Multi-dimensional flow and transport modeling of a surface water body in a semi-arid area: the case of the Icó-Mandantes Bay, Northeast Brazil

vorgelegt von

Elena Matta, M. Sc.

geb. in Turin, Italien

von der Fakultät VI – Planen Bauen Umwelt

der Technischen Universität Berlin

zur Erlangung des akademischen Grades

Doktor der Ingenieurwissenschaften

Dr.-Ing.

genehmigte Dissertation

Promotionsausschuss:

Vorsitzender: Prof. Dr. Johann Köppel

Gutachter: Prof. Dr.-Ing. Reinhard Hinkelmann

Gutachter: Priv.-Doz. Dr. rer. nat. Günter Gunkel

Gutachter: Prof. Dr. rer. nat. Gunnar Nützmann

Gutachter: Prof. Dr.-Ing. Michele La Rocca

Tag der wissenschaftlichen Aussprache: 5. Januar 2018

Berlin 2018

To You, my Master, my Savior

Acknowledgments

This doctoral thesis is the fruit of my efforts as a PhD student at Technische Universität Berlin since the year 2014.

First, I would like to express most sincere gratitude to my supervisor Prof. Reinhard (Phillip) Hinkelmann, for his continuous guidance and support. Professors like you are incredibly rare to find. Thank you for the trust and the great opportunities that you have given to me in the last years, for all what I have learned and experienced, at this Chair and around the world.

Sincere gratitude is expressed as well to my other supervisors, part of the thesis committee: P.D. Günter Gunkel, for his great expertise concerning the 'water quality issues' and his constant availability; to Prof. Gunnar Nützmann, Prof. Michele La Rocca and Prof. Johann Köppel, for their constructive critics and useful advices.

I gratefully acknowledge the German Federal Ministry of Education and Research (BMBF) for supporting the biggest part of this work, as part of the INNOVATE project.

My gratitude goes to Dr. Ilhan Özgen, for being my office-mate, colleague and friend; to Mr. Ralf Duda, for your incomparable technical support and great humanity; still, to Dr. Florian Selge and Dr. Hagen Koch, for the nice collaboration and your scientific support.

To Giacomo, who hold my hand almost until the end of this path, always believing in me, I am truly thankful. It is also because of you that I have arrived until here.

Dearest gratitude is also expressed to Anastasia, who the angels sent to me in a particularly hard time of my life and, when I thought to find a flatmate, I got a friend instead.

In conclusion, I would like to thank all my friends, the life-time and the new ones met around the world. I cannot name you all, but each of you know what you mean to me.

Last but not least, to my wonderful family. You have surrounded me with so much love that nobody would ever be able to match. The extreme efforts and the hard times that I have been gone through in these years could have never been overcome without you. You are the most amazing gift of God to me and I thank you from the deepest of my heart for being with me, since always.

Thanks to You, my Lord. NOTHING would have ever been possible without You.

Berlin, 27 Sept. 2017

Publications of cumulative doctoral thesis

Journal papers

1. Matta, E.; Selge, F.; Gunkel, G.; Rossiter, K.; Jourieh, A.; Hinkelmann, R. Simulations of nutrient emissions from a net cage aquaculture system in a Brazilian bay. *Water Sci. Technol.* **2016**, 73(10), 2430–2435, with permission from the copyright holders, ©IWA Publishing; doi:10.2166/wst.2016.092. Postprint.
2. Matta, E.; Koch, H.; Selge, F.; Simshäuser, M. N.; Rossiter, K.; Nogueira da Silva, G. M.; Gunkel, G.; Hinkelmann, R. Modeling the impacts of climate extremes and multiple water uses to support water management in the Icó-Mandantes Bay, Northeast Brazil. *J. Water Clim. Chang.* **2017**, *under review.*
3. Matta, E.; Selge, F.; Gunkel, G.; Hinkelmann, R. Three-dimensional modeling of wind- and temperature-induced flows in the Icó-Mandantes Bay, Itaparica Reservoir, NE Brazil. *Water (Switzerland)* **2017**, 9(10), 772; doi:10.3390/w9100772. Postprint.

Supplementary contributions

Journal papers

1. Gunkel, G.; Matta, E.; Selge, F.; Silva, G. M. N. da; Sobral, M. do C. Carrying capacity limits of net cage aquaculture in Brazilian reservoirs. *Rev. Bras. Ciências Ambient.* **2015**, 128–144, doi:10.5327/Z2176-947820151008.
2. Rossiter, K. W. L.; Morais, M. M.; Calado, S. C. S.; Benachour, M.; Matta, E. Diagnóstico da Qualidade da Água ao longo de um Canal de concreto: Um estudo de caso do Canal do Sertão Alagoano. *Rev. Bras. Ciencias Ambient.* **2015**, 157–167, doi:10.5327/Z2176-947820151010.
3. Selge, F.; Matta, E.; Hinkelmann, R.; Gunkel, G. Nutrient load concept-reservoir vs. bay impacts: A case study from a semi-arid watershed. *Water Sci. Technol.* **2016**, *74*, 1671–1679, doi:10.2166/wst.2016.342.
4. Gunkel, G., Selge, F., Keitel, J., Lima, D., Calado, S., Sobral, M., Rodriguez, M., Matta, E., Hinkelmann, R., Casper, P., Hupfer, M. Impacts of water management on aquatic ecosystem services of a tropical reservoir (Itaparica, São Francisco, Brazil) and development of advanced reservoir management tools. *Reg. Environ. Chang.* **2018**, doi:10.1007/s10113-018-1324-8.
5. Hattermann, F. F.; Koch, H.; Liersch, S.; Silva, A. L.; Azevedo, R.; Selge, F.; Silva, G. N. S.; Matta, E.; Hinkelmann, R.; Fischer, P.; Venohr, M. Climate and land use change impacts on the water-energy-food nexus in the semi-arid northeast of Brazil – scenario analysis and adaptation options. *Reg. Environ. Chang.* 2017, *subm.*
6. Rodriguez, M.; Koch, H.; Hartje, V; Matta, E.; Casper, P. How water level fluctuation impacts greenhouse gas emissions from a tropical semi-arid hydropower reservoir: Economical evaluation and management implications, *subm*.

Conference papers

1. Broecker, T.; Özgen, I.; Matta, E.; Cabral, J.; Candeias, A. L.; Hinkelmann, R. Simulation of Flow and Transport Processes in a Brazilian Reservoir. In *International Conference on Hydroscience & Engineering (ICHE)*; Lehfeldt, R. & Kopmann, R. (eds), Ed.; Bundesanstalt für Wasserbau ISBN 978-3-939230-32-8: Hamburg, Germany, 2014.
2. Matta, E.; Özgen, I.; Cabral, J.; Candeias, A. L.; Hinkelmann, R. Simulation of Wind-induced Flow and Transport in a Brazilian bay. In *International Conference on Hydroscience & Engineering (ICHE)*; Lehfeldt, R. & Kopmann, R. (eds), Ed.; Bundesanstalt für Wasserbau ISBN 978-3-939230-32-8: Hamburg, Germany, 2014.
3. Matta, E.; Selge, F.; Gunkel, G.; Rossiter, K.; Jourieh, A.; Hinkelmann, R. Quantification of exchange processes between a bay and a river using a two-dimensional high-resolution transport model. In *IWA-DIPCON Conference*: Berlin, Germany, 2015.

4. Matta, E.; Simshäuser, M. N.; Koch, H.; Selge, F.; Gunkel, G.; Rossiter, K.; Hinkelmann, R. Modeling the interaction of multiple uses, climate and land-use changes in a bay of Itaparica reservoir, São Francisco river. In *Proceedings XXI SBRH Conference*: Brasilia, Brazil, 2015.
5. Gunkel, G.; Selge, F.; Keitel, J.; Lima, D.; Calado, S.; Sobral, M.; Rodriguez, M.; Matta, E.; Hinkelmann, R.; Casper, P.; Hupfer, M. The Itaparica reservoir – Aquatic ecosystem functions: Impact, vulnerability and development of an adapted management. In *BMBF Final Conference – Sustainable Land Management: Challenges and Opportunities*: Berlin, Germany, 2016.
6. Hattermann, F.; Koch, H.; Liersch, S.; Silva, A. L.; Azevedo, J. R.; Selge, F.; Silva, G. N. S.; Matta, E.; Hinkelmann, R.; Fischer, P.; Venohr, M. Climate and land use change impacts on the water-energy-food nexus in the arid northeast of Brazil – scenario analysis and adaptation options. In *BMBF Final Conference – Sustainable Land Management: Challenges and Opportunities*: Berlin, Germany, 2016.
7. Matta, E.; Silva, G. M. N.; Lorenz, R.; Gunkel, G.; Hinkelmann, R. Estimation of water residence time in Icò-Mandantes bay using the TELEMAC-2D modeling system. In *I SBHSF Conference*: Juazeiro, Brazil, 2016.
8. Silva, G. M. N.; Matta, E.; Gunkel, G.; Hinkelmann, R.; Severi, W.; Sobral, M. C. Modelling nutrient emissions from a net-cage aquaculture system in Northeastern Brazil. In *IWA DIPCON Conference*: Dublin, Ireland, 2016.
9. Matta, E.; Selge, F.; Gunkel, G.; Hinkelmann, R. 3D wind effects on hydrodynamics and transport in a Brazilian bay. In *37th IAHR World Congress*: Kuala Lumpur, Malaysia, 2017.

Policy paper

Berger, V., Fan, F., Gabel, F., Galvão, P., Gies, M., Grabner, D., Langhans, S., Machado, A., Manzione, R., Matta, E., Andreu, A., de Moraes, M., Morihama, A., Macedo-Moura, P., de Paiva, A., Periotto, N., Porst, G., Rigotto, C., Roters, B., Schulz, S., S, C. *How Do We Want to Live Tomorrow? Perspectives on Water Management in Urban Regions*; German National Academy of Sciences Leopoldina, Brazilian Academy of Sciences, Centre for Water and Environmental Research at the University of Duisburg-Essen (Publishers); Halle/Saale, Rio de Janeiro, Essen, 2017.

Abstract

Since approximately 2012, Northeast Brazil dramatically suffers from the harshest drought in the recent history, with serious consequences on water resources, anthropogenic uses and ecosystem services. Among else, the hydropower production, irrigation agriculture, water supply and net cage aquaculture are the principal uses adopted in the Itaparica Reservoir, located in the Sub-Middle São Francisco River. Due to the often uncontrolled water withdrawals, the climate and land use change effects, the water quantity and quality in the reservoir has deteriorated, leading to socio-economic and environmental problems. E.g., phenomena such as harmful algae blooms (HAB) in the lentic areas are attributed to the high fluctuations of the water levels in the reservoir (up to maximum 5 m per year), due to hydropower production. Moreover, the newly built and highly argued water diversion project will withdraw water from Itaparica via two channels, the eastern one located in one of the major branches of the reservoir: the Icó-Mandantes Bay, focus of this study.

Two (depth-averaged) and three-dimensional hydrodynamic and transport models have been implemented using the open TELEMAC-MASCARET modeling system (2D, 3D). The aim was to provide a pioneer tool for the region, capable to simulate different (combined) climate-, issues- and stakeholders-oriented scenarios and, thus, to support water management and decision-making. In this work: (1) high-resolution unstructured grids for low and high water levels (respectively LWL and HWL) have been set up, to assess their impact on hydraulics, tracer transport and exchange processes between the bay and the reservoir main stream; (2) an alternative approach was implemented to estimate the water residence times of the bay's complex system; (3) nutrient emissions (e.g. phosphorus) from a net cage aquaculture system were investigated on half-year cycles; moreover, (4) the impacts on the flow field of the eastern channel of the water diversion; (5) the effects of a flash flood combined with tracer transport from an intermittent tributary and finally (6) the 3D effects induced by moderate or extreme winds as well as by heating of the water surface have been assessed.

The findings showed that (1) the dynamics of the bay and the reservoir main stream followed different velocity regimes (at least one order of magnitude higher for the latter, i.e. range of 10^{-2} to 10^{-1} m/s for reference conditions); (2) the bay's water residence times were estimated to be higher than six months (about two months for the reservoir), higher for HWL and high discharges, compared to LWL and low discharges; (3) a relevant increase of phosphorus due to a

small fish production of 130 t/y was observed, higher for LWL on the short term and for HWL on the long term; (4) the eastern diversion channel did not influence significantly the hydrodynamics of the bay; although, it is important to monitor constantly water quality parameters, especially during rainy periods after prolonged droughts; (5) during such events, the nutrient inputs from the tributary and the nearby drainage systems overflows will affect the water withdrawals (irrigation, water supply); (6) a windstorm increased the flow velocities (at least one order of magnitude, i.e. up to 10^{-1} m/s) without altering significantly the flow circulation patterns; this occurred substantially for the heating scenario, which had in contrast a lower effect on velocities.

