto 2013).

4.3. Data for the model

4.3.1. Spatial discretization

The discretized flow domain was developed through a triangular mesh with 5 000 nodes, 5 slices and 4 layers (Figure 29). The number of nodes mentioned was chosen in order to obtain a mesh with equilateral elements of similar size. This condition facilitates the numerical process in the solution of the water balance equations established in the model.

Subsequently, based on the geological data previously mentioned, the thickness value of each geological media values was assigned. With respect to the base of the system was delimited at an altitude of -70 masl, because there are not hydrogeological data measured at greater depths. The maximum altitude of the terrain represented in the model is approximately 19 masl at south of Mérida and the minimum is 0 masl in the coastal area.

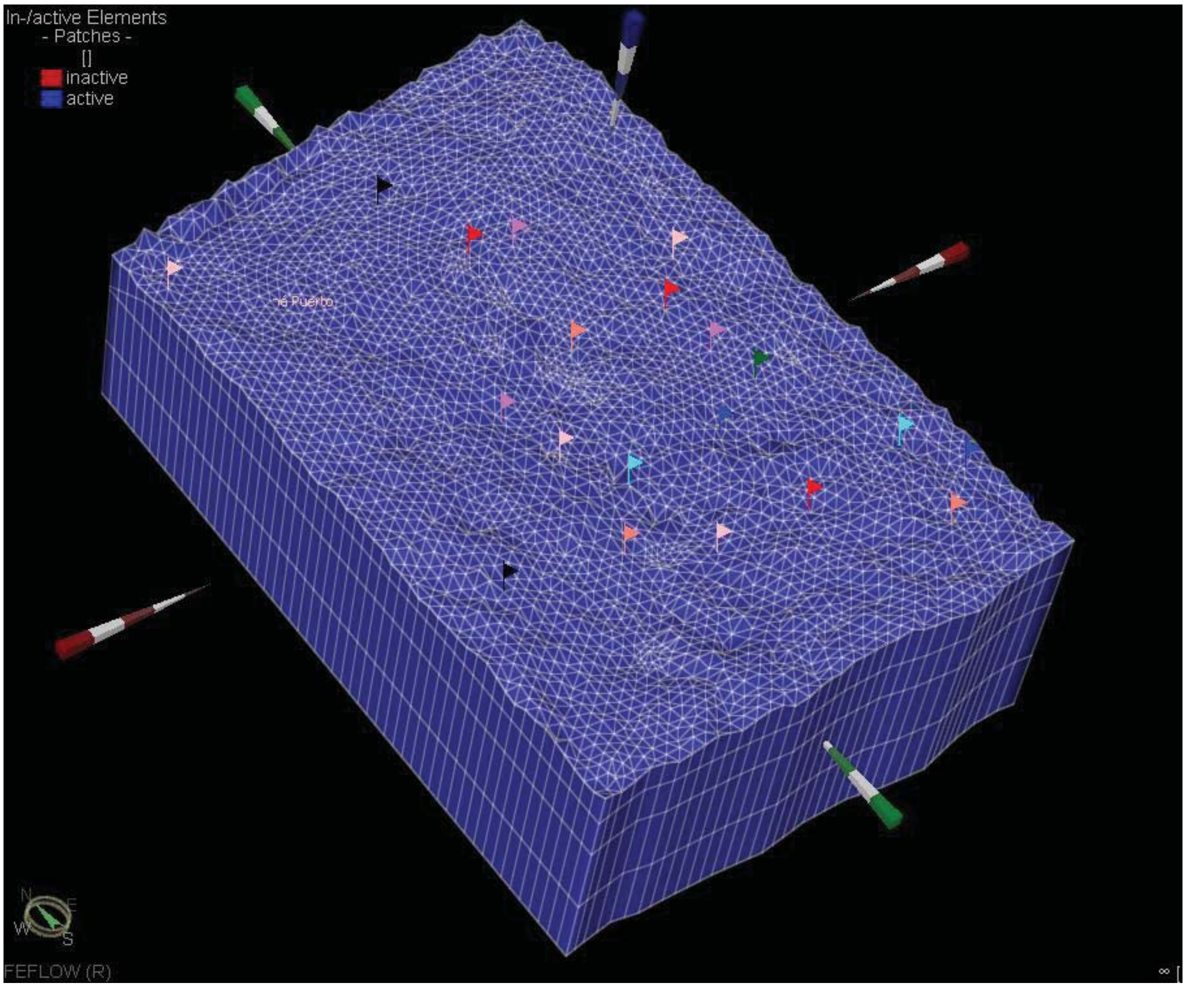


Figure 29. Spatial discretization.

4.3.2. Temporal discretization

The calibration process of groundwater flow was performed in steady and transient state regimes. In steady state regime the period was 1 year. The selected time range in transient state regime was from January 1995 to June 2012 (6371 days, around 18.5 years), the time steps were annual, except 2012 and 2013 which they were monthly.

The calibration process of groundwater flow, was performed based on the comparison between observed and calculate hydraulic heads; 3 observation periods were established: January 1995-August 1995 (227 days), August 1995-May 2006 (2312 days) and May 2006-June 2012 (2221 days).

The date for the validation process in groundwater flow calibration process was October 2013 (day 6858 since January 1st, 1995).

The calibration process of transport of solutes, in this case N-NO_3, was performed based on the comparison between observed and calculate concentrations; 1 observation period was established: January 1995-February 2012 (6620 days).

Subsequently for the development of future scenarios the groundwater model of flow and transport of solutes was projected until January 1, 2030 (12 775 days since January 1995).

4.3.3. Geologic units and hydrostratigraphy (Hydraulic conductivities, Specific storage and porosity)

The initial hydraulic properties were assigned in the calibration process, corresponding to hydraulic conductivity (K) both horizontal and vertical, the specific storage coefficient (Ss) and drain/fillable porosity (dfP), according with each type of rock which the geology in the study region is formed. The geological units implemented in the groundwater model are: (1) sandy-clay limestone, (2) mollusk limestone (3) dolomitic limestone (Figure 30).

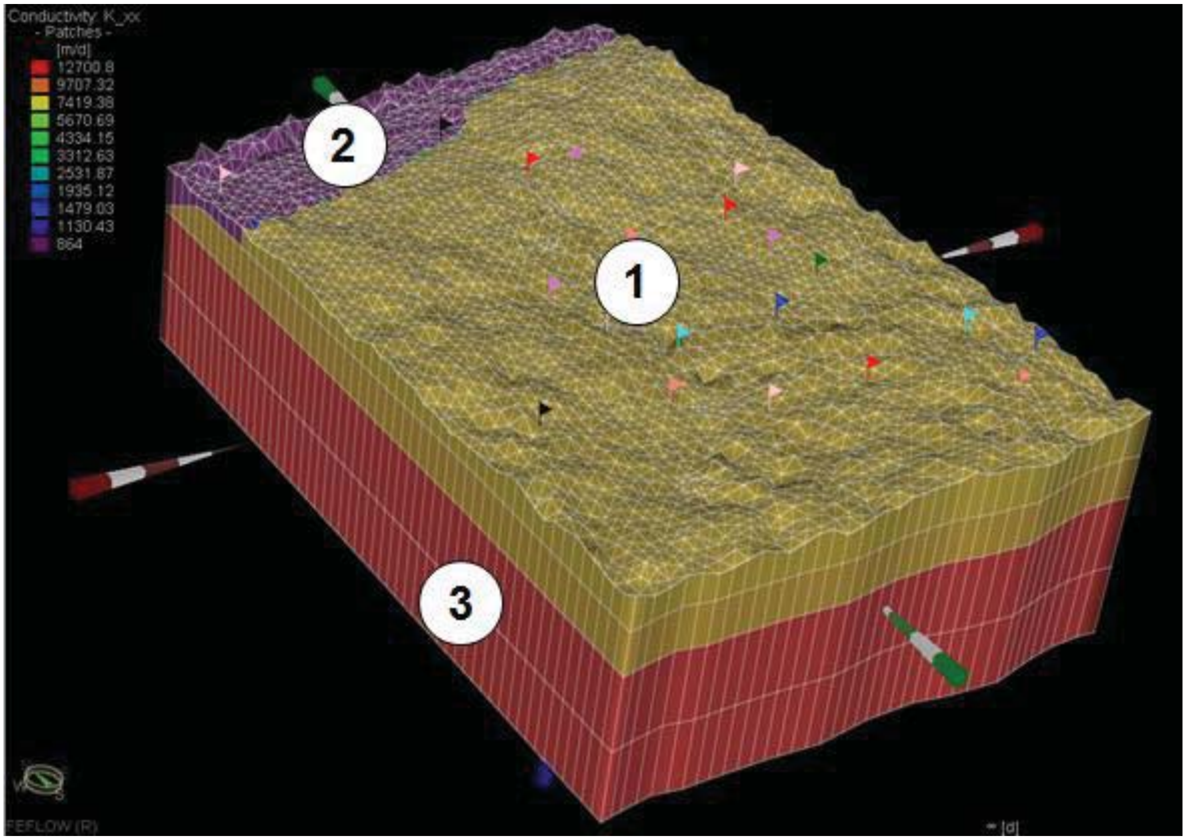


Figure 30. “K” values in different hydrogeological units.

4.3.4. Groundwater recharge

For implementation of recharge in groundwater model 4 kind of zones were defined: (a) recharge area by precipitation, (b) recharge area by precipitation plus agricultural wastewater returns, (c) recharge area by precipitation plus urban wastewater returns and (d) impermeable zone, where due to geological conditions infiltration does not occurs. Groundwater recharge as implemented temporally (year by year) according to calculations obtained in the water balance (Figure 31).