The main implications for water management derived from the findings summarized above are outlined hereafter. (1) It is not advisable to increase the discharges and the water levels in the reservoir to stimulate water exchange processes, because it could and increase the risk of development of HAB; (2) given to the low exchange rates between the reservoir main stream and the bay, it is suggested not to install an aquaculture system inside the bay or at least to ensure sufficient water depth beneath the cages, in order to allow translocation and dilution of organic material and avoid an extreme increase of sediments; (3) the withdrawals for drinking water and irrigation agriculture should stop working during flash floods from the intermittent tributaries, as well as during windstorms, and at least three days afterwards; (4) monitoring the water quality in the eastern diversion channel is of vital importance, due to the low water depth and the high evaporation rates; (5) a heating of the water surface would likely increase the risk of development of HAB in the shallow areas, so that further assessments with a water quality module are needed to support advanced remediation measures; (6) the 3D model proves to be a necessary tool to identify high risk contamination areas, e.g. for installation of new aquaculture systems, capable of additionally taking into account wind and heating effects. In conclusion, the complex water system investigated urges of adaptive and differentiated measures to the continuously changing natural conditions and anthropogenic impacts. An efficient communication and collaboration is needed between the water users, managers and researchers, e.g. to discuss the feasibility of the proposed operation measures, such as the inversion of the water flow withdrawn by the eastern diversion channel, in the case of alarming nutrient overloads and high amount of algae in the shallow stagnant areas.

In future work, the existent models should be coupled with a water quality module to address some of the still open research questions, such as focusing on (1) the risk of HAB development, mainly on their inoculation in the lentic bay areas and their interaction with the reservoir main stream, (2) the impact of HAB on the withdrawals for drinking water or irrigation agriculture and (3) the adaptation of hydroelectric production to reduce water level fluctuations, in order to minimize the introduction of nutrients from the desiccated soils in the shallow areas and, thus, the greenhouse gases (GHG) emissions as well. Moreover, external forces such as wind, heating and cooling processes should be always included in the modelling, since they influence indeed the hydraulics of water bodies such as the Icó-Mandantes Bay.

Zusammenfassung

Seit dem Jahr 2012 leidet Nordostbrasilien an der härtesten Dürre seiner jüngsten Geschichte, mit schwerwiegenden Folgen für Wasserressourcen, anthropogene Nutzungen und Ökosystemdienstleistungen. Wasserkraftproduktion, Bewässerungslandwirtschaft, Wasserversorgung und Aquakulturen sind die wichtigsten Nutzungen des Wassers im Itaparica-Stausee (Mittellauf des São Francisco Flusses). Aufgrund von oft unkontrollierten Wasserentnahmen und Auswirkungen von Klima- und Landnutzungsänderungen haben sich die Wassermenge und die Wasserqualität im Stausee verschlechtert, was zu einer Belastung der sozioökonomischen Entwicklung und Umweltproblemen geführt hat. So kann beispielsweise das Auftreten schädlicher Algenblüten in stehenden flachen Wasserbereichen auf die hohen Schwankungen der Wasserstände im Stausee (bis zu maximal 5 m pro Jahr) aufgrund der Wasserkraftproduktion zurückgeführt werden. Darüber hinaus finden im Rahmen des häufig kritisierten Wasserumleitungsprojektes Wasserentnahmen an zwei Stellen im Itaparica-Stausee statt, wobei sich eine dieser Entnahmestellen in einem der wichtigsten Zweige des Stausees, der Icó-Mandantes-Bucht befindet, welche Schwerpunkt dieser Arbeit ist.

Mit dem Open-Source-TELEMAC-MASCARET Modellierungssystem wurden zwei- (tiefengemittelte) und dreidimensionale Berechnungen zu Hydrodynamik und Transport durchgeführt. Ziel war es, erstmalig ein Werkzeug für die Region bereitzustellen, das in der Lage ist, verschiedene Szenarien zu simulieren, um Fragestellungen zu Klimaänderungen und Stakeholder-Interessen zu untersuchen, um damit das Wassermanagement und die Entscheidungsfindung zu unterstützen. In dieser Arbeit wurden (1) hochauflösende unstrukturierte Gitternetze für niedrige und hohe Wasserstände (LWL und HWL) erstellt, um ihre Auswirkungen auf die Hydraulik, den Stofftransport und Austauschprozesse zwischen der Bucht und dem Hauptstrom des Stausees zu beurteilen; (2) ein alternativer Ansatz zur Abschätzung der Aufenthaltszeit des Wassers in der komplexen Icó-Mandantes-Bucht entwickelt; (3) Nährstoffemissionen (z.B. Phosphor) aus einem Aquakultur-System untersucht; (4) die Auswirkungen des östlichen Kanals der Wasserumleitung auf das Strömungsfeld in der Bucht abgeschätzt; (5) die Auswirkungen einer Sturzflut zusammen mit Stofftransport aus einem Nebenfluss untersucht und schließlich (6) 3D Strömungseffekte abgeschätzt, die durch mäßige und extreme Winde sowie durch die Erwärmung der Wasseroberfläche hervorgerufen werden.

Die Ergebnisse zeigen, (1) dass die Dynamik der Bucht und des Stausee-Hauptstroms unterschiedlichen Fließgeschwindigkeitsbereiche aufweisen (mindestens eine Größenordnung höher im Hauptstrom im Bereich von 10^{-2} bis 10^{-1} m/s für Referenzbedingungen); (2) dass die Aufenthaltszeiten des Wassers in der Bucht mehr als sechs Monate betragen (etwa zwei Monate für den Stausee), höher für HWL im Vergleich zu LWL; (3) dass die Phosphorkonzentrationen aufgrund einer kleinen Aquakultur beträchtlich zunehmen, mehr für LWL auf kurze Sicht und für HWL auf lange Sicht; (4) dass der östliche Umleitungskanal die Hydrodynamik der Bucht nicht wesentlich

beeinflusst; trotzdem ist es insbesondere während der Regenzeit nach längeren Dürren sehr wichtig, Wasserqualitätsparameter in diesem Kanal ständig zu überwachen; (5) dass während Sturzflutereignissen die Wasserentnahmen (Bewässerung, Wasserversorgung) durch Nährstoffeinträge aus dem Nebenfluss und nahe gelegenen Entwässerungssystemen beeinträchtigt werden; (6) und dass ein Sturm die Strömungsgeschwindigkeiten erhöht (mindestens um eine Größenordnung, d.h. bis zu 10^{-1} m/s), ohne die Muster der Strömungszirkulation maßgeblich zu verändern; dies trat in großem Maße für das Erwärmungsszenario auf, welches aber eine geringere Auswirkung auf die Geschwindigkeitsgrößen hatte.

Die wichtigsten daraus resultierenden Schlussfolgerungen für das Wassermanagement werden nachfolgend zusammengefasst: (1) Es wird nicht empfohlen, die Zuflüsse und die Wasserstände im Stausee zu erhöhen, um Wasseraustauschprozesse zu stimulieren, weil es kontraproduktiv sein und das Risiko der Entwicklung von schädlichen Algenblüten erhöhen kann. (2) Es wird vorgeschlagen, keine Aquakulturen innerhalb der Bucht zu betreiben oder zumindest eine ausreichende Wassertiefe unterhalb der Systeme vorzusehen, um eine Verlagerung und Verdünnung des organischen Materials zu ermöglichen und eine extreme Zunahme von Sedimenten zu vermeiden. (3) Die Entnahmen für Trink- und Bewässerungswasser sollten während Sturzflutereignissen der Nebenflüsse sowie bei Windstürmen mindestens drei Tage ausgesetzt werden. (4) Die Überwachung der Wasserqualität im östlichen Umleitungskanal ist aufgrund der geringen Wassertiefe und der hohen Verdunstungsrate von entscheidender Bedeutung. (5) Eine Erwärmung der Wasseroberfläche wird voraussichtlich das Risiko der Entwicklung von schädlichen Algenblüten in den flachen Gebieten erhöhen, so dass weitere Untersuchungen mit einem Wasserqualitätsmodell anzustreben sind, um weitergehende Sanierungsmaßnahmen abzuleiten. (6) Das 3D-Modell sollte zur genaueren Abschätzung von Kontaminationsbereichen eingesetzt werden, z.B. für die Installation von neuen Aquakultur-Systemen, da Wind- und Wärmewirkungen berücksichtigt werden. Abschließend wird festgestellt, dass das komplexe Wassersystem Icó-Mandantes-Bucht differenzierte und anpassungsfähige Maßnahmen erfordert, die sich an die ständig verändernden natürlichen Bedingungen und anthropogenen Einflüsse anpassen. Es ist eine effiziente Kommunikation und Zusammenarbeit zwischen Wassernutzern, Managern und Wissenschaftlern erforderlich, um die Machbarkeit der vorgeschlagenen Maßnahmen zu überprüfen, wie beispielsweise die Rückleitung der Wasserentnahme im östlichen Umleitungskanal im Fall von zu starken Nährstoffbelastungen und Algenblüten in Bereichen der Icó-Mandantes-Bucht.

In Zukunft sollten die vorhandenen Modelle mit einem Wasserqualitätsmodul gekoppelt werden, um einige der noch offenen Fragestellungen zu untersuchen, wie (1) die Entwicklung von schädlichen Algenblüten, vor allem in den flachen Bereichen mit fast stehendem Wasser und deren Interaktionen mit dem Hauptstrom des Stausees, (2) die Auswirkungen von schädlichen Algenblüten auf Entnahmen für Trink- oder Bewässerungswasser und (3) die Anpassung der Wasserkraft zur Reduzierung von Wasserstandsschwankungen, um das Auswaschen von Nährstoffen aus ausgetrockneten Böden in Uferzonen und damit auch Treibhausgasemissionen zu minimieren. Darüber hinaus sollten antreibende Größen wie Wind und Temperatur bei der Modellierung berücksichtigt werden, da sie die Hydraulik der Icó-Mandantes-Bucht nachgewiesenermaßen beeinflussen.

Contents

Chapter 1

1. Introduction

This chapter addresses some of the actual challenges in reservoirs management in semi-arid areas, it presents the research project, to which this specific work belongs, the study area and the related aspects; finally, it shows some of the modeling systems available, as well as provides the structure of the entire document.

1.1 General

In the last years, the dramatically increasing number of scientific reports assessing the consequences of climate change on water resources is crying out not only for the attention of institutions and researchers, but for a worldwide awareness-raising. Scientists together with decision makers are called to identify the actual challenges and their impacts, finding adaptive measures to the changes. Among global warming and sea level rise, many dry regions are expected to become drier, wet regions wetter. Moreover, it is very likely that many countries already facing water shortages today will suffer from increased water stress and that major investments in water management infrastructure will be needed (e.g. [1]). This is the case of Northeast Brazil (NE), where high rainfall variability, land degradation, and desertification are some of the factors that lead this region to be defined as one of the most vulnerable to climate change in the entire world [2,3]. Brazil is one of the countries owning the highest amount of water resources (approx. 5,418 km^3 of annual surface waters, according to [4]; although, about 73% of the fresh water available is located in the Amazon Basin, where less than 5% of the population lives [5]. Moreover, the Brazilian semi-arid region is the world's most densely populous dry land region [6]. This, combined with the rainfall deficit and increased aridity foreseen for the next century, does not lead to the most daring expectations for the future and generates increasing concerns among water managers, researchers, farmers, development specialists and policy makers [3]. According to Tundisi and Matsumura-Tundisi [7], reservoirs construction in South America was particularly intense during the last 50 years of the 20th century. In general, such huge human interventions influence the natural water systems, modifying its ecosystem functions and leading to positive and negative repercussions, in regards to both water quantity and quality [8,9]. Nowadays, the large impoundment of lands by building dams in response to droughts seems to be no longer the solution, or at least not the unique. Moreover, due to the pressure of water resources allocation to multiple uses, population growth, and economic factors, water resources managers face a number of challenges to overcome [7]. The anthropogenic impacts on the aquatic environment show the urgency of a responsible use of our natural resources to guarantee sustainable conditions [10]. Looking at the picture drawn by global climate modeling regarding future projections (e.g. [11]), considering the multiple stressors on the existent reservoirs worldwide, the environmental impacts must be assessed, in order to mitigate the negative effects and to plan prompt response measures. Indeed, there is a strong need for effective, sustainable water management strategies, supported by strong policies, stakeholder and water users' dialogues, as well as modeling support for scenarios and possible strategies evaluation [12].

1.2 How to deal with the actual challenges?

Some recent research studies in semi-arid areas

Several researchers are struggling with these challenges over the last years. E.g., Bond et al. [13] provided an overview over the impacts of droughts on freshwater ecosystems in Australia. Gophen [14] presented some perspectives for lake management in arid and semi-arid climate (among others, some study cases were lake Wadi El-Rayan and lake Quarun in Egypt), assessing the eco-hydrological changes in arid and semi-arid aquatic ecosystems due to climate fluctuations and human intervention. A sufficient water availability (quantitative and qualitative) in those areas is considered the key factor for the economic and cultural growth and might raise geo-political conflicts. Further, Sousa Júnior et al. [15] assessed the governance issues in Australia and Brazil, having to deal with heavy prolonged droughts. Both countries had to modify relevantly their water policy issues, both introducing a legal foundation to enhance a more integrated and participatory management at the catchment scale, based on the best information available. About limnology, ecology and environmental assessment, Tundisi and Matsumura-Tundisi [7] elaborated a wide review over the reservoirs in South America and in particular for Brazil for the period of 1970 to 2000. Gunkel and Sobral [9] analyzed the aquatic ecosystem services of reservoirs in semi-arid areas to stimulate a more sustainable reservoir management. Several articles produced by the authors assessed the water quality aspects in particular in the Itaparica reservoir, in Northeast Brazil (e.g., [16]; [17]).

In many countries, new construction measures are currently adopted in reaction to the impacts of climate change, such as droughts. E.g. the first water diversion project pioneer for Brazil was implemented in the State of Ceará [18] and construction works are near to be finished for the huge new diversion project in the Itaparica Reservoir (State of Pernambuco) (e.g., [19]). Further, the Los Vaqueros Reservoir is one of the large water bodies in California seriously affected by frequent and severe dry periods. The enlargement project of its major bay is planned as an adaptation measure [20]. Martin et al. [21] tried in their research to predict the changes on the hydrodynamics of the reservoir after the expansion, to support design decisions, e.g. for the oxygenation system and aid the water management. Further moving to Kenya, the new construction of the Thwake Dam at the confluence of Thwake and Athi Rivers is supposed to supply water to over one million residents of Machakos, Makueni and Kitui counties, generating 20 megawatts of electricity to power Konza Tech City in Makueni County. Political leaders retain that the project will stimulate the economic growth that the region needs; however, the irrigation component should be prioritized over the generation of electricity [22]. In India, Jadhav et al. [23] discussed about the need of sand-dams in semi-arid regions, in respond to the episodic and frequent shortages of water. Elshemy [24] studied the water quality of the large Lake Nasser in Egypt, assessing the impacts of climate change.

Figure 1.1 An impression of the Folson Lake (California), during a long period of drought (source: California Department of Water Resources, date: January 16, 2014).

A brief overview of previous studies in the semi-arid Northeast Brazil

Cirilo [25] modelled the runoff discharges for the entire catchment of the São Francisco River using an hydrological model during his PhD studies. He also measured the flow, the water level and the bathymetry in several sections along the river, calibrating the roughness friction coefficients. Güntner et al. [26]

used dynamic integrated models to develop a hydrological model for the quantification of water availability in the Federal State of Ceará (Northeast Brazil), in view of the environmental change over a large geographic domain of semi-arid environments. Still in Ceará, de Araújo et al. [11] investigated (and predicted) different global scale scenarios and regional development between the years 2001 and 2025, assessing the water scarcity issue. Ferreira Junior [27]studied the Reservoir Moxotó (between the States of Pernambuco, Alagoas and Bahìa) during his PhD studies, proposing a methodology to determine the capacity of the reservoir to support intensive aquaculture production, which might be a relevant push for economic development in the area. Kwon et al. [28] identified the runoff volumes of the Iguatu Basin in the State of Ceará with hydrologic and forecast models. Cantalice et al. [29] modelled the sediment transport to obtain a relationship between the bedload and the suspended sediments in the sand-bed Exu River in the State of Pernambuco. Pereira et al. [30] used a global meteorological and ecosystem modeling approach, studying the effect of oceans on droughts and vegetation, considering the entire Northeast Brazil. Koch et al. [31] modelled different scenarios of climate and land-use change, water demand and water availability for the São Francisco River Basin using the eco-hydrological model SWIM [32]. Oliveira de Assis et al. [33]) conducted a climate analysis of the rainfall on the Sub-Middle São Francisco River Basin based on the rain anomaly index. Marengo et al. [3] provided an historic overview of drought events in Northeast Brazil. Silva et al. [34] assessed the surface water flows for the Sobradinho Reservoir under the effects of drought using multi-temporal Landsat images. Remote sensing tools were also applied by Farias et al. [35], to conduct a temporal analysis of the droughts and the related effects. Santos et al. [36] studied the water quality in the large Orós Reservoir in the State of Ceará, assessing the land use and trophic state dynamics. For the same reservoir, Trejo and Barbosa [37] enriched a remote sensing approach for drought monitoring with the launch of the Soil Moisture and Ocean Salinity (SMOS), occurred in November 2009 by the European Space Agency (ESA).

Why is there at all interest in small inland water bodies?

Small water systems as reservoirs' bays are often used for multiple purposes such as water supply, irrigation and fishing; in this way, they enhance rural development, health improvement and poverty reduction as access to safe drinking water [38]. Being off-stream and thus having lower flow velocities, they are easier to be reached and exploited. As also discussed in Abbasi [39], such water bodies are in fact able to stimulate agricultural economy, making possible livestock farming and fishery. Nevertheless, they are often neglected in hydrological and water resources management plans, because of the difficulty in monitoring them, since they are scattered in large numbers and have usually limited in-situ measurements. This may lead to undesired consequences at the local scale, such as nutrient overloads, depletion of water transparency and oxygen rates, impacting negatively the larger scale as well. Further researchers investigated the thermal stratification patterns with the hydrodynamic modeling: e.g., Abeysinghe et al. [40] in the Kotmale Reservoir (Sri Lanka), in order to prevent it for further water quality issues due to algae blooms and eutrophication. Liebe et al. [38] presented the Small Reservoirs Project, investigating some semi-arid areas in Africa (Ghana, Burkina Faso, Zimbabwe, and Brazil), with the aim to assess their impacts on the rural communities and thus stimulate the improvement of water availability and economic development through a proper planning, maintenance and operation. Chitata et al. [41] estimated the sedimentation processes and impacts in a small reservoir in the Semi-Arid Southern Zimbabwe. Abbasi et al. [42] investigated heat exchange processes and temperature dynamics between water and air in the small Lake Binaba in Ghana, as a tool to identify the impacts on the water quality, enabling biological and environmental assessments.

Figure 1.2 Algae bloom and drought in the Icó-Mandantes Bay, Itaparica Reservoir (Brazil) (*left*). Pumping station of the eastern channel of the water diversion project (source: photos taken by the author, date: October 28, 2014)

Limited studies have been found in international and Brazilian literature for the Itaparica Reservoir (State of Pernambuco, NE Brazil) and even less for the Icó-Mandantes Bay, one of its major branches, which is used for water multiple uses. As previously mentioned, Cirilo [25] applied a hydrological model to compute the runoff discharges in the entire catchment of the São Francisco River, including the some bathymetry sections, flow and water level measurements for several reservoirs along the stream. No further literature sources have been found concerning modeling applications using Computational Fluid Dynamics (CFD) tools in the region. The research studies in the area increased relevantly approx. from the year 2012, with the kick-off meeting of the INNOVATE project, a joint collaboration between German and Brazilian scientists and experts (s. next sub-chapter). In 2012, Melo et al. [43] conducted a research to assess the future impact of the controversial water diversion project on water quality of the Itaparica Reservoir, among others. Governance, management and water quality challenges (e.g. computing the reservoir's nutrient capacity limits) were explored by Gunkel and Sobral [9], Gunkel et al. [17,44], Rodorff et al. [45]. Remote sensing studies, e.g. to evaluate the spatio-temporal behavior of chlorophyll-a in the Itaparica Reservoir and to assess potential eutrophication processes were conducted by Lopes et al. [46]. Intense limnological studies concerning water quality and, specifically, e.g. reaction processes in desiccated sediments, macrophyte growths, nutrient loads and temperature profiles were the focus of several research studies conducted by Arruda [47], Keitel et al. [48], Selge [49], Lima

[50] where the water level variations of the reservoir were considered responsible water quality deterioration and issues such as algae blooms and eutrophication potential in shallow branches of the reservoir. Silva et al. [51] focused their analyses on ecosystem's conservation, in particular fish species, and protection of artisanal fishery of the communities located along the reservoir, in particular next to the Icó-Mandantes Bay.

The first modeling approaches concerning hydrodynamics and tracer transport in the Itaparica Reservoir and the Icó-Mandantes Bay were conducted by Özgen et al. [52], Broecker et al. [53] and Matta al. [54] assessing the influence of wind-induced flow, drought- or flood- made-up scenarios on the flow field and the exchange rates between the bay and the reservoir main stream. The main outcomes were that the bay is characterized by almost stagnant water and that the main driver of water movement is the wind. Further research was conducted by Matta et al. ([12,55]), which investigated the impacts of stakeholders- and issue-oriented scenarios, wind and temperature dynamics on the flow field with a two-dimensional depth-averaged and a three-dimensional model of the Icó-Mandantes Bay and part of the reservoir main stream. Specifically, the setup of those models and the most relevant results are presented in this document and discussed later on. Additional work concerning e.g. the estimation of residence times of the domain using the Lagrangian particle tracking under different water level and flow conditions is not shown here. Additionally, many of the outcomes of the subject author's research were presented at several conferences worldwide: among others, the 11th ICHE (International Conference on Hydroscience & Engineering) in 2014 in Hamburg, Germany [54], the IWA-DIPCON conference in Berlin, Germany [56]; the XXI SBRH (Simpósio Brasileiro de Recursos Hídricos) in 2015 in Brasilia and the I SBHSF (Simpósio da Bacia Hidrográfica do Rio São Francisco) in 2016 in Juazeiro, both in Brazil [57,58]) The three-dimensional wind effects on the spreading of nutrient emissions coming from fish net cages were presented at the 37th IAHR World Congress in Kuala Lumpur, Malaysia [12]. Several joint journal and conference papers were written with the project partners, touching several of the above-discussed challenges, e.g. [17,55,59]. Finally, a policy paper was the product of an interactive and interesting workshop organized by the Academy Leopoldina (Germany) and the Academia da Ciências (Brazil) in the University of Duisburg-Essen [60]. Twenty-five selected German and Brazilian young scientists discussed and proposed future research questions in the context of urban and land integrated water management. All these publications are not included in this document.

1.3 The INNOVATE project

The INNOVATE project started (i.e. INterplay among multiple uses of water reservoirs Via inNOvative coupling of Aquatic and Terrestrial Ecosystems), a joint collaboration between Brazilian and German institutions started in January 2012 and finished in December 2016. Among others, the principal bodies involved were the Technische Universität Berlin, the Potsdam Institute for Climate Impact Research (PIK), the Leibniz-Institute of Freshwater Ecology and Inland Fisheries (IGB) and the Federal University of Pernambuco (UFPE). The INNOVATE was one of the 12 regional projects settled worldwide and included in the Sustainable Land Management program, in the framework of the Research for Sustainability (FONA) of the German Federal Ministry of Education and Research (BMBF). Co-founders were the Brazilian Ministry of Science, Technology, Innovation and Communication (MCTIC, formerly MCTI) through the Brazilian National Council for Scientific and Technological Development (CNPq). The controversial environmental and governmental situation in Northeast Brazil was a strong call for an integrative and adaptive approach to manage the natural resources of water and land, as well as governance at different levels. In order to reach this goal, a multi-scale, inter- and transdisciplinary research was necessary, organized in seven sub-projects and twenty-two research modules, covering topics such as aquatic and terrestrial ecosystem functions and services, biodiversity, modeling, economy, decision support and governance approaches. The project's studies were conducted mainly at two different scales: a large scale including the entire basin of the São Francisco River and a smaller one, comprising the Itaparica Reservoir and the semi-arid area north of it, in the so-called Sub-Middle.