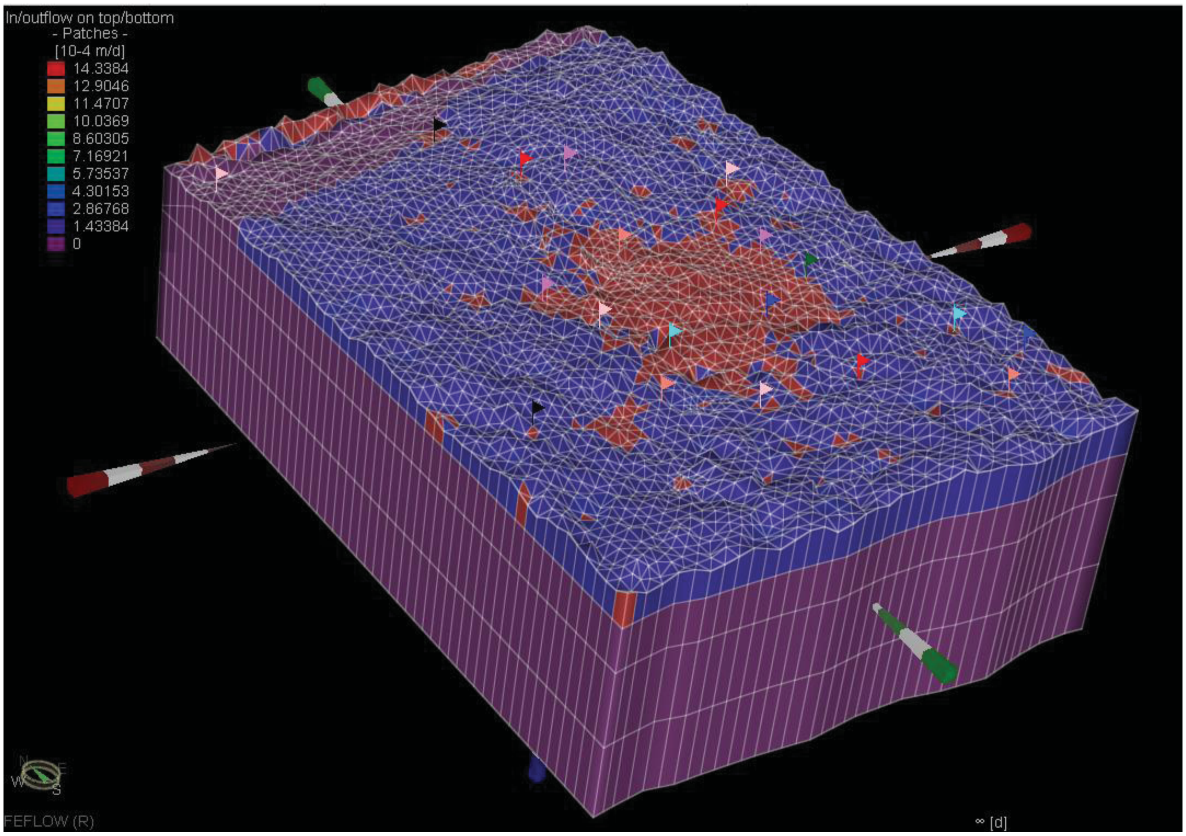


Figure 31. Recharge areas.

4.3.5. Groundwater flow inputs and outputs

According to the characteristics of groundwater flow in the study region, the flow direction is mainly from south to north.

To simulate the groundwater flow inputs and outputs were used constant head (Dirichlet's condition) and fluid flux (Neumann's condition) boundary conditions. The constant head boundary condition was implemented in the northern area (sea groundwater discharge and mean sea level); normally this kind of boundary condition is used for simulate surface water bodies, such perennial rivers, lakes, canals and sea coast interact freely with the aquifer. And fluid flux boundary condition was implemented in the southern area; flux boundary conditions are applied in cases where the gradient or inflow/outflow velocity is known in advance. In this case fluid flux boundary condition was applied by trial and error to achieve water balance previously calculated.

Based on the hydraulic heads in the study region, a constant head of 2.6 masl was implemented in the southern border and 0 masl in the coastal area (northern border) that simulates the sea. The tidal effect was not considered because the simulation is long term and can be considered as a non-variable constant head (Figure 32).

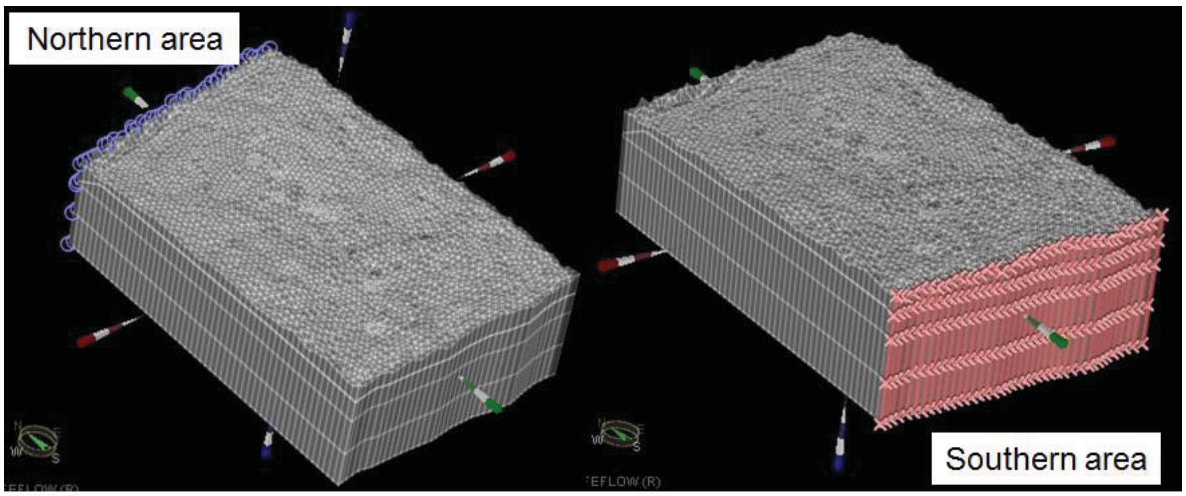


Figure 32. Border conditions (Southern border and coastal area (northern border)).

Normally in this case of boundary conditions is use the Prescribed flux or 2nd kind or Neumann's condition because through this function, it is possible to simulate a variable hydraulic head over time; however, this boundary condition requires the implementation of values of hydraulic parameters which are not measured in the study region.

4.3.6. Hydraulic heads

The initial values of hydraulic heads for the calibration process corresponded to the static levels of 1980 for the monitoring wells of Conagua (Table 3). These same monitoring wells were used for the calibration process with their respective historical records. Then for the validation process, hydraulic heads recorded in October, 2013 in the monitoring wells of this project were used (Table 3).

4.3.7. Concentrations of N-NO_3

For the simulation of solute transport (in this case N-NO_3), the boundary conditions Mass Concentration BC, Longitudinal dispersity (0.055 m), Transversal dispersivity (1.6 m), Molecular diffusion (4E-9 $m^2 \cdot s^{-1}$) and Decay-rate constant (0 E-04$\cdot s^{-1}$) were implemented. Solute dispersion: Nonlinear. Sorption type: Henry. Fluid viscosity: Constant. Mathematical formulation of transport equation: Convective form.

The mass concentration (Figure 33) presented above was used (18.15 $mg \cdot L^{-1}$ in urban areas) and in the agricultural areas the same boundary condition was proposed with a concentration of 4 $mg \cdot L^{-1}$ because there are not records of the possible contribution derived from fertilizer.

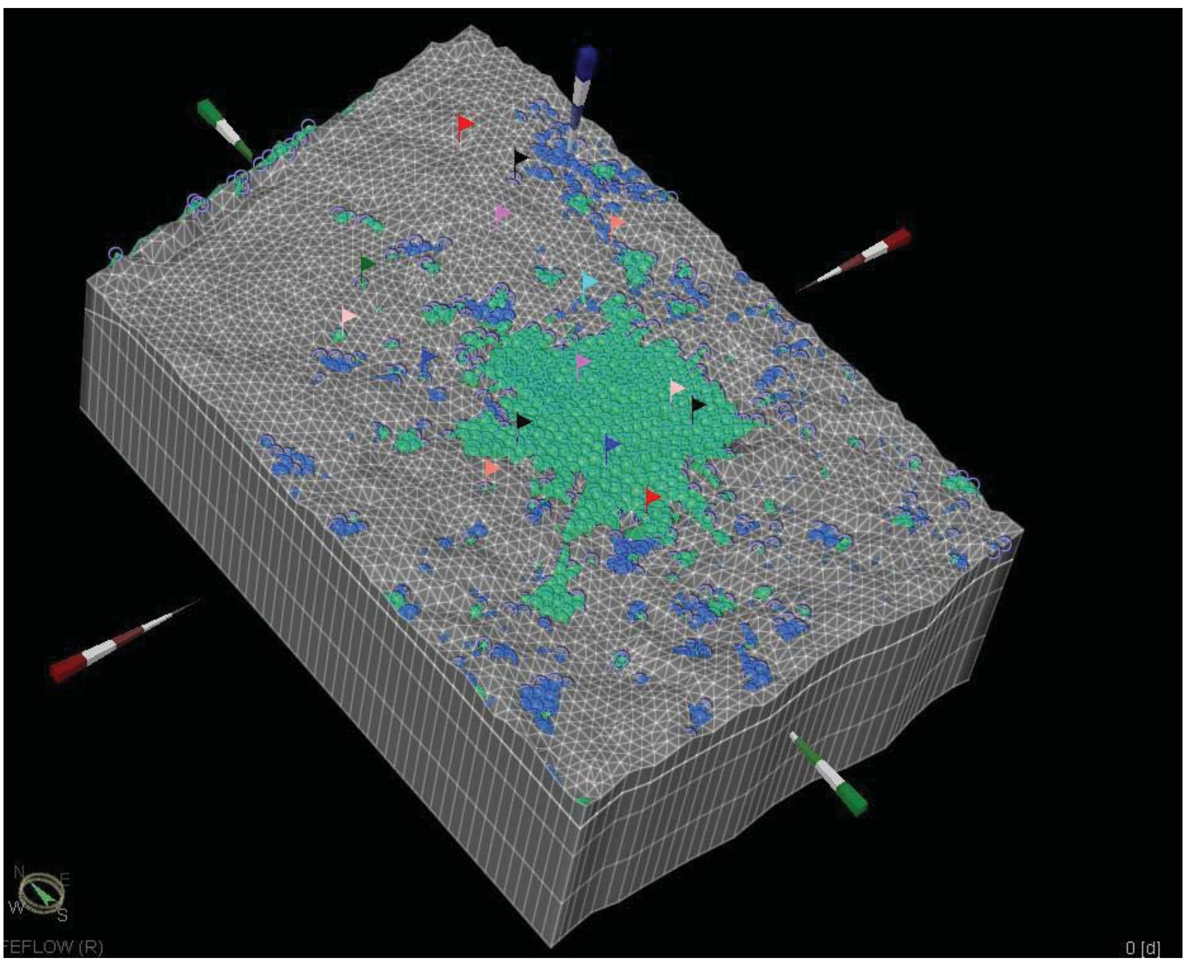


Figure 33. Mass concentrations of N-NO_3.

4.4. Calibration

Calibration is the process of refining the model representation of the hydrogeological framework, the hydraulic properties, and the boundary conditions to achieve a desired degree of correspondence between the model simulations and the observations of the groundwater flow system (ASTM 1993). Model calibration requires that field conditions at a site are properly characterized. A lack of proper site characterization may result in a model calibrated to a set of conditions that are not representative of actual field conditions (Reisinger 2013).

Trial and error calibration method is applied by selecting values for the uncertain parameters and the model runs until a satisfactory result (small discrepancy between calculated and observed heads or concentrations) is obtained (Reisinger 2013).

In FEFLOW the Scatter-plot chart provides the possibility to compare observed and calculated values. It is essential to prove the calibration by using a scatter plot. A scatter plot can show that there is no systematic error involved in the spatial distribution of differences between calculated and observed heads. An assessment of the quality of the groundwater flow model is recommended, preferably by comparing the consistency of the calculated contours in relation to the spot heights of the observed groundwater levels (Middlernis 2000). The chart shows in addition to the residual mean difference, the root mean square error and the standard deviation.

To quantify the calibration processes, statistical equations of error analysis are needed to be counted. The residual mean difference and the root mean square error are important (Reisinger 2013).

The residual mean difference is calculated from the individual differences.

Calibration Residual (Ri): $Ri = Xcal - Xobs$

Residual Mean (Ṙ): $\dot{R} = \frac{1}{n}\sum_{i=1}^{n} R_i$ (4)

The root mean square error equation is shown in the following equation.

Root Mean Squared error (RMS): $RMS = \sqrt{\frac{1}{n}\sum_{i=1}^{n} R_i^2}$ (5)

The test method Rate Budget Panel displays the budget at the current simulation step. The boundary flows are divided in positive flows (into the model) and negative flows (out of the model) (Diersch 2005) and are shown in bars for the different kinds of boundary conditions and the area/volumetric sources or sinks in FEFLOW. The Balance bar shows the sum of all the other values. The groundwater balance term referred to an imbalance in DHI-WASY FEFLOW 6.1. The imbalance corresponds to the sum of all entering and exiting amounts.

4.4.1. Flow

Steady state

Figure 34 and Table 7 show the calibration and the water balance for calibration in steady state.

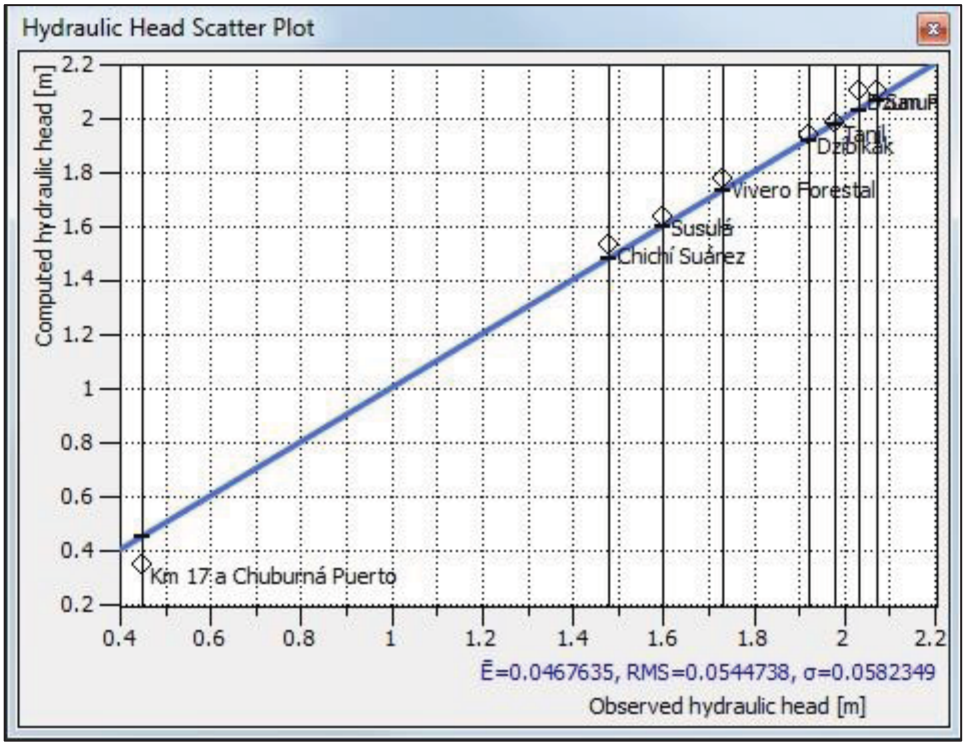


Figure 34. Calibration in steady state.

Concept	Water balance (A)	Model balance (B)	B/A
	(Mm^3)	(Mm^3)	(%)
Groundwater flow outputs	605	475	79
Groundwater flow inputs	482	612	127
Pumping rate	206	206	100
Recharge	328	343	104

Table 7. Water balance calibration in steady state.

Transient state

Figure 35, Figure 36 & Figure 37, and, Table 8, Table 9 & Table 10 are showed the calibration results of the groundwater numerical model in transient state for the different dates.

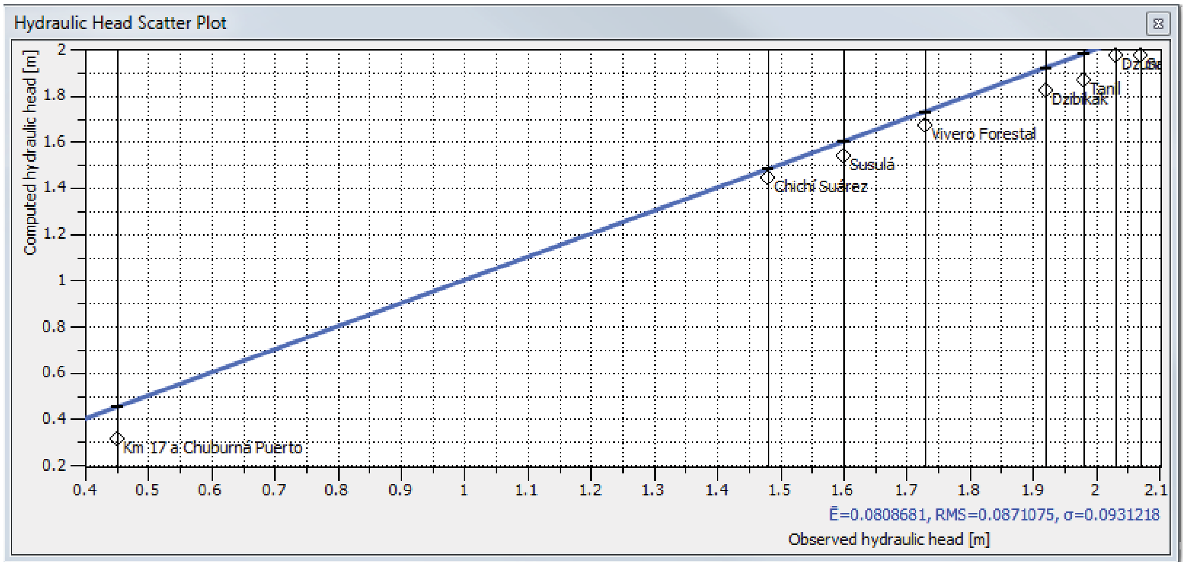


Figure 35. Calibration in transient state (August, 1995).

Concept	Water balance (A)	Model balance (B)	B/A
	(Mm^3)	(Mm^3)	(%)
Groundwater flow outputs	605	421	70
Groundwater flow inputs	482	271	56
Pumping rate	206	129	63
Recharge	328	193	59

Table 8. Water balance in transient state (August, 1995).

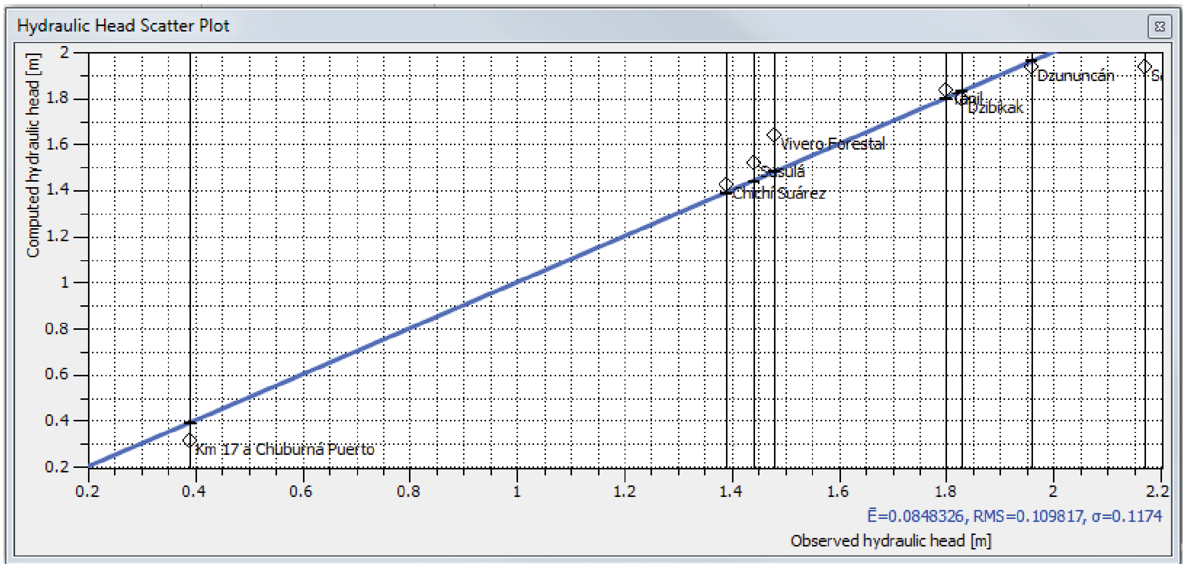


Figure 36. Calibration in transient state (May, 2006).

Concept	Water balance (A) (Mm^3)	Model balance (B) (Mm^3)	B/A (%)
Groundwater flow outputs	6153	7293	119
Groundwater flow inputs	4196	5366	128
Pumping rate	2785	2648	95
Recharge	4769	4483	94

Table 9. Water balance in transient state (May, 2006).