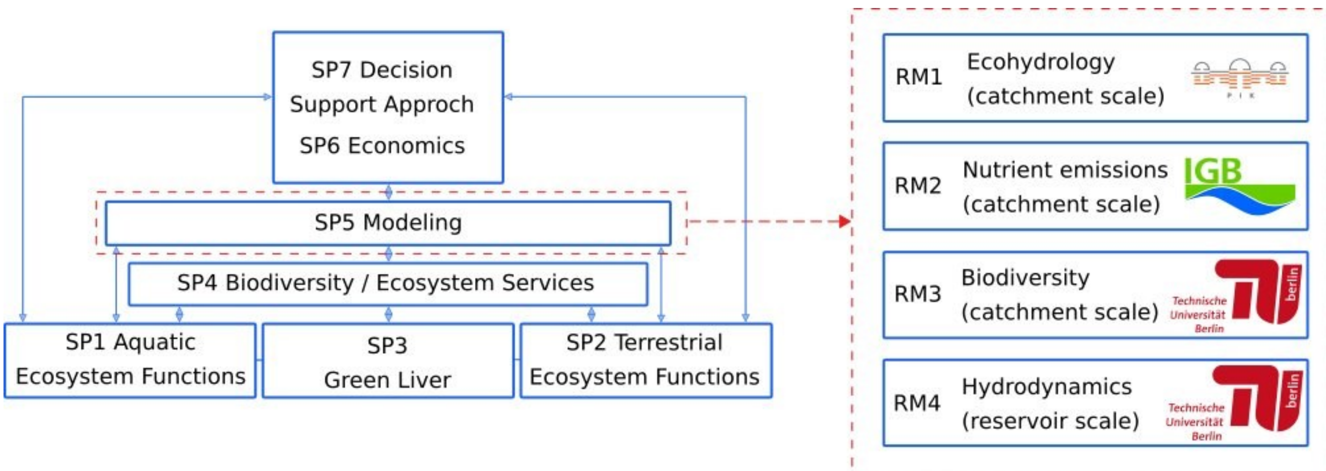

Figure 1.3 Scheme of the structure of the INNOVATE project, divided in seven subprojects (*left*) and twenty-two research modules. The research modules of the subproject 5 are shown on the *right* side. This work belongs to the subproject (SP) 5 and research module (RM) 4. (source:[61], adapted by the author)

This work belongs to the subproject (SP) 5 and research module (RM) 4, dealing with high-resolution numerical modeling of hydrodynamics and transport processes at the reservoir's scale. In particular, the research conducted merges the large-scale analyses of the eco-hydrological model SWIM (SP5-RM1) and the water quality model MONERIS (SP5-RM2) (e.g., [59]) with the local scale studies concerning limnological and biological aspects (SP1-1, SP1-3, SP4-3) (e.g., [17,49,50]). A very fruitful collaboration was established with the project partners of TU Berlin, PIK and IGB, shown by several joint publications. The work done was the result of different scenarios designed together with project partners, coordinators and stakeholders (e.g., AGB Peixe Vivo, Belo Horizonte, Brazil), that embraced climate aspects, simplified water quality processes and political and social issues.

1.4 Itaparica Reservoir and Icó-Mandantes Bay, Northeast Brazil

Itaparica Reservoir is located in the Sub-Middle São Francisco River, in the semi-arid area of Pernambuco, in Northeast Brazil. The artificial lake has a meandering shape constituted by a deeper part referred as the main stream (the former riverbed) and several branches along the shores, where the water is shallower. One of its major off-stream bays is Icó-Mandantes, focus of these modeling studies. The computational domain chosen for the model covers a larger area i.e. of around 100 km^2, including the bay itself and part of reservoir main stream, in order to assess water exchange processes, enabling inflow and outflow for the bay (Fig. 4). The climate is semi-arid, characterized by the unique Caatinga biome, a dry forest ecosystem, which covers large parts of the Northeast [62]. Some of the principal characteristics of the reservoir are summarized in Table 1.

Table 1.1 Principal hydraulic, hydrologic, morphologic and water quality parameters of the Itaparica Reservoir. Data sources: [55,63].

Parameter	Value and Unit
Water level	299-304 m a.s.l. [(a)]
Mean regulated discharge	2,060 m^3/s [(a)]
Current discharge	479 m^3/s (30.07.2017) [(a)]
Installed power	1,480 MW [(a)]
Area of the normal operating reservoir	828 km^2 [(a)]
Mean annual precipitation	475 mm/y [(b)]
Mean annual evaporation	> 1,500 mm/y [(b)]
Temperature	24.8-27.7 °C [(b)]
Secchi depth	4.8-0.8 [(b)]
Conductivity	79-70.6 µS/cm [(b)]
Total nitrogen (TN)	0.2-0.6 mg/L [(b)]
Total phosphorus (TP)	21.2-42.3 µg/L[(b)]

[a] Data from CHESF [63]

[b] Data from Selge et al. [55], respectively from field campaigns of September 2012 (dry period) and March 2013 (rainy period)

Flowing briefly through the history of the reservoir, the construction of the Luiz Gonzaga dam was completed in 1988 with the consequent formation of the Itaparica Reservoir and the resettlement of about 40,000 people, forced to change their extensive traditional systems with intensive irrigated vegetable and fruit production, not without adaptation issues [62]. The dam was primarily built for energy production and water storage. Besides these main uses, the water serves also for irrigation agriculture (approx. 70 % of the economic activities, according to FAO [4]), water supply, water- and land-based aquaculture, navigation, recreation and fishery.

Around 2007, the construction works of the largest water supply infrastructure project of the country began: the controversial São Francisco River Integration Project (in some sources is shortened as PISF, commonly known and indicated as water diversion project, also in this document). This project, promoted by the Brazilian Ministry of National Integration in response to the increasingly frequent and prolonged dry periods affecting the region in the last decades, attempts to transfer water via two channel systems, in order to supply over 12 million people in 390 municipalities of Pernambuco, Ceará, Paraíba and Rio Grande do Norte by 2025 [64]. The two channels (North and East axis) have currently a total length of more than 600 km and they are both installed in the Itaparica Reservoir; in particular, the eastern axis will withdraw water directly from the Icó-Mandantes Bay, crossing some of the irrigated lands [47]. According to ANA 411/05 [65] and De Castro [19], the total continuous withdrawal of water is planned to be 26.5 m^3/s (approx. 1.4% of the normal-operating discharge from the Sobradinho Reservoir of about 1,850 m^3/s, upstream to Itaparica), while the maximum intake is fixed to 127 m^3/s. In detail, the eastern channel is expected to withdraw a continuous minimum of 10 m^3/s up to a maximum allowance of 28 m^3/s. This huge project raised strong political and social debates between governmental bodies, environmentalists, local stakeholders and native people, which in particular are already mourning their "lost" São Francisco River and now additionally concerned about the decrease in water availability and the future anthropogenic impacts to the environment.

Since at least 2012, the area suffers for a severe drought, which more recently lead the hydroelectric company of the São Francisco River (CHESF) to reduce the water discharges released at the outlets of the reservoirs (Sobradinho, Itaparica, Xingó) below the standard minimum of 1,300 m^3/s, to minimize the risks and maintain electricity generation [66]. The current alarming situation is expected to worsen, since the already low averaged rainfall rates (Table 1), occurring only in few months of the year, are likely to decrease progressively in the next decades. Currently, the discharge flowing from Sobradinho to Itaparica is approx. 600 m^3/s, while from Itaparica downstream to Moxotó and Paulo Alfonso is about 500 m^3/s [63].

Aside to the water quantity issues, degradation in water quality is expected, if remediation measures are not embraced soon [17]. Given to hydropower generation and to the high evaporation rate (s. Table 1), the water elevation [m a.s.l.] in the Itaparica Reservoir is characterized by a high variability (up to maximum 5 m/y). Recent limnological findings in the area showed that the water level fluctuations are able to trigger many undesirable phenomena such as desiccation of the shores and nutrients release from sediment mineralization, nutrients overloads, algae blooms and decrease of macrophyte's diversity [48–50]. This concerns especially the shallower parts of the reservoir (e.g., the Icó-Mandantes Bay), characterized by low velocities and low water exchange, making them prone to eutrophication.

At this point, it becomes important to discern the reasons why the Icó-Mandantes Bay in particular has a strategic importance in the region and why it is worth the effort of research studies. The multi-functionality of the bay is schematized in Fig. 4 (*right*) and some of the principal triggering points are explained hereafter:

- four pumps for irrigation agriculture are located along the south-eastern shores of the bay (total intake of approx. 1.3 m^3/s, according to Arruda [47]);
- the eastern channel of the water diversion project is directly withdrawing water from the bay and is located right next to the intermittent tributary Riacho dos Mandantes;

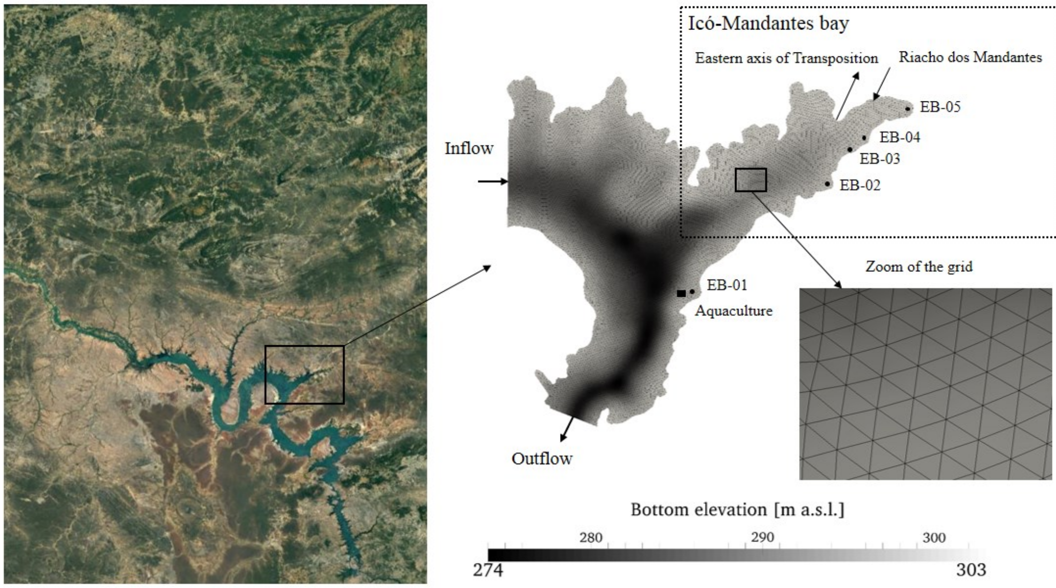

Figure 1.4 Study area and computational domain: Itaparica Reservoir (*left*); unstructured triangular high-resolution grid for high water level scenarios (*right*), where the multiple uses and a zoom of the mesh are shown. (Source: elaborated by the author after Arruda [47], Matta et al. [67] and Google Earth 2016: image recorded on 1 January 1970, coordinates in WGS84 zone 24L 629106.53 m E and 9028941.12 m S).

- the intermittent tributary Riacho dos Mandantes (mean flow rate of approx. 1.18 m^3/s) is one of the main sources of pollution in the bay, because of its dry bed and flash floods during the rare and intense rain events [55];
- residents are living next to the bay, out of fishery and/or agriculture [47]; they use the water of the bay for human and animal consumption, irrigation agriculture, fishery and recreation;
- the sewage treatment of the water coming from the agricultural villages is insufficient and also the drainage water is not treated before flowing into the reservoir [17];
- the bay is affected by serious algae bloom in particular in the shallow areas [50], creating problems e.g. to fishes and fishery;
- up until now, no water-based aquaculture systems are yet installed inside the bay, but the nearest is around 5 km far away from the bay, while there are several in the reservoir mostly nearby the inflow of Itaparica (e.g. [51]). The nutrient emissions (predominantly phosphorus) from the fish net-cages are another relevant source of water contamination.

Out of all these reasons, it is mandatory to prevent this bay from water quality deterioration and associated health risks for drinking and irrigation water. Such water uses and effects must be considered and effectively managed. Additional social and governmental issues are present in the study area, e.g. concerning the consequences of the water diversion project, the artisanal fishers or the water rights. To have broader overview regarding all these topics, it is suggested to refer e.g. to the Guidance Document of the INNOVATE project, one of its final products [66].

1.5 Multi-dimensional numerical modeling

Modeling approach and numerical settings

Surface water bodies such as lakes and reservoirs have to deal with complex phenomena related to natural as well as anthropogenic impacts: among others, the consequences of climate change such as droughts, human interventions, e.g. the installation of water withdrawals, water quality processes or yet interactions between water and atmosphere. Numerical models, or Computational Fluid Dynamics (CFD) software products, are nowadays widely used to simulate complex hydrodynamics and transport scenarios according to variable inputs and outputs (e.g. flow conditions, water uses) in various natural systems. In general, modeling is the use of numerical models to simulate the behavior of water bodies in response to a specific set of forcing conditions; in particular, they allow to identify the effects of particular factors and thus future research needs [68,69]. Models are powerful tools to conceptualize complex interactions in natural resource management and to develop appropriated policies, supporting a systematic, integrative and multidisciplinary assessment at various scales [70].

The processes occurring in a water body are described by mathematical models, often a set of coupled, non-linear, partial differential equations, which are known as the Navier-Stokes equations for momentum and the continuity equation (e.g. [69,71]). In order to determine flow and transport in complex natural hydrosystems, time and space are discretized through various methods, leading to an approximated solution, which must be fairly close to the reality and should be reached sufficiently fast. As presented in detail, e.g. in Hinkelmann [71], numerical models can be classified according to:

- numerical methods: finite difference (FDM), finite element (FEM) and finite volume (FVM);
- grid type: structured or unstructured grid;
- time differencing scheme: explicit, implicit, semi-implicit;
- advection schemes: e.g., upwind, total variation diminishing (TVD).

Approaching a new model setup, the researcher needs first to identify the key hydrodynamic processes, the water quality concerns, as well as the proper scaling (time, space) and the most suitable simulation scenarios, to support decision making and water management [69]. This first step is directly connected to the selection of the model and, in case of bays and reservoirs, the choice often lays between a vertical one-dimensional (1D), a laterally- or depth-averaged two-dimensional (2D) or a three-dimensional (3D) approach. The formers are commonly used when one of the three dimensions can be neglected: e.g., the horizontal, in narrow reservoirs, or the vertical, in shallow large lakes. On the contrary, when the wind-driven currents or thermal processes enhance a vertical variability of velocities or for complex bathymetries, 3D modeling is usually preferred. Physical forces as wind are applied on the free surface of a water body and transferred along the water depth by turbulence in the vertical plane; thus, precise advection time scales and flow paths at specific depths should be determined [72]. Most researchers retain that in case of large lakes, the horizontal uniformity is rarely valid, hence the application of 3D hydrodynamic models is necessary for proper calculations (e.g. [42,73]). Surely, the choice is also influenced by further important aspects, such as the availability of measurements (field data) and the CPU

(Central Processing Unit) time consumption, directly linked with the speed of the computation. Nevertheless, this last point can be currently handled better than in the recent past, thanks to parallel processing on supercomputers (e.g. [71,74]) and to faster or more efficient numerical schemes (e.g., [75]).

Once that the model type is selected (about the modeling systems will be discussed later on), field or laboratory data, as well as measurements, should be collected and elaborated (e.g., statistical analyses for meteorological data, interpolation methods for bathymetry). At this point of the work flow, an unstructured or structured grid can be built and the simulation of the desired scenario can start, under proper initial and boundary conditions. An unstructured mesh is preferable for hydrosystems with complex boundaries and inner structures, as well as complex bathymetry. The governing equations, combined with the numerical methods and schemes, lead to the numerical solution of the specific processes investigated, which can be then visualized and analyzed.

At this point, the so-called *verification* can be conducted, which is a procedure to check the reliability of the results and consists in the comparison with analytical solutions, only available for simple systems and single processes, or in plausibility tests, in the case of lack of data. E.g., the researcher can control the mass conservation of the system at each time step, as well as after the entire computation, and conduct some sensitivity analyses. Further, qualitative comparisons with the real behavior of the water system, as far as possible, contributes to the verification of the results. In the ideal situation of having enough data available, which is often not the case, the researcher conducts a *calibration* and *validation* of the model. With the first, the numerical results are compared with experimental or field data, varying e.g. the friction coefficient in the case of a surface flow simulation. With the second, the solution is further proven, using a new data set, under similar conditions (e.g. if mean flow was assumed for calibration, then one can validate the model taking into account high flow for validation). Further information regarding such aspects can be found in Hinkelmann [71] and Ji [69]. In this specific work, as no (hydraulic) field campaign could be conducted to enable a proper calibration and validation for velocities, concentrations and temperatures, values of a calibration undertaken by Cirilo [25] have been used for the Strickler friction coefficient. Further, sensitivity studies have been carried out concerning also the turbulent viscosity and diffusion and the results did not show high sensitivity to friction and turbulence. Thus, the model is reliable, with certain constraints. E.g., Zamani et al. [76] assessed the eutrophication potential in the Abolabbas Reservoir (Iran) using a not-calibrated 3D and water quality model with standard coefficients (and sensitivity analyses).

As mentioned above, hydrodynamic and transport processes in surface water bodies are governed by the Navier-Stokes equations, together with a turbulent model, solved at each time step and point of the mesh. For this study case, in regards to the 3D simulations, a free surface changing in time, an incompressible fluid, the hydrostatic pressure hypothesis and the Boussinesq approximation for the momentum were assumed [71,77]. Even if many researchers encourage the use of the non-hydrostatic hypothesis for 3D studies (e.g. [78,79]), the choice of the hydrostatic pressure instead is not considered here a limitation, since the 3D results showed a negligible change when assuming one or the other. Concerning the 2D simulations, the equations must be further reduced, averaging the continuity and momentum equations over the depth (vertical) and thus obtaining the Saint Venant equations. Different models can be used to estimate turbulence in the different dimensions. Simple models, such as the constant viscosity or the Elder's, take into account a constant turbulent viscosity or an easily computable one with algebraic equation, respectively. Mixing length models such as the Prandtl's [80] or Smagorinsky's [81] for the vertical direction (just for 3D applications) provide the vertical viscosities. Complex models such as the k-ε or the k-ω depend on physical quantities, which represent the transport of turbulent structures in the flow [77]. E.g., Mahgoub [79] used the Prandtl mixing length and the k-ε model to define respectively the vertical and the horizontal turbulent viscosity and diffusivity, in order to simulate the 3D flow and salinity transport in the Nile estuary. For this work, the constant viscosity model was chosen for turbulence, yielding nearly same results as those of more complex models (e.g. k-ε), but faster and less CPU time consuming. Additionally, the turbulent viscosity was set always equal to the turbulent diffusivity. Also Jourieh [82] used simple turbulence models to simulate multi-dimensional hydrodynamic and transport processes in the Unterhavel water system in Berlin.

Review of some existent modeling systems

Nowadays, the modeling systems available are numerous and classifiable according to the processes, the dimensions and the numerical methods considered. Moreover, some of them own a graphical user interface and some not. In this last case, the use of pre-processors, to build the bathymetry of the model, creating the structured or unstructured grid, and post-processors, to visualize and analyze the results, is mandatory, increasing the level of difficulty on the one hand, but also the level of expertise. The next part is a brief review of the modeling systems most commonly used to study water bodies similar as the one investigated in this work. In order to provide also an example of 2D models laterally averaged, the freely available model CE-QUAL-W2 is briefly presented. Additionally, among the hydrodynamic models, some of the water quality models available are exposed.

- **TELEMAC-MASCARET** (Hervouet [77], EDF-R&D, 2014)

The open TELEMAC-MASCARET system (often abbreviated in this document as TELEMAC) is an integrated modeling tool for developments and applications in the field of free-surface flows, managed by a consortium of core organisations, which are Artelia (formerly Sogreah, France), Bundesanstalt für Wasserbau (BAW, Germany), Centre d'Etudes et d'Expertise sur les Risques, l'Environnement, la Mobilité et l'Aménagement (CEREMA, France), Daresbury Laboratory (United Kingdom), Electricité de France R&D (EDF, France), and HR Wallingford (United Kingdom). It contains various simulation modules using estabilished algorithms based mainly on the FEM. The modules consist in subroutines, which can be modified by the user when needed, written in the programming language FORTRAN 90. Space-discretization is in form of unstructured grids made of triangular cells, which can be refined in special areas of interest. It was developed by the Laboratoire National d'Hydraulique, a department of Electricité de France's Research and Development Division and is open source since 2010. Further support and developments are conducted by the Open Telemac-Mascaret Consortium. The system is available in 2D and 3D and capable of simulating different flow and transport processes, according to the dimension chosen for the specific model. Among others, the phenomena included are the effects of bottom friction, wind, rain or evaporation and turbulence (2D and 3D), as well as tracer transport (mass-conservative in

2D or not in 3D) and the influence of temperature and salinity gradients on density (better 3D). The implementation of particle tracking and computation of Lagrangian drifts is possible as well.

This modeling system has been chosen to conduct the analyses presented in this work. Some of the aspects influencing the decision were the previous positive experience at the Chair of Water Resources and Modeling of Hydrosystems TU Berlin with this tool (e.g. [71,79,82]) and the open source availability at the starting point of this research. TELEMAC has no graphical interface, thus, it requires the use of pre- and post-processors. For the 2D cases investigated, ParaView was sufficient [83], while for 3D applications POSTEL-3D, Rubens (integrated in the TELEMAC modeling system) and Blue Keneu (Canadian Hydraulics Centre of the National Research Council, Ottawa) were additionally adopted. The use of these different tools according to the simulations is explained in detail in each chapter (2-4). Finally, the open source availability implies continuous updates of the software. In this work, the versions used were the 6.3 and 7.0. The latest currently available is the 7.2, which intends to overcome some bias and includes the water quality module WAQTEL.

In previous research, Kopmann and Markofsky [84] coupled TELEMAC-3D with the water quality Ecosystem Model of the IGB (Berlin) for the lake Müggelsee in Berlin, Germany. Mahgoub [79] used TELEMAC-2D and -3D to study the flow and salinity processes at the estuary of the Nile River in Egypt, while Jourieh [82] to assess wind-induced flow and contamination issues in the Unterhavel system in Berlin.

- **MIKE** powered by DHI (DHI, 2017)

The MIKE family is a group of commercial software products developed and distributed by the Danish Hydraulic Institute (DHI) for more than 25 years. They are mainly based on the FDM and available in different dimensions (from 1D to 3D). The field of applications is very broad, e.g., it covers runoff processes in cities and flood predictions (e.g. MIKE URBAN), hydrodynamics and transport of coastal areas and seas (e.g. MIKE 21, MIKE 3) or of rivers and reservoirs (e.g. MIKE HYDRO River, MIKE 21C), as well as groundwater and porous media related dynamics (FEFLOW). Eco-modeling (ECO Lab), dealing with water quality aspects, is also offered. These tools are rather user-friendly, since they are featured by a graphical user interface.

E.g., Sinha et al. [85]) used MIKE 3 to reveal the flow velocities and the potential water stagnation of the reservoir at the confluence of the rivers Bhagirathi and Bhilangana in the Garhwal Himalayan region.

- **Delft3D** (Deltares, 2017)

The last released Delft3D Flexible Mesh Suite (Delft3D FM) is a commercial software package, successor of the structured Delft3D 4.02 Suite, developed by the Deltares institute for applied research in the field of water and subsurface waters. Similarly as Delft3D 4.02, the Delft3D FM Suite is capable of simulating wind-, tides- and density-induced flows (e.g., storm surges, hurricanes, tsunamis), detailed flows and water levels, waves, sediment transport and morphology, water quality and ecology, and to handle the interactions between these processes. The suite is designed for use by domain experts and non-experts alike, ranging from consultants and engineers or contractors, to regulators and government officials. It includes 1D, 2D and 3D modules, as well as water quality (DELWAQ). DELWAQ is the engine of the D-Water Quality and D-Ecology programs of the Delft3D suite. It is based on a library from which relevant substances and processes can be selected to couple water and sediment quality models. Likewise the MIKE's products, these tools have an user-friendly graphical interface.