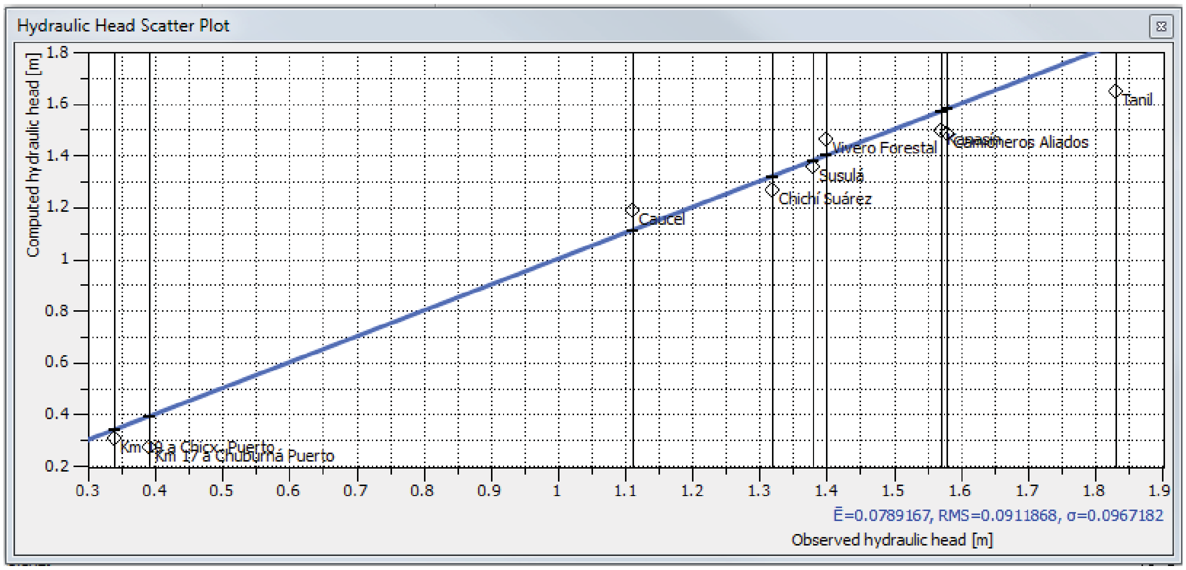


Figure 37. Calibration in transient state (June, 2012).

Concept	Water balance (A) (Mm^3)	Model balance (B) (Mm^3)	B/A (%)
Groundwater flow outputs	8589	11050	129
Groundwater flow inputs	5847	8250	141
Pumping rate	4175	4357	104
Recharge	6917	6984	101

Table 10. Water balance in transient state (June, 2012).

In Table 11 the results of the hydraulic parameters of the calibration process are shown.

Geology	Layer	Kxx (m·s^{-1})	Kyy (m·s^{-1})	Kzz (m·s^{-1})	dfP	Ss
(1) Sandy-clay limestone	1	9.50E-02	9.50E-02	9.50E-03	0.32	2.00E-04
(2) Mollusk limestone	1	1.00E-01	1.00E-01	1.00E-02	0.32	2.00E-04
(1) Sandy-clay limestone	2	1.50E-01	1.50E-01	1.50E-02	0.32	2.00E-04
(3) Dolomitic limestone	3	1.53E-01	1.53E-01	1.53E-02	0.32	2.00E-04
(3) Dolomitic limestone	4	1.53E-01	1.53E-01	1.53E-02	0.32	2.00E-04

Table 11. Hydraulic parameters of the model obtained in the calibration process.

The hydraulic conductivity (k) values obtained during the calibration process of this model, are similar to other ones calculated by another researches in different parts of the YP as is shown in the Figure 38 showed by Bauer-Gottwein *et al.* 2011

K (m s^{-1})	Aquifer type	Scale	Method	Location	Source
0.0116	U	10s of meters	Test pumping	21.0591 N, 87.0270 W	Aguakan S.A de C.V. (2009)
0.004	U	10s of meters	Test pumping	21.0637 N, 87.0331 W	Aguakan S.A de C.V. (2009)
$9 \cdot 10^{-4}$–$1 \cdot 10^{-2}$	U	10s of meters	Test pumping	Mérida	Andrade-Briceño (1984)
0.1	U	10s of km	Numerical model calibration	Northwest Yucatán state	Marín (1990)
1	HPZ	10s of km	Numerical model calibration	Northwest Yucatán state	Marín (1990)
0.55–1.115	U	10s of km	Numerical model calibration	Northwest Yucatán state	Gonzalez-Herrera et al. (2002)
6	HPZ	10s of km	Numerical model calibration	Northwest Yucatán state	Gonzalez-Herrera et al. (2002)
0.0055	LPZ	10s of km	Numerical model calibration	Northwest Yucatán state	Gonzalez-Herrera et al. (2002)
0.064	U	10s of km	Numerical model calibration	Mérida	Mendez-Ramos (1991)
0.36–2.59	U	100s of km	Numerical model calibration	Southern Quintana Roo	(B.R.N. Gondwe, Technical University of Denmark, unpublished data, 2010)
0.26–68.84	HPZ	100s of km	Numerical model calibration	Southern Quintana Roo	(B.R.N. Gondwe, Technical University of Denmark, unpublished data, 2010)
0.014–2.48	U	100s of km	Numerical model calibration	Yucatán Peninsula	Charvet (2009)
7.38–295.8	HPZ	100s of km	Numerical model calibration	Yucatán Peninsula	Charvet (2009)
0.19–0.65	U	10s of km	Darcy's law	Playa del Carmen	Moore et al. (1992)
10^{-6}–$5 \cdot 10^{-3}$	M	10s of cm	Hydraulic testing of core samples	Mérida	Gonzalez-Herrera (1984)
$3 \cdot 10^{-4}$–$5 \cdot 10^{-2}$	M	10s of cm	Hydraulic testing of core samples	North of Mérida	Reeve and Perry (1990)

Figure 38. Summary of published effective hydraulic conductivity estimates for the YP (Bauer-Gottwein *et al.* 2011).

4.4.2. Transport

Figure 39 shows the transport of $N\text{-}NO_3$ calibration in transient state.

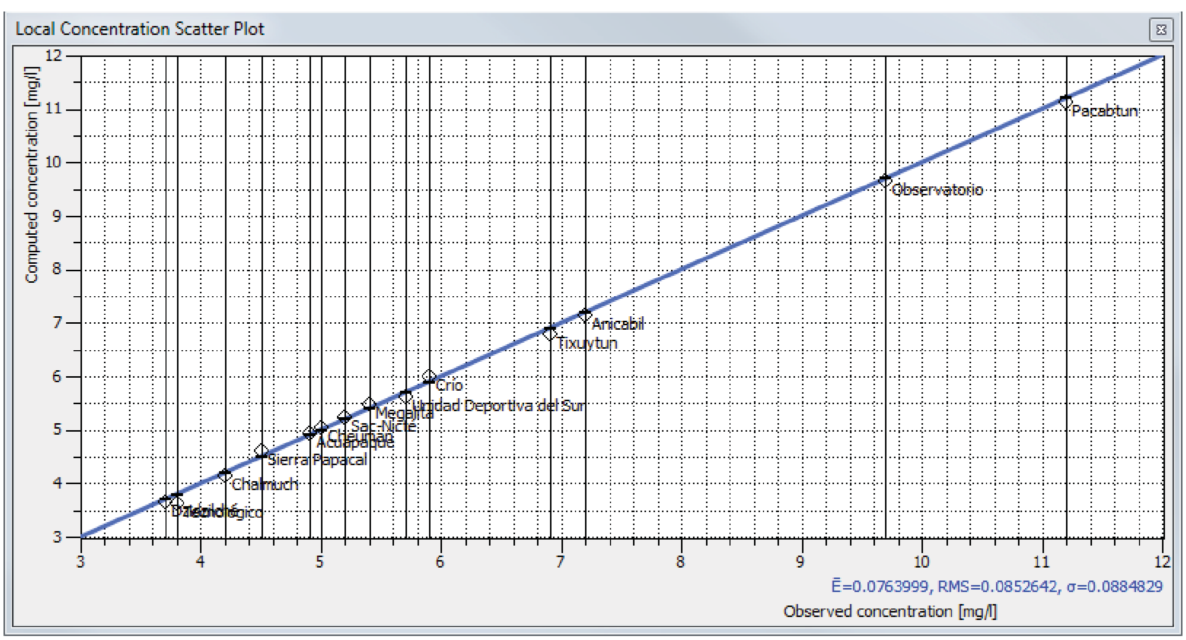


Figure 39. Transport of $N\text{-}NO_3$ calibration.

4.5. Validation

Figure 40 shows the validation graphic for groundwater flow calibration.

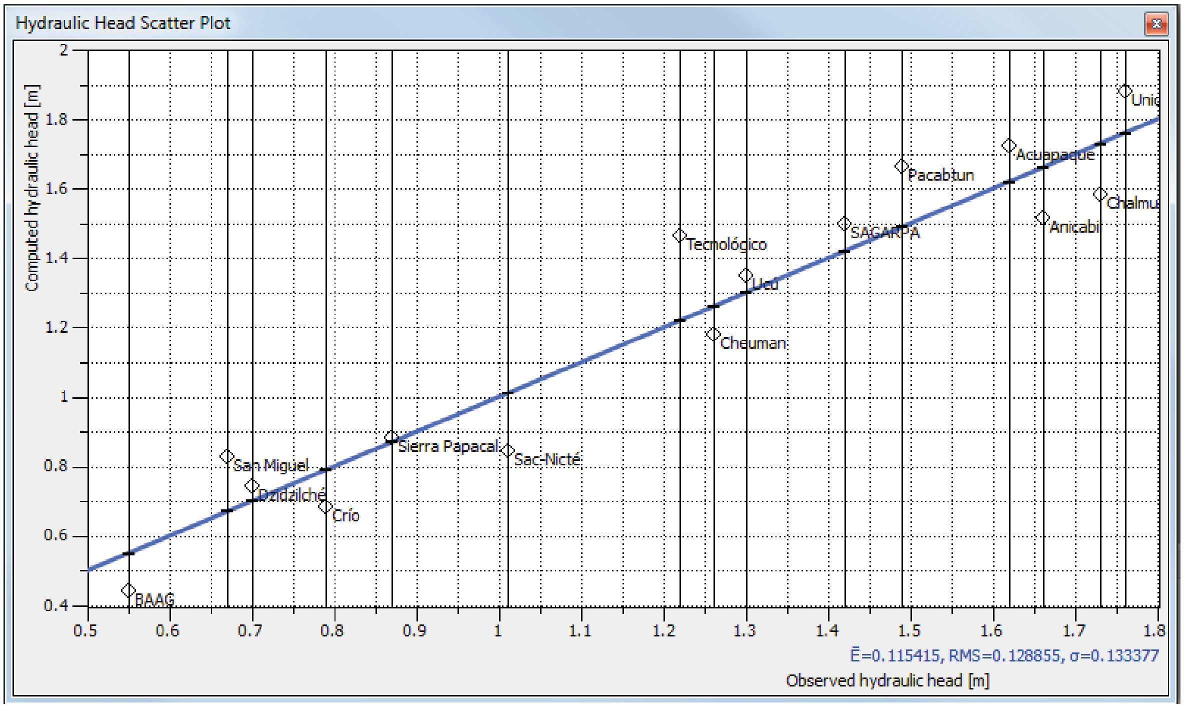


Figure 40. Validation of flow calibration.

4.6. Sensitivity analysis

Sensitivity analysis aims to describe how much model output values are affected by changes in model input values. It is the investigation of the importance of imprecision or uncertainty in model inputs in a decision-making or modelling process. The exact character of a sensitivity analysis depends upon the particular context and the questions of concern. Sensitivity studies can provide a general assessment of model precision when used to assess system performance for alternative scenarios, as well as detailed information addressing the relative significance of errors in various parameters. As a result, the sensitivity results should be of interest to the model users and developers (UNESCO 2005).

A sensitivity analysis is the process of varying the model input parameters over a reasonable range and observing the relative change in the model response (Reisinger 2013).

The first step for performing a sensitivity analysis is to identify which model input parameters should be varied. Then, the calibrated input value will be changed by some factors (Putranto 2013).

Once the groundwater model was calibrated for pumping periods between 1980-1986, 1986-1996 and 1996-2006 in transient state, different simulations were performed to determine the sensitivity of the model to measure the susceptibility of the behavior system to changes in parameters such as hydraulic conductivity, specific storage coefficient and recharge. Changes were performed independently for each of these parameters, affecting every layer particularly and all layers at the same time which represent the geological media.

The method used, consisted of modifications to the final values for each parameter of the calibration process and compare the resulting hydraulic head (with modified parameters) with respect to the calibrated values in terms of standard deviation of the differences of the calibrated and modified hydraulic heads . Hydraulic conductivities, specific storage coefficient and recharge were changed in 10%, 30% and 50% above and below of the calibrated values.

In Figure 41 and Figure 42 graphics of sensitivity analysis results are shown.

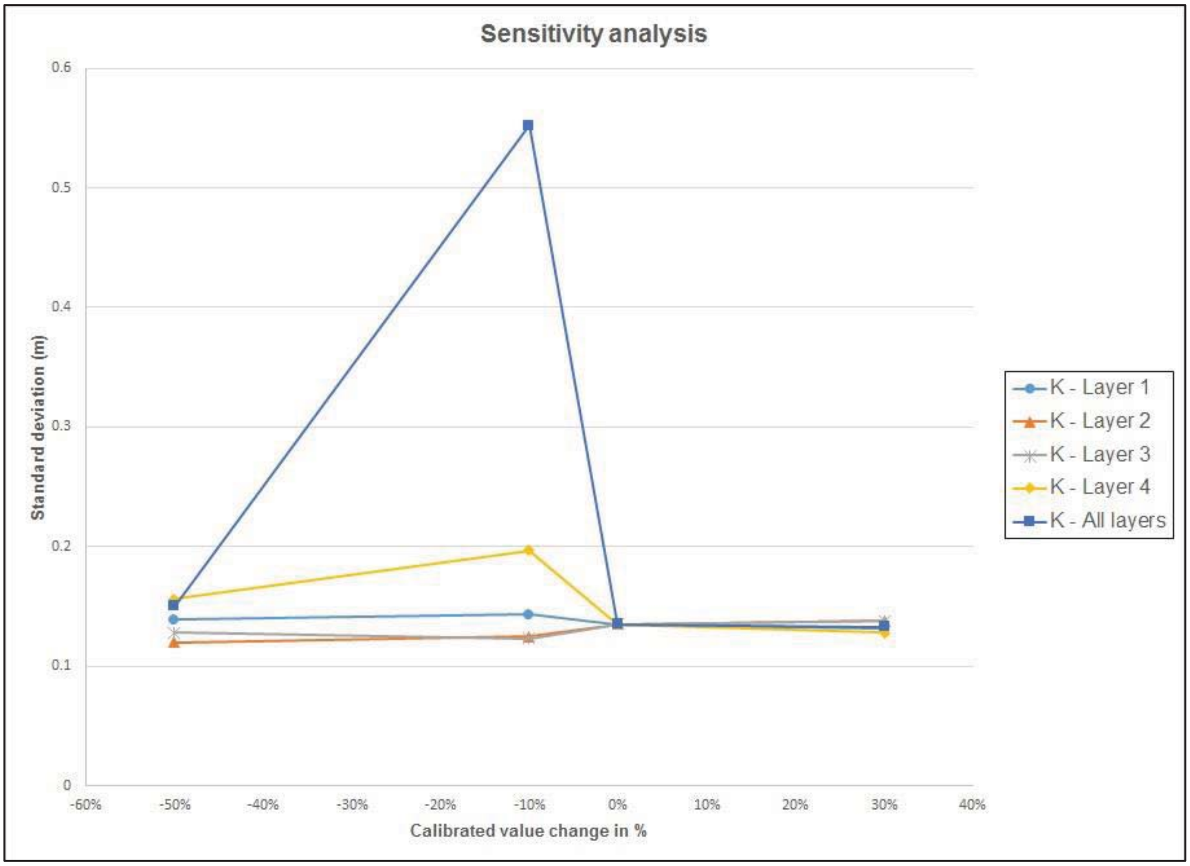


Figure 41. Sensitivity analysis from K values.

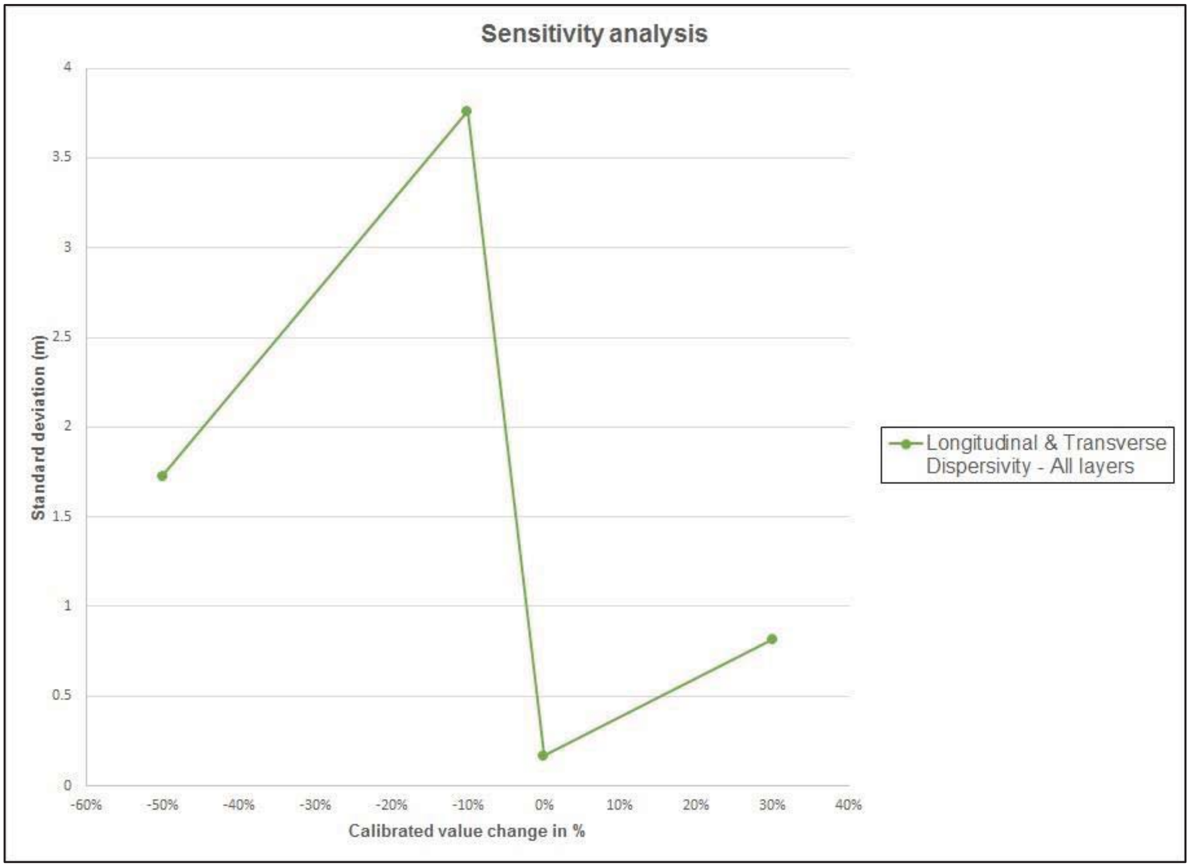


Figure 42. Sensitivity analysis for transport calibration in Longitudinal and Transversal Dispersivity.

5. Experimental phase: Future scenarios modeling (2030)

Given the sets of elements that formed the groundwater model of flow and transport of the aquifer and the calibration process, concern arises about to know the aquifer response to possible future scenarios of groundwater use.

In the course of this investigation, three future scenarios of groundwater use were developed to predict the state of the study region and the coastal area in 2030; that is, 17 years to the future taking into account that the most current available information that is the year 2013 (in addition to being the final year considered in the calibration process). 17 years it is considered, taking into account that the calibration period was 19 years (Jan 1st, 1995-Dec 31st, 2013); normally, the period used for calibration, is the maximum number of years that theoretically can be projected to the future in the simulation to obtain reliable results.

The proposed and developed scenarios were designated as follows:

- Groundwater scenario 1: Existing state (2013)
- Groundwater scenario 2: Increased groundwater extraction by the population growth.
- Groundwater scenario 3: Increased groundwater extraction by the population growth and decreased precipitation in a 50%.