E.g., Morelissen et al. [86] coupled the Delft3D-FLOW with the CORMIX mixing zone model and decision support system, supported by the USEPA (U.S. Environmental Protection Agency) for environmental impact assessment, and applied them in an engineering project, to study the effects of multiple large-scale cooling water outfalls.

- **OpenFOAM** (Greenshields, 2015)

OpenFOAM (Open Field Operation and Manipulation) is another open source CFD software, released and developed primarily by OpenCFD Foundation Ltd since 2004 and wholly owned subsidiary by the ESI Group. It is based on the FVM and written in C++. It has a large user base across many areas of engineering and science, from both commercial and academic organizations. Within its features, it is capable to resolve complex fluid flows in 2D and 3D, involving chemical reactions, turbulence and heat transfer, acoustics, solid mechanics and electromagnetics. This modeling system is also used to solve the Navier-Stokes equations, e.g. in the near field of hydraulic structures as piles or for two-phase flow (water-gas) and is currently used by some colleagues at the Chair of Water Resources and Modeling of Hydrosystems TU Berlin [87,88]. Like TELEMAC, it has no graphical interface, thus, needs pre- and post-processing tools. New versions are released every six months.

E.g., Abbasi [39] used the OpenFOAM CFD toolbox, to simulate the temperature dynamics in the small Lake Binaba (in the Northeast of Ghana), implementing complex surface boundary conditions to include the thermal effects of heat exchange.

- **CE-QUAL-W2** (Cole and Wells, 2015)

The two-dimensional laterally averaged, hydrodynamic and water quality model CE-QUAL-W2 is suited for relatively long and narrow water bodies exhibiting longitudinal and vertical water quality gradients. The model has been applied to rivers, lakes, reservoirs, estuaries, and combinations of them, including entire river basins with multiple reservoirs and river segments. Among others, the software is capable of simulating longitudinal-vertical hydrodynamics and water quality in stratified and non-stratified systems, nutrients-dissolved oxygen-organic matter interactions, fish habitat, sediment and multiple algae, as well as to include hydraulic structures. It is written in FORTRAN90 and uses the hydrostatic assumption for the vertical momentum equation. The current model release is Version 4.0 (the first was in 1975).

E.g., Lian et al. [89] used the hydrodynamic and water quality model CE-QUAL-W2 to obtain the reservoir operation rules that would reduce the level of algal blooms in the Xiangxi River, enhanced by the Impoundment of Three Gorges Dam (China).

- **Further models and applications**

Hodges et al. [90] used the 1D-vertical model DYRESM [91] and water quality model CAEDYM [92] to assess the hydrodynamics processes in stratified lakes, e.g. Lake Burragorang in Australia. Hein et al.

[93] coupled the 1D hydraulic model HYDRAX to the water quality model QSim (Quality Simulation) to simulate the impacts of climate change in the Elbe River. Ladwig et al. [94] coupled the 1D-vertical General Lake Model (GLM) with the water quality AED2 to study wind-induced flow and nutrients spreading in the Lake Tegel in Berlin. Wu et al. [95] applied a two-dimensional, laterally averaged, finite-difference hydrodynamic, and water quality model to the Shihmen Reservoir in Taiwan, to simulate the water quality conditions and define appropriate management strategies in response to eutrophication. De Marchis et al. [73,96] used PANORMUS [97], a 3D finite volume model, employing the k–ε turbulence model for the Reynolds stresses, to assess wind- and tide-induced currents in the Stagnone di Marsala Lagoon and in the Augusta Bay in South Italy. Fenocchi et al. [72] investigated the effects of wind and complex bathymetry, comparing a 2D shallow water solver and a 3D Reynolds-averaged Navier-Stokes one, for the Superior Lake of Mantua, a shallow fluvial lake in Northern Italy. Li et al. [98] used the EFDC model to investigate the thermal structure and water age of Lake Mead (largest of the U.S., located in Arizona and Nevada). Martin et al. [21] modelled the Los Vaqueros Reservoir with the Estuary Lake and Coastal Ocean Model (ELCOM) coupled with the Computational Aquatic Ecosystem DYnamics Model (CAEDYM), trying to predict the potential effects of the future lake expansion, planned in response to the droughts.

1.6 Synthesis of the research gaps filled by this work

Numerical models to investigate flow and transport processes were missing in the study area; thus, the depth-averaged two-dimensional and three-dimensional models set up for the Icó-Mandantes Bay and exposed in this work are the first modeling tools available in the region at the reservoir scale. A very scarce literature was found and the available previous studies had in focus either the entire São Francisco River Basin, e.g. modeling the global impacts of climate change or using remote sensing approaches to determine macrophyte growth, either the very local scale such as the estimation of nutrient loads in some shallow branches. The complex challenges to face (e.g. drought, multiple uses) required a CFD tool, in order to merge the research at the different scales, as well as support the water management and academic future studies.

Some of the main research questions addressed in this work can be formulated as in the following:

- What is the impact on water quantity and quality of the water multiple uses in the reservoir, such as the aquaculture production (nutrient emissions) and the water supply (withdrawals; e.g. eastern channel of the diversion project), or of the climate extremes, such as a flash flood from the intermittent tributary Riacho dos Mandantes or a prolonged drought?
- Does the wind (moderate wind, windstorms) influence significantly the two- and three-dimensional flow circulations in the Icó-Mandantes Bay and in which way? How do e.g. the flow velocities change and to which extent?
- Does the surface heating alter the hydraulics in the bay? How (e.g. velocity profiles, intensities)? Which are the consequent three-dimensional effects (e.g. stratification, flow configuration)?

- How do the outcomes of this research influence the management of the bay? Which are the recommendations and the measures to be embraced (adaptive management)?
- What can and should still be done in the future?

In addition, one of the advantages of this study is the use of an open-source software (TELEMAC-MASCARET), which is widely used nowadays in similar water surface flow applications.

The tool developed and the approaches presented are pioneer for the Itaparica Reservoir and can be refined and improved in future studies, since they do represent the essential missing part for a concrete integrated water resource management in the São Francisco River Basin.

1.7 The structure of the thesis

This document is structured in five chapters, comprising an introduction (the current **Chapter 1**), three peer-reviewed journal articles (one published, two submitted) and a synthesis.

Chapter 2 presents the 2D hydrodynamics and transport model of the Icó-Mandantes Bay. Given to the significant water level fluctuations in the reservoir and thus to avoid numerical errors due to drying and wetting of the shores, two unstructured meshes were setup: one suitable to simulate low water level and the other one mean and high water level scenarios. The emissions of dissolved phosphorus and nitrogen ions measured from an aquaculture system hypothetically located inside the bay with a productivity of 130 t/y were investigated, using a punctual tracer source and differentiating the results according to the different water levels. In fact, still no aquaculture systems are located into the bay (the nearest is at about 5 km distance), but it is expected that further fish net cages could be installed inside Icó-Mandantes. Therefore, assessing the potential impacts of the related nutrient emissions on the water quality was necessary, leading to important outcomes for the water users and managers.

Chapter 3 shows the analyses of climate- and stakeholders-oriented scenarios, conducted with the 2D model using the different water levels' grids. During the INNOVATE Status Conference (October 2014, Recife, Brazil), several urgent questions were raised by project partners and stakeholders, in particular concerning the consequences of the water diversion project on water quantity or of the flash floods from the intermittent tributaries concerning the water quality issues. Finally, an alternative approach to estimate the water residence times for the Icó-Mandantes Bay was applied for constant and variable flows and water levels. Assessing the fate and effects through the design of the different scenarios, the specific results are useful for the limnology studies and to support the water management in the bay, providing practical suggestions and measures.

Chapter 4 deals with the implementation of the 3D model of the Icó-Mandantes Bay and present the meticulous analysis of the 3D effects on the flow field driven by wind (moderate and extreme) and density (due to temperature and heating of the water surface), exploring the capabilities of the 3D model and discussing about the choice between the use of 2D or 3D modeling. The 3D analyses enabled the assessment of the changes concerning in particular velocities, water depths, flow configuration and eventual stratification patterns, not only over the different horizontal layers (fourteen), but also at specific depths along the water column. The results provide a higher developed tool for the region in order to deepen the understanding of the complex dynamics of the system, as well as to save time and resources when approaching future studies.

Chapter 5 syntheses the principal outcomes of the work and gives an outlook for the future.

Chapter **2**

2. Simulations of nutrient emissions from a net cage aquaculture system

Reproduced from:
[67] Matta, E.; Selge, F.; Gunkel, G.; Rossiter, K.; Jourieh, A.; Hinkelmann, R. Simulations of nutrient emissions from a net cage aquaculture system in a Brazilian Bay. *Water Sci. Technol.* **2016**, 73(10), 2430–2435, with permission from the copyright holders, ©IWA Publishing; doi:10.2166/wst.2016.092. Postprint.

2.1 Abstract

Hydrodynamics and transport simulations were conducted with the software TELEMAC-2D on Icó-Mandantes Bay, a branch of the Itaparica Reservoir. The bay has a maximal operational water level amplitude of 5 m and is suffering for eutrophication and algae bloom. Therefore, we investigated low and high water level scenarios with two different high resolution meshes, with the purpose to deeper understand their impact on transport of substances and to improve the watershed management. In particular, nutrient emissions from a hypothetical net cage aquaculture system located in the bay were investigated on half-year cycles. We observed a relevant impact on water quality for a tilapia production of 130 t/y, i.e. after 6 months simulation we obtained around 8 µgP/L and 6 µgP/L at the source of emissions, for low and high water scenario, respectively.

2.2 Introduction

Many reservoirs in Brazil were built within the last 50 years, primarily for water storage and energy production, without a conscious consideration of the environment. As a general consequence, large-dam construction in the 1960s and 1970s strongly interfered with river functioning and the hydrological cycles, producing many changes in these cycles and in the biodiversity related to the rivers [7]. Human intervention affects irreversibly water flows natural state, with a huge social and ecological impact. In Itaparica Reservoir, located in the semi-arid Pernambuco, Northeast Brazil, climate and land-use changes as well as multiple uses of water lead to water quality problems [16]. Surface water conservation, both for water quality and quantity aspects, is strategic for the sustainable development of the region [11]. Therefore, it is necessary to face the social, political and ecological issues with the help of multi- and trans-disciplinary studies, in order to find enhanced management options for the future. This is one of the purposes of the INNOVATE project (Interplay among multiple uses of water reservoirs via innovative coupling of substance cycles in aquatic and terrestrial ecosystems), a joint research in collaboration between Germany and Brazil, which this work belongs to.

Object of the study is Icó-Mandantes Bay, a shallow eutrophic bay, located approximately in the middle of Itaparica Reservoir. A map of the study site can be found in Matta *et al.* [54]. Previous research in the area showed that exchange with the reservoir main stream hardly occurs, as long as wind is neglected [52–54]. Water multiple uses (e.g. irrigation agriculture), water level fluctuations and shore's desiccation, caused by high evaporation rates (ca. 2,000 mm/y), are overstressing the bay, isolating it from the river [55]. In this work, we simulated hydrodynamics and transport using TELEMAC-2D, in order to quantify the mechanisms and timescales of exchange between Icó-Mandantes Bay and the reservoir main stream, according to different water elevations. We investigated in particular nitrogen and phosphorus dissolved ions emissions from an aquaculture system hypothetically located in the bay, to quantify the potential impacts on water quality.

2.3 Material and Methods

Modeling tools

The bathymetry of the model was set up using measured data mapping, conducted by echo sounder profiling during different field campaigns, performed between 2012 and 2014 [55]. The data were imported and elaborated with the help of Janet (Smile Consult GmbH), an efficient tool to generate and edit grids for numerical simulations. TELEMAC-2D, a module of the TELEMAC-MASCARET system (Laboratoire National d'Hydraulique et Environnement (LNHE), part of the R&D group of Électricité de France), was used as processor. It is a powerful integrated modeling tool for free-surface flows and it solves the two-dimensional shallow water and transport equations with complex algorithms mainly based on the Finite Element Method, computing the water depth, the two velocity components and the depth averaged concentration at each point of the mesh [77]. After each computation, the results were examined with the help of ParaView, an open-source multi-platform data analysis and visualization application [83].