5.1. Groundwater scenario 1: Existing state (2013)

The development of this scenario, consisted in predicting the groundwater conditions to 2020, maintaining the current (2013) conditions of use.

The model was run with the same groundwater recharge and extraction conditions in 2013 and until 2030 (year by year). According to the results of time series analysis of precipitation and temperature, apparently there are not implications to implement these conditions (there is not trends in the behavior of these variables, at least in the calibration period), only in the pumping scheme the limitation is that possibly would not be according to the projection of population growth by 2030 and consequently with the increase in pumping rate.

In the case of transport of N-NO_3 it remained steadily with the concentrations indicated in Figure 33.

5.2. Groundwater scenario 2: Increased groundwater extraction by the population growth

The development of this scenario, consisted in predicting the groundwater conditions to 2030 increasing pumping groundwater extraction by in proportion to population growth based on 2013 data.

The model was run with the same groundwater recharge conditions in 2013 and until 2030 (year by year). According to the results of time series analysis of precipitation and temperature, apparently there are not implications to implement these conditions (there is not trends in the behavior of these variables, at least in the calibration period), only in the pumping scheme was increased according to the projection of population growth by 2030.

In the case of transport of N-NO_3 was calculated the contribution of this by the human beings, based on the 2030 population and their wastewater contribution (induced recharge) for to obtain the concentration.

Was discarded the implementation of a future scenario with the conditions that could consider the influence of climate change, because at least in terms of precipitation and temperature there are not effects or trends of these phenomena for the analyzed period (1995-2013).

5.3. Groundwater scenario 3: Increased groundwater extraction by the population growth and decreased precipitation in a 50%.

The development of this scenario, consisted in predicting the groundwater conditions to 2030 increasing pumping groundwater extraction by in proportion to population growth based on 2013 data (same scheme of scenario 2) and a proposal of a decreased precipitation in a 50%, to observe the behavior of groundwater to a possible decrease in precipitation and transport behavior of $N\text{-}NO_3$.

6. Results and discussion

In this chapter, the results about the experimental phase are presented and analyzed.

6.1. Groundwater quantity

According to the results of the future scenarios a pumping scheme with the conditions of 2013 (scenario 1, Figure 43) will not bring changes in the hydraulic behavior of the aquifer. It can be interpreted as being influenced by meteorological phenomena and demonstrated in an analysis of time series in the last 19 years (1995-2013) there are no variations in precipitation and temperature and to a pattern of constant pumping, no drawdowns will be taken or damage systems aquifer flow. Figure 43 shows the water table configuration in 2030.

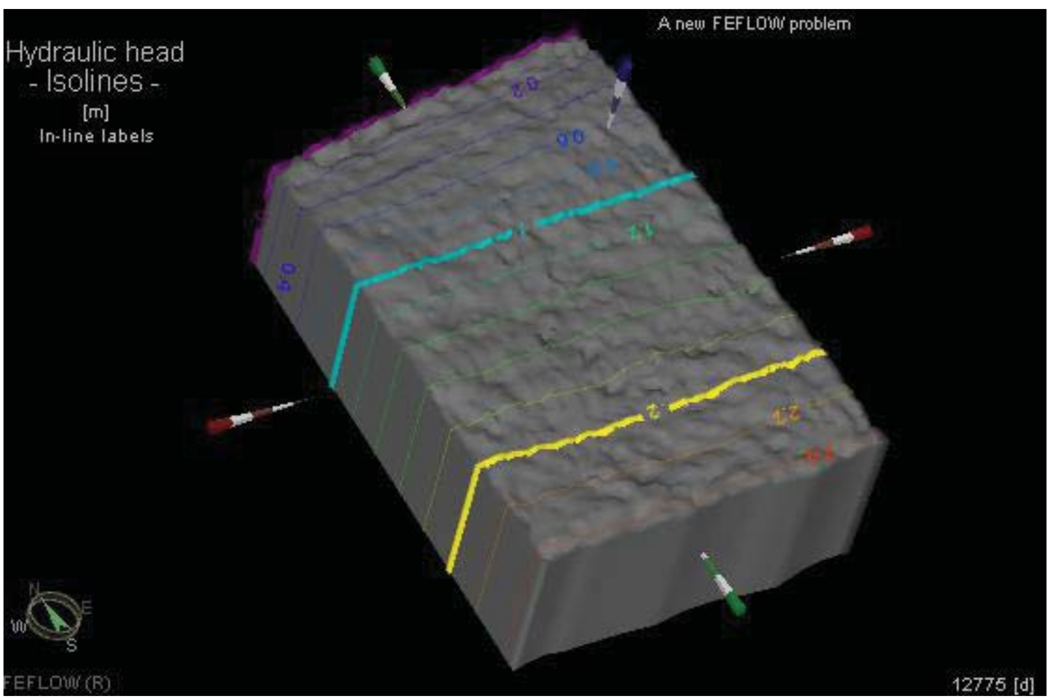


Figure 43. Hydraulic heads (m) in 2030, scenario 1.

Similarly happens with a steady increase in the pumping of 2.13% (scenario 2, Figure 44) equal to the population growth rate in the period (1995-2013). Apparently pumping with this increase has not significant influence based on the volume of precipitation that result in the vertical groundwater recharge coming from the south. Figure 44 shows the water table configuration in 2030.

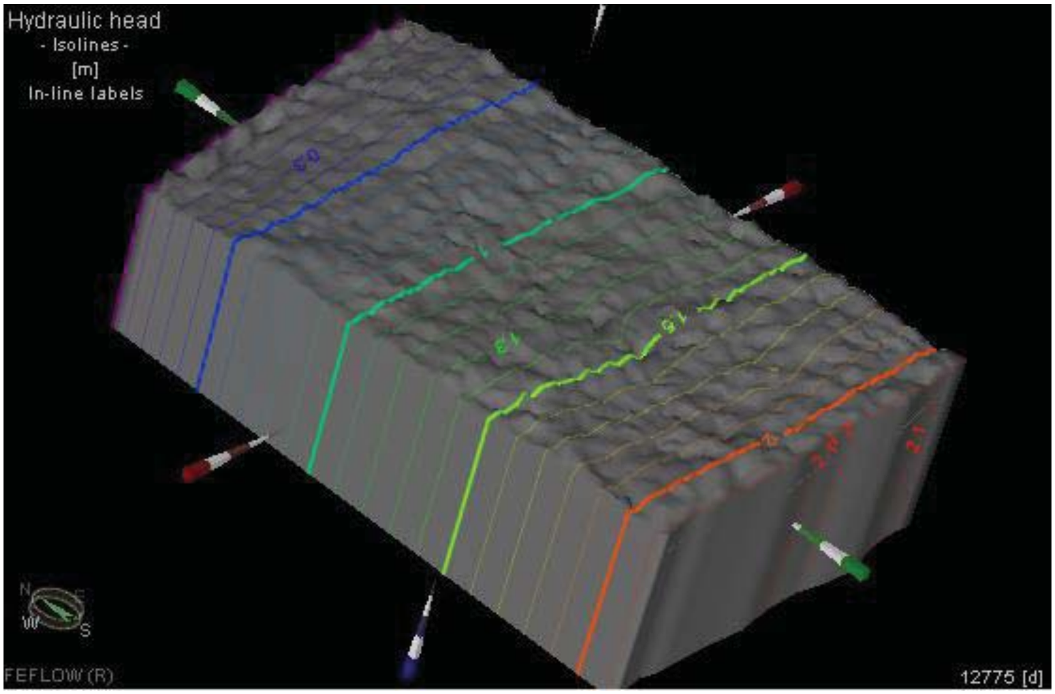


Figure 44. Hydraulic heads (m) in 2030, scenario 2.

On scenario 3 (Figure 45) significant variation occurs in the configuration of the water table; this scenario which has the same conditions of pumping scenario 2 and a reduction in rainfall by 50% of annual precipitation filed in the period (1995-2013). This allows to infer that the behavior of groundwater in the study area is highly influenced by weather events and a possible reduction or increase in precipitation would affect directly and quickly in the behavior of groundwater and consequently in the volume of exploitable water in the region. Figure 45 shows the water table configuration in 2030.

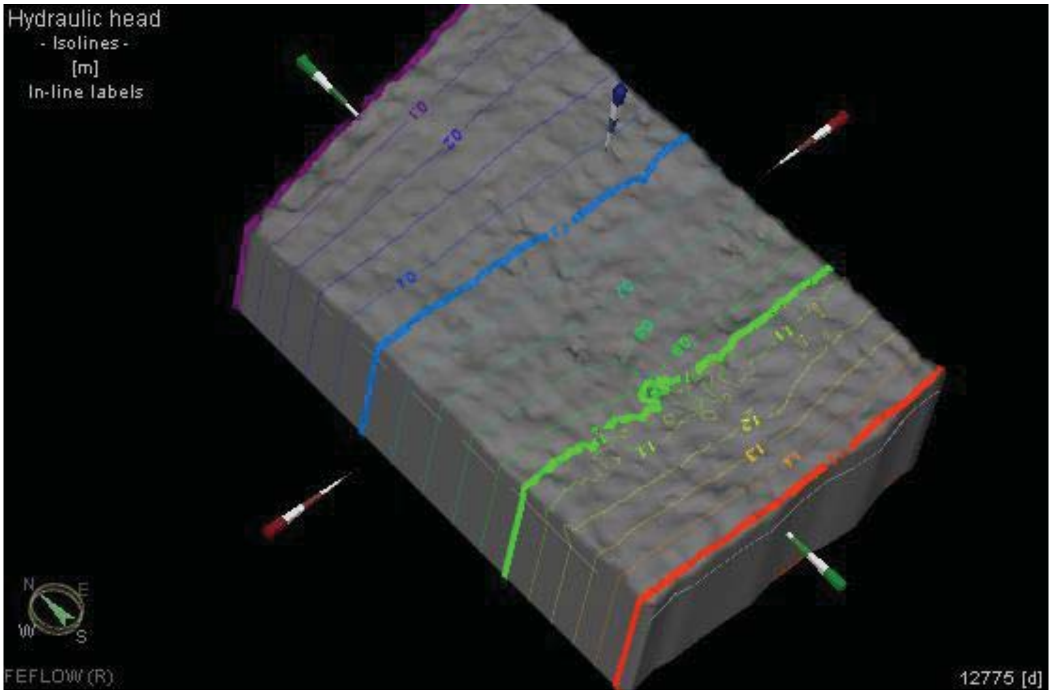


Figure 45. Hydraulic heads (m) in 2030, scenario 3.

6.2. Groundwater quality

According to the scenario 1 (Figure 46 & Figure 47), the transport of N-NO_3 support an accumulation of the solute within the study region. This is due to the combination of two factors: (i) took into account the contribution of N-NO_3 be constant throughout the period of the future projection, and (ii) is conjugated to a pumping scheme unchanging from 2013 to 2030. Displacement of N-NO_3 occurs from south to north (coastal area) reaches the mangrove area in concentrations greater than 10 $mg \cdot L^{-1}$. Also, concentrations are presented in virtually the entire thickness of the aquifer, and apparently in the future there is a possibility that the quality of freshwater in the Mérida-Progreso region will be severely affected by the accumulation of N-NO_3.

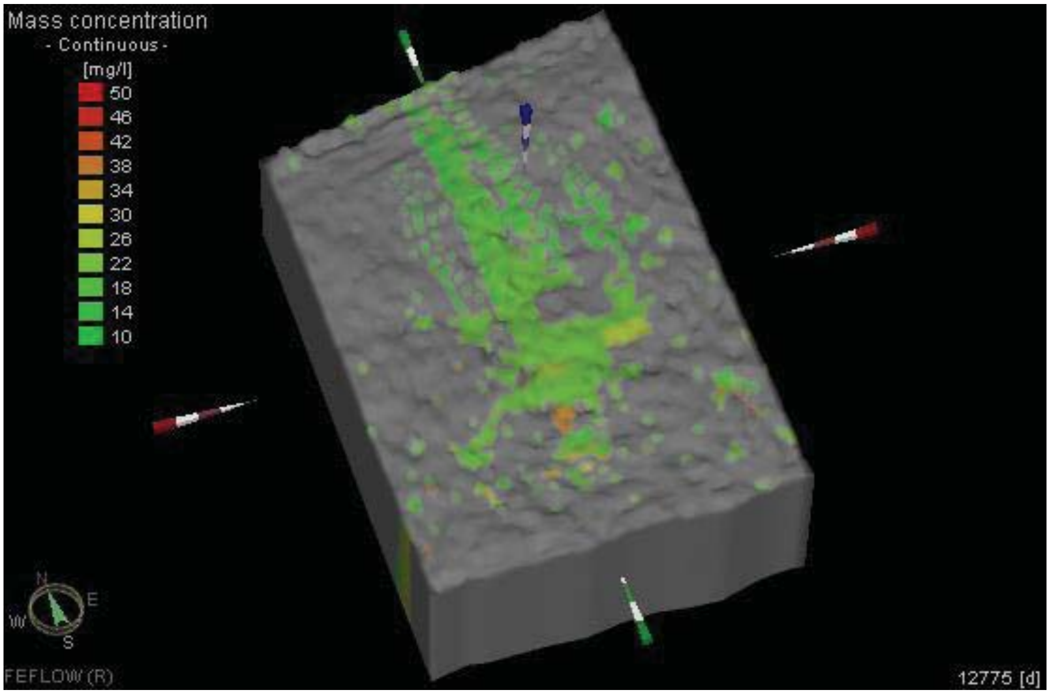


Figure 46. N-NO_3 concentrations ($mg \cdot L^{-1}$) in 2030, scenario 1.

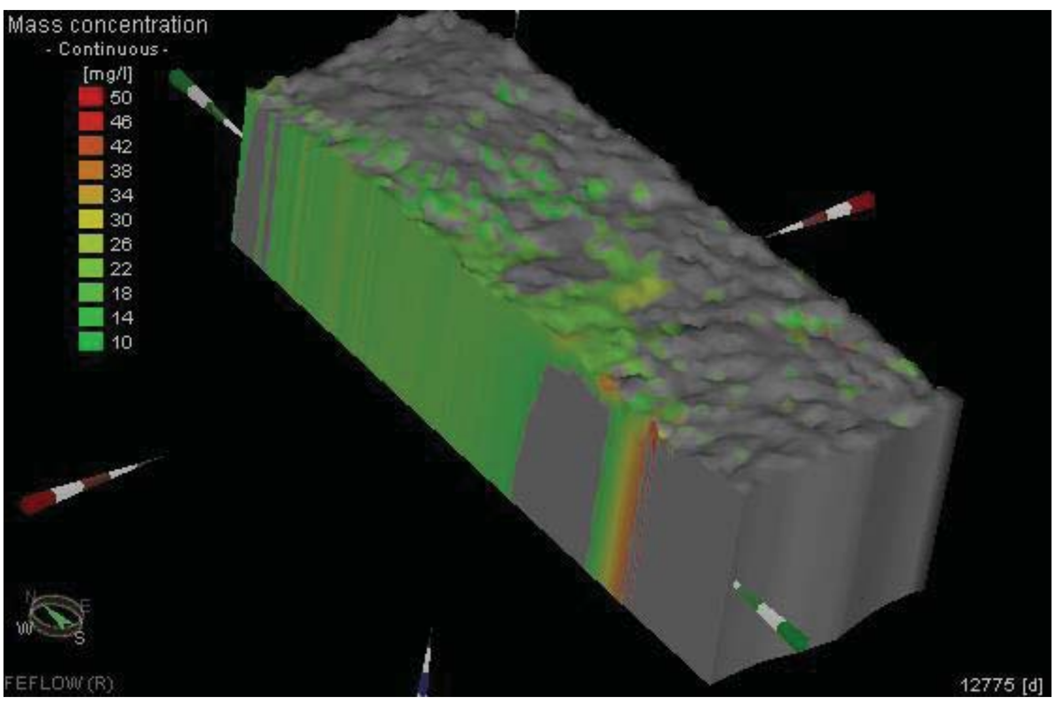


Figure 47. N-NO_3 concentrations ($mg \cdot L^{-1}$) in 2030 (N-S sectional profile), scenario 1.

In the case of scenario 2 (Figure 48 & Figure 49) remains constant the N-NO_3 contribution, however, the groundwater pumping increases annually by 2.13% (as is the population growth rate in the period 1995-2013). In this scenario less accumulation of nitrates is observed within the study region. In the first instance, it can be concluded that when comparing the two scenarios, scenario 2 presents less accumulation of N-NO_3 because the increased water extraction would also help in the removal of N-NO_3 out of the system.

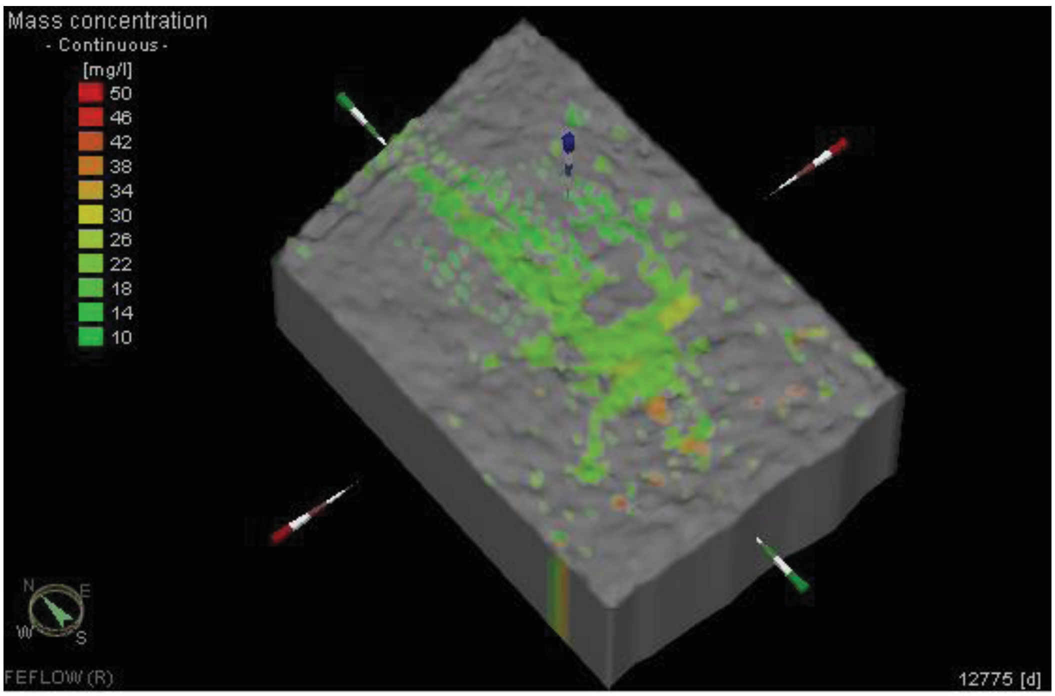


Figure 48. N-NO_3 concentrations ($mg \cdot L^{-1}$) in 2030, scenario 2.

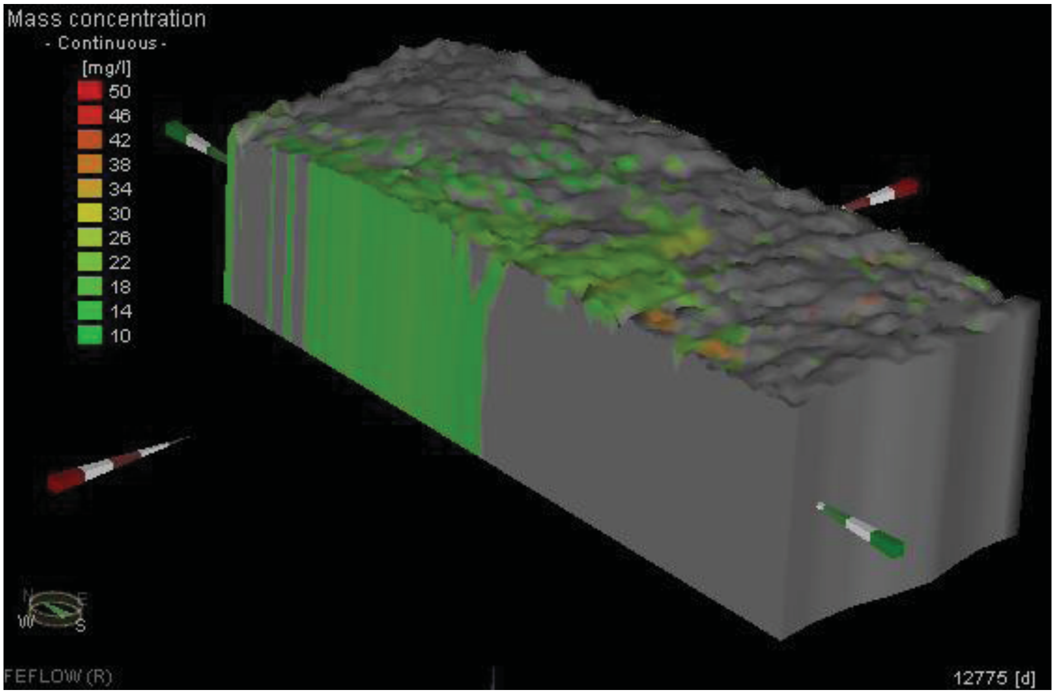


Figure 49. N-NO_3 concentrations (mg·L^{-1}) in 2030 (N-S sectional profile), scenario 2.