Governing equations

The governing equations are the two-dimensional depth-averaged shallow water and transport equations. The shallow water equations consist of the continuity and the momentum equations in x- and y-direction, reported in Equation 2.1 to 2.3:

$$\frac{\partial h}{\partial t}+\frac{\partial uh}{\partial x}+\frac{\partial vh}{\partial y}=0 \tag{2.1}$$

$$\frac{\partial uh}{\partial t}+\frac{\partial u^2h}{\partial x}+\frac{\partial uvh}{\partial y}-\frac{\partial}{\partial x}\left(\nu_t\frac{\partial u}{\partial x}h\right)-\frac{\partial}{\partial y}\left(\nu_t\frac{\partial u}{\partial y}h\right)=h(\frac{f_x}{\rho}-g\frac{\partial(h+z_b)}{\partial x}) \tag{2.2}$$

$$\frac{\partial vh}{\partial t}+\frac{\partial uvh}{\partial x}+\frac{\partial v^2h}{\partial y}-\frac{\partial}{\partial x}\left(\nu_t\frac{\partial v}{\partial x}h\right)-\frac{\partial}{\partial y}\left(\nu_t\frac{\partial v}{\partial y}h\right)=h(\frac{f_y}{\rho}-g\frac{\partial(h+z_b)}{\partial y}) \tag{2.3}$$

where u and v are the x- and y-component of the velocity vector, respectively, ν_t is the turbulent viscosity (assumption: $\nu_{t,t}$ equal to 10^{-4} m^2/s), f_x and f_y are the shear stresses (bottom and surface) in x- and y- direction, respectively, h is the water depth, g is the gravity acceleration, ρ is the fluid density and z_B is the bottom elevation.

The bottom and the surface friction (i.e. wind) are respectively determined through the Strickler law and the empirical Flather's approach, where the relevant parameters are the Strickler coefficient for the first, the wind velocity and a wind shear stress coefficient, dependent on wind velocity and direction, for the second. More information about the consideration of wind forcing in the TELEMAC system may be found in [77]. A mean wind of 5.5 m/s blowing from South-East with an angle of 140° [54] and a Strickler bottom friction coefficient of 30 $m^{0.33}/s$ [25] were chosen for each case studied.

The depth-averaged transport equation is shown in Equation 2.4:

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}-\frac{\partial}{\partial x}\left(\nu_{t,t}\frac{\partial c}{\partial x}\right)-\frac{\partial}{\partial y}\left(\nu_{t,t}\frac{\partial c}{\partial y}\right)=r \tag{2.4}$$

where c is the tracer concentration and $\nu_{t,t}$ is the turbulent diffusivity (assumption: $\nu_{t,t}$ equal to 10^{-4} m^2/s).

We considered only conservative transport in our study, simulating phosphorus and nitrogen emissions. This means that biological or chemical reactions and feedback effects of the transport with the flow are not taken into account. The evolution in time of the transported substances depends on advection (most relevant) and diffusion, whose terms are shown in Equation 2.4.

Further, two-dimensional simulations are carried out, i.e. vertical variations of the velocity or concentration are also not considered.

Preprocessing

Water level fluctuations are common phenomena in semi-arid areas due to rain seasons, high evaporation rates and hydropower generation. These changes play an important role for water quality by aquatic biodiversity development, nutrient release from desiccated areas and therewith water quantity management becomes a major tool for aquatic ecosystem control in these regions. Therefore, the study cases were investigated according to high and low water levels, in order to compare the respective results. Two unstructured triangular grids with high resolution were set up with the software Janet, one for low water level (LWL) and one for high water level scenarios (HWL) (Table 2.1).

Table 2.1 Characteristic parameters of the grids.

High resolution models with unstructured mesh			
Water level	Maximum bottom elevation (m a.s.l.)	Prescribed water elevation (m a.s.l.)	Number of triangular cells (-)
LWL	299.5	300.0	17,000
HWL	302.8	304.0	23,000

The computational domain has an area of around 100 km^2: it covers Icó-Mandantes Bay and it includes a part of São Francisco River, concerning the inflow and the outflow (Figure 2.1). São Francisco river, the longest in Brazil with about 2,914 km length, crosses the area and it is interrupted in its flow by the Luiz Gonzaga dam, forming the Itaparica Reservoir: a large basin of about 828 km^2, with a regulated mean flow of 2,060 m^3/s and a mean water elevation of 302.8 m a.s.l.

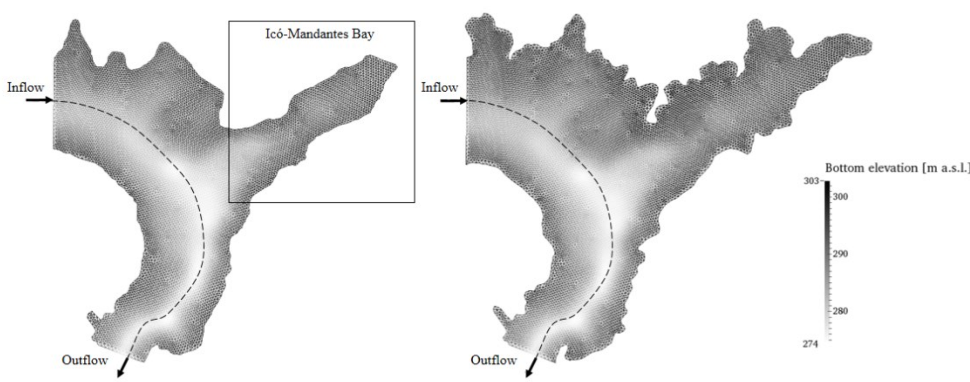

Figure 2.1 Unstructured high resolution grid for LWL (*left*) and for HWL (*right*). The black frame in the LWL grid (*left*) highlights Icó-Mandantes Bay.

2.4 Results and Discussion

A low water level of 300 m a.s.l. and a high water level of 304 m a.s.l. were imposed as constant water elevation for low water level (LWL) and for high water level (HWL) at the outflow boundary, respectively, and a controlled discharge of 2,060 m^3/s as boundary condition at the inflow from Itaparica.

Aquaculture nutrient emissions

Tilapia production in Itaparica Reservoir amounts to 20,000 tons per year. In Brazil, 1% of the lake surface is allowed to host aquaculture (43,267 t/y), but there are concerns about the sustainability to this regulation [44]. Net cage fish culture brings a desirable economic development, but can also contaminate water bodies with eutrophication and sediments leading to anoxic conditions [44]. Thus far, Icó-Mandantes Bay is not yet interested by any aquaculture system, although it is used e.g. for fishery, irrigation agriculture. Therefore, we thought to model the accumulation of nitrogen and phosphorus dissolved ions emissions from a hypothetical location inside the bay. Their spreading, as well as their retained mass quantities, were observed in time and space.

The choice of the emissions site required a specific care. Since it is necessary to guarantee enough space to allow translocation and dilution of particulate organic material to avoid an extreme sediment increase beneath the cages [44,99], we adopted a point of 5 m and 9 m water depth for LWL and HWL respectively, near the southeastern shore of the bay. We assumed a productivity of 130 t/y, which means that Dissolved Nitrogen (DN) and Dissolved Phosphorus (DP) are equal to around 17.359 kg/d and 1.302 kg/d, respectively. The emissions were simulated as a daily accumulation of nutrients, implementing a tracer source in TELEMAC-2D. The results were observed after 1 week and 6 months computation. In Table 2.2 we reported the values of DN and DP in 4 observation points chosen inside the domain (Figure 2.2), considering the modeled aquaculture impact for LWL and HWL.

Table 2.2 DN and DP concentrations [µg/L] at 4 observation points chosen inside Icó-Mandantes Bay after 1 week and 6 months simulation.

LWL 1 week			HWL 1 week		
Observation points	DN [µg/L]	DP [µg/L]	Observation points	DN [µg/L]	DP [µg/L]
1224	0	0	1224	0	0
3972 – source point	103.120	7.735	3972 – source point	53.164	3.988
6479	0	0	6479	0	0
8536	0	0	8536	0	0
LWL 6 months			**HWL 6 months**		
Observation points	DN [µg/L]	DP [µg/L]	Observation points	DN [µg/L]	DP [µg/L]
1224	0.683	0.051	1224	0.403	0.030
3972 – source point	110.575	8.294	3972 – source point	74.815	5.612
6479	0.012	0.001	6479	0.008	0.001
8536	7.497	0.562	8536	4.580	0.344

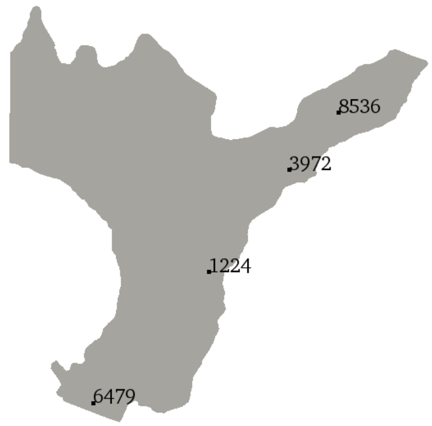

Figure 2.2 Observation points shown for the LWL grid (3972 is the source of nutrient emissions).

Considering a critical DP concentration of 25 µg/L [55] the accumulation of nutrients inside the bay is relevant: after 6 months simulation we obtained around 8 µg/L and 6 µg/L at the source of emissions (3972), while about 0.6 µg/L and 0.3 µg/L in point 8536, for LWL and HWL respectively. We can notice that the former gained higher concentrations in all observation points compared to the latter. We can state that with low water conditions, nutrients reached higher concentrations inside the bay and they spread faster. For high water conditions, the accumulation lasted longer and substances flew harder out of the bay. The final quantities [kg] that remained inside the bay after 1 week, 1 month and 6 months computation are reported in Table 2.3.

After 1 week, the entire quantity created by the source term is still inside the domain (s. Figure 2.1). After 6 months, 56 % of the initial quantity left the domain for LWL, while for HWL only 36 %. Spreading and exchange processes inside Icò-Mandantes Bay are slow, given to the extreme slow flow velocities, mainly driven by wind [54]. The study conducted shows that installation of a net cage aquaculture system inside Icò-Mandantes Bay would affect more the water quality of the area under low water conditions on a shorter term, but under high water conditions on a longer term. We can add that concentrations reached higher values for LWL, because water depths and surface are smaller, compared to HWL (Volume $_{LWL}$ = 66 % Volume $_{HWL}$). Figure 2.3 shows the spreading of DN in the computational domain after 6 months simulation.

Table 2.3 DN and DP mass quantities [kg] still retained inside Icó-Mandantes bay after 1 week, 1 month and 6 months simulation.

	1 week		1 month		6 months	
	DN [kg]	DP [kg]	DN [kg]	DP [kg]	DN [kg]	DP [kg]
Source	121.513	9.114	520.770	39.060	3176.697	238.266
LWL	121.504	9.114	502.092	37.663	1385.204	103.908
HWL	121.504	9.114	519.644	38.980	2037.925	152.870

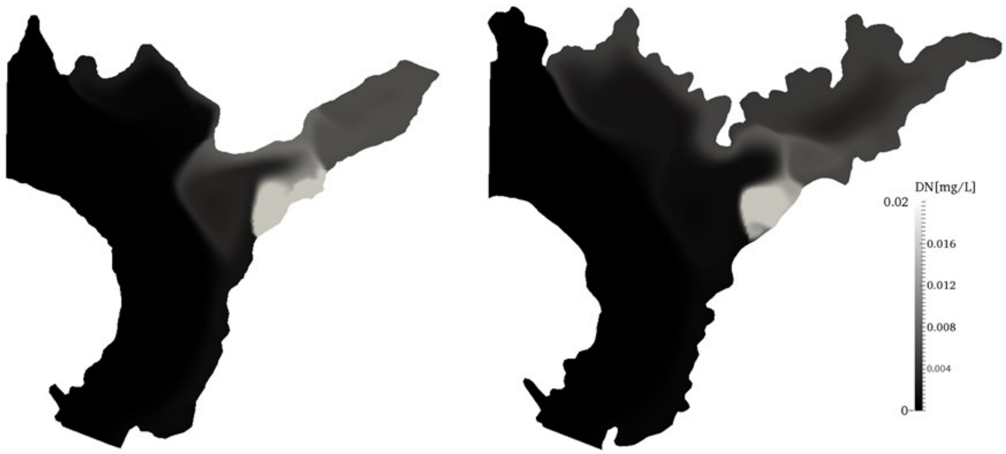

Figure 2.3 Spreading of DN concentrations [mgL^{-1}] inside Icó-Mandantes bay, after a computation of 6 months for LWL (*left*) and HWL (*right*).