In scenario 3 (Figure 50 & Figure 51) less displacement of N-NO_3 occurs, this could be because the groundwater recharge by precipitation was reduced, it helps that there is not a rapid displacement of the solute to the coastal zone. It is noteworthy that a reduction of recharge from the groundwater flow was not established and the same input volumes were considered from the south, although a decrease in precipitation, would imply a reduction in recharge from the groundwater flow also. This means that the displacement of N-NO_3 would be eventually even smaller in this scenario.

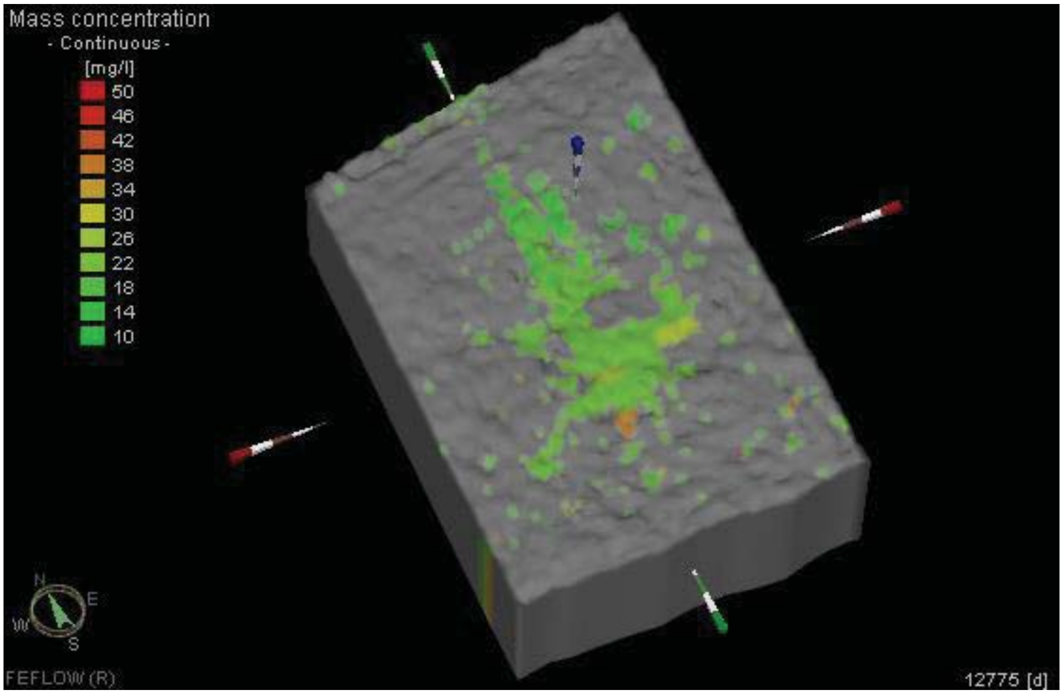


Figure 50. N-NO_3 concentrations ($mg \cdot L^{-1}$) in 2030, scenario 3.

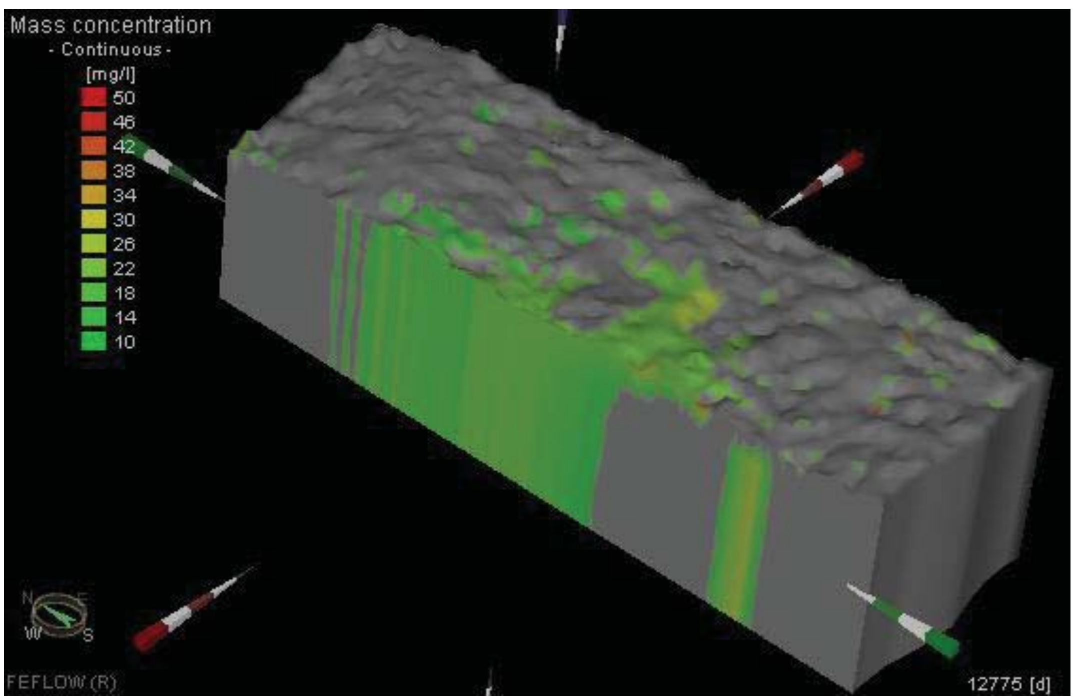


Figure 51. N-NO_3 concentrations ($mg \cdot L^{-1}$) in 2030 (N-S sectional profile), scenario 3.

The three scenarios indicate an accumulation of $N\text{-}NO_3$ greater than 10 $mg \cdot L^{-1}$ (maximum allowed by the official Mexican standard for human use) in the thickness of freshwater and its displacement to the coastal zone.

The sense-dispersed occurs in S-N and that is well explained by the advection phenomena and demonstrates how valid the hypothesis of this study

6.3. Probable effects on the coastal zone ecosystems

First, to meet the probable effects on the coastal zone ecosystems it should be studied the hydrodynamics of these areas. The arrival of $N\text{-}NO_3$ in these ecosystems can be a benefit or a problem; this is, can act as a nutrient and in the worst case, it can cause eutrophication (in its case "cultural eutrophication", Smith and Smith 2001).

Among the adverse effects presented by the phenomenon of eutrophication are: changing the characteristics of the water body, leading to a loss of quality thereof; replacement of desirable fish species, by other ones less valued; production of toxins by particular types of algae, oxygen depletion, causing mortality of dependents living in these ecosystems; increase of bacterial activity (Moreta 2008). Such effects could trigger the decline in mangrove area, which are ecosystems in which essential phenomena are developed for the life of many organisms; also function as natural barriers to weather events such as cyclones, hurricanes and severe storms.

Based on the above, a fundamental activity to be implemented in the immediate future would be to make a wastewater treatment prior to being deposited back into the aquifer.

Conclusions and recommendations. Initial strategies for sustainable management of groundwater

The study process included four important phases: (1) data collection, (2) implementation and (3) calibration of the numerical model of the aquifer and development of future scenarios and (4) analysis of implications of groundwater use in the coastal area.

Information gathering was a hard work due to limited uniformity of information previously generated; this data were tried to sort and deliver more smoothly herein.

Calibration of the numerical model was one of the most challenging and demanding activities, but it was very useful as it was possible to draw conclusions of great importance.

Establish a management program is complicated when previously it is necessary to implement a series of activities to improve the characterization and therefore the knowledge of the behavior of groundwater in the region. Therefore, the following proposals are made for the benefit of improving the quality of the information in the study region. The following strategies that emerged based on the problems faced during the fieldwork of the project:

It is important to improve the quality of information generated, have greater continuity and establish periodic programs for obtaining field data.

Generate information regarding the whole aquifer and in major depths, because in the analyzed studies, it was observed that each year, often study certain areas, which sometimes are usually very small and does not represent the behavior of flow systems in the aquifer.

Increased pumping tests, including that will be applied in a more distributed way, to define in detail the hydraulic parameters throughout the aquifer. So it is necessary to pump tests are carried out in observation wells.

Install flowmeters to define in greater detail the flow of extraction wells and, with this, update and refine the census data about extractions.

Generate better quality information about climatic variables like precipitation, temperature and evapotranspiration to understand with greater certainty the phenomena about water movement.

Establishing an optimal groundwater monitoring network to achieve periodic measurements at different times of the year and to achieve a better understanding of the behavior of the fluctuations in groundwater in terms of quantity and quality.

Collect all data (hydrological, hydrogeological, geological and meteorological) in a GIS that allows easy management of all information aquifer.

In general, the proposed strategies are aimed at a wider generation of meteorological, hydrological and hydrogeological information, so that it can be manipulated reliably in a "desk" and can be easily manipulated for implementation in the numerical model.

The development of future strategies for the sustainable use of water of the Mérida-Progreso region cannot be conceived without full knowledge of the factors affecting the operation and without the active participation of users and water management authorities.

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Appendix

Note: See electronic files

Appendix 1. Water balance calculations.

Appendix 2. Rocha, H., Cardona, A., Graniel, E., Alfaro, C., Castro, J., Rüde, T., Herrera, E., Heise, L. (2015). Fresh-brackish water interfaces in the Mérida-Progreso region Yucatán (in Spanish). Tecnología y Ciencias del Agua, 6(6), 89-112.

Appendix 3. Complete census of pumping wells.

Appendix 4. Census of pumping wells by type of water use.

Appendix 5. Time series analysis of meteorological data.

Appendix 6. Groundwater numerical model files.

Appendix 7. Geodatabase data.