2.5 Conclusions

Exchange processes between Icó-Mandantes Bay and Itaparica Reservoir main stream, Northeast Brazil, were investigated for low and high water conditions (abbreviated as LWL and HWL, respectively) using the TELEMAC-2D modeling system. Nutrient emissions were simulated on the long term (6 months), in order to understand the potential impacts of a hypothetical net cage aquaculture system inside the bay. The results showed that concentrations of DN and DP reached higher values for LWL and they spread faster inside the bay, while for HWL the mass quantities [kg] are retained longer in the area (56 % left the domain after 6 months for LWL and only 36 % for HWL). The results of this study are an additional tool for local companies and decision makers, which can be particularly helpful regarding water quality control, water level regulation of the reservoir, placements of new pumps for irrigation agriculture or of a new net cage aquaculture system. In further work, also 3D effects (e.g. wind, stratification) will be investigated to observe hydrodynamic changes over the vertical, fulfilling the lacks of 2D modeling.

Chapter 3

3. Modeling the impacts of climate extremes and multiple water uses to support water management

Submitted in September 2017 and currently under review as:
[12] Matta, E.; Koch, H.; Selge, F.; Simshäuser, M. N.; Rossiter, K.; Nogueira da Silva, G. M.; Gunkel, G.; Hinkelmann, R. Modeling the impacts of climate extremes and multiple water uses to support water management in the Icó-Mandantes Bay, Northeast Brazil. *J. Water Clim. Chang.* (©IWA Publishing)

3.1 Abstract

The hydropower production, water supply and aquaculture services of the Itaparica Reservoir are of immense importance for the Brazilian Northeast. Due to the uncontrolled water resources consumption (e.g. irrigation, water supply), climate and land use change effects, the water quantity and quality in the reservoir has deteriorated, leading to socio-economic and environmental problems. In this work, a depth-averaged shallow water model was set up for the Icó-Mandantes Bay, one of the major branches of the reservoir, using the open TELEMAC-MASCARET system. The aim was to assess the impacts of the newly built water diversion channel, as well as the effects of a flood and tracer transport from an intermittent tributary, both located in the bay. An alternative approach to estimate the water retention times was additionally implemented. The simulations showed that though the diversion channel did not influence significantly the hydrodynamics of the bay, it is necessary to continuously monitor water quality parameters, especially during rainy periods after long droughts, because the nutrient inputs from the tributary and the overflows of the nearby drainage systems will affect the withdrawals. Such events urge of management measures adapting to the continuously changing natural conditions and anthropogenic impacts, whereby the model presented can be adopted as supporting tool.

3.2 Introduction

The current drought in Northeast Brazil is considered the harshest in the recent decades, if not of the last 100 years, devastating agricultural, livestock, and industrial producers [100]. The consequent water scarcity, mostly attributed to climate change [101], the illegalities in water withdrawals [102] and the water quality issues [7,16] generate concern among Brazilian government, water managers and academic institutions, which endeavor to understand the extent of such impacts [3]). Nowadays, due to the pressure of water resources allocation to multiple uses, population growth, and economic factors, water resources managers face a number of challenges to overcome [7]. Such natural phenomena as droughts or floods can aggravate existing problems, affecting irrigation and agriculture as well as key water uses including hydropower and industry, and thus, the welfare of the residents [3]. To cope with such complex tasks there is a strong need for effective, sustainable water management strategies, supported by strong policies, stakeholder and water users' dialogues, as well as modeling support for scenarios and possible strategies evaluation.

The INNOVATE project, a joint trans-disciplinary research project in collaboration between German and Brazilian institutions, emerged in this context, with the aim to find solutions and strategies to enhance a more sustainable watershed management for the São Francisco River Basin [66]. The project is embracing different disciplines, objectives and scales, e.g. catchment scale hydrological (SWIM) and water quality (MONERIS) modeling [59]. This work is part of the project and provides the hydrodynamic modeling at the reservoir scale. During the INNOVATE Status Conference and the so-called Environmental Days workshops in October 2014 in Recife and Petrolândia (Brazil), the existing challenges in the Itaparica Reservoir were discussed and specific requests were raised by water authorities and local stakeholders, which we intend to address in this paper.

The focus of this work is the Icó-Mandantes Bay, part of the meandered Itaparica Reservoir, in the Sub-Middle São Francisco River, Northeast Brazil (Figure 3.1). Similarly to other big reservoirs in Brazil [7], the main use of the Itaparica Reservoir is water storage for hydropower production (HPP). Nowadays, the reservoir also serves to develop large areas of irrigation agriculture, abstraction of drinking water, fishery, aquaculture and recreation activities. Over the past twenty years, the demand for energy has increased. The adopted practices for fertilization and the release of sewage from urban areas, combined with the climate change, lead to significant environmental impacts, as well as increasing pressure on the aquatic systems and sedimentation in the inflow area, water losses and a trophic upsurge with severe eutrophication related processes, concerning in particular Icó-Mandantes Bay [16,47].

In previous studies in the region, Cirilo [25] analyzed the formation process of surface runoff for the entire São Francisco Basin, with the purpose to identify the potential inundation areas in case of floods during and after dam construction. Another group of Brazilian scientists works since several years on remote sensing techniques (e.g. Landsat-TM) in the Itaparica Reservoir, with the aim to improve water management, in particular analyzing chlorophyll a dynamics, to assess potential eutrophication processes (e.g. [46]). Nevertheless, very limited studies can be found in this region, especially concerning CFD (Computational Fluid Dynamics) applications at the reservoir scale.

This article presents the application of a depth-averaged modeling tool for hydrodynamic and transport processes in the Icó-Mandantes Bay, developed using the modeling system TELEMAC-2D [77], in order to simulate climate, stakeholders- and project issue-oriented scenarios. This bay is over-stressed by various factors and gained increasing attention in the last years [55,67]. Withdrawals for human and animal consumption, as well as for irrigation agriculture, are located there. Moreover, the eastern channel of the controversial water diversion project (e.g., [19]) is withdrawing water directly from Icó-Mandantes, to transfer it to nearby watersheds. This bay is rather isolated from the dynamics of the reservoir main stream, behaving as two separated systems with different flow velocities (one order of magnitude higher in the main stream, i.e. about 10 cm/s); thus the exchange hardly occurs [54].

In this work, we investigated the effects of the eastern channel of the water diversion project and a flood from the intermittent tributary Riacho dos Mandantes, combined with tracer transport, on the bay's water dynamics. Since the reservoir is characterized by high water level fluctuations up to maximum 5 m per year due to HPP [48] the simulations have been run alternating low and high water level conditions. Moreover, in order to quantify the mechanisms and timescales of exchange between the Icó-Mandantes Bay and the reservoir main stream, we applied an alternative method, imposing an initial uniform distribution of a mass-conservative passive tracer, tracking its evolution in time and, thus, estimating water residence times.

The aim of this research is to provide a first modeling setup for the region, capable of simulating hydrodynamic and transport processes at the local scale, in order to respond to the above-mentioned urgent challenges in the Itaparica Reservoir. The methodology presented integrates the large scale modeling studies [59] and the São Francisco River Basin Management Plan 2016-2025 [103] in order to provide state-of-the art support for water management in the region.

3.3 The study site

The Icó-Mandantes Bay is located in Itaparica Reservoir, in the Sub-Middle São Francisco River Basin. The São Francisco River with its length of 2,914 km is the longest river that runs entirely in Brazilian territory. The reservoir is characterized by a total capacity of 10,781 hm^3 and an active capacity of 3,549 hm^3, with an installed power of 1,480 MW. Its flow is regulated by the upstream reservoir Sobradinho and has a mean discharge of 2,060 m^3/s and a mean water elevation of 302.8 m [63], fluctuating seasonally up to 5 m between 299 and 304 m above sea level (a.s.l.) every six months. The average and the maximum water level of the reservoir are respectively 13 and 42 m. The climate conditions are semi-arid: the average annual temperature is 26 °C and the rainy season extends from January to April with an average annual precipitation of 475 mm. The Icó-Mandantes Bay covers approximately 3% of the annual mean surface area of the reservoir.

Figure 3.1 provides information on the multi-functionality of the bay. As depicted, there are four pumps (named EB-n), irrigating large agricultural areas: Block-3 and Block-4, of respectively 149.81 and 79.99 km^2, and supplying water for human and animal consumption. The total withdrawal reaches about 1.3 m^3/s [47]. Further, there are the intermittent tributary Riacho dos Mandantes (mean flow rate of 1.18 m^3/s) and the eastern channel of the water diversion project. In the outer bay, there is a net-cage aquaculture system and another water intake for irrigation agriculture and human consumption (EB-01). In the Fig. 1, one can also observe the consequences of the recent drought: EB-04 and EB-05 used to be wet (Google Earth 2014), but currently they are dry, with a minimum distance from water of about 1.7 km (Google Earth 2016).

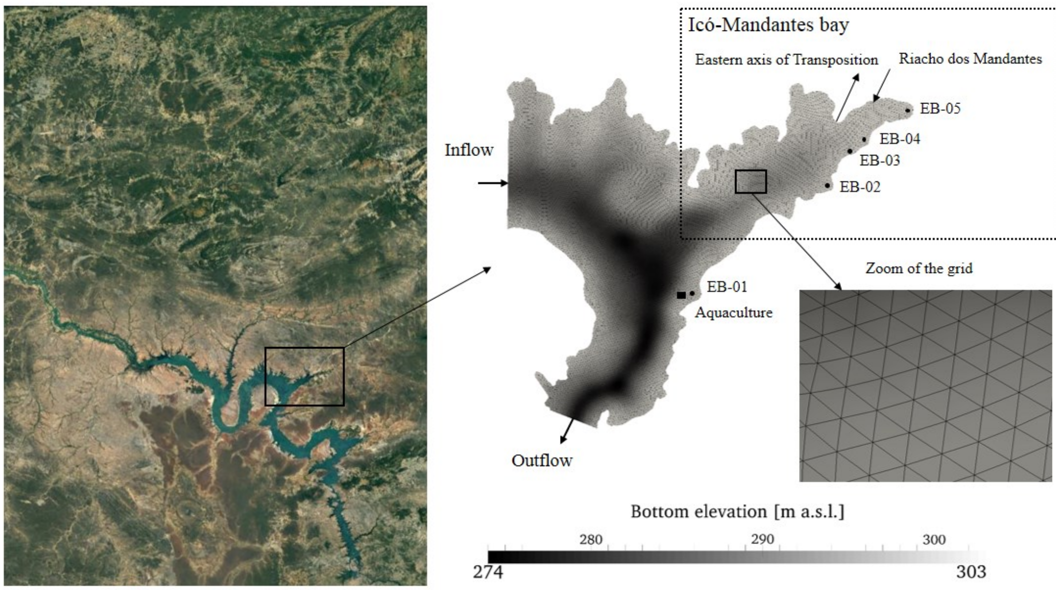

Figure 3.1 Study area and computational domain: Itaparica Reservoir (*left*); unstructured triangular high-resolution grid for high water level scenarios (*right*), where the multiple uses and a zoom of the mesh are shown. Figure elaborated by the author after Arruda [47], Matta et al. [67] and Google Earth 2016 (image recorded on 1 January 1970, coordinates in WGS84 zone 24L: 629106.53 m E and 9028941.12 m S).

The water diversion project of the São Francisco River is the largest water infrastructure project in the country, which raised strong political and social debates between governmental bodies and local stakeholders. The project aims to ensure water supply (human and animal consumption) of 12 million people in 390 municipalities through two axes (East and North) in the states of Pernambuco, Ceará, Rio Grande do Norte and Paraiba, in particular to the big cities of the region i.e. Fortaleza, Juazeiro do Norte, Crato, Mossoró, Campina Grande, Caruaru, partly to mitigate the effects of frequent droughts in those regions. The project belongs to the Federal Government, under the responsibility of the Ministry of National Integration and its costs are currently estimated at R$ 8.2 billion. For this study, we considered only the eastern channel of the project, as it diverts water directly from Icó-Mandantes Bay, supplying it to the wild regions of Pernambuco and Paraíba. The planned operational flow for the eastern channel is 10 m^3/s, which can be increased up to 28 m^3/s maximum flow, exclusively when precise restrains concerning the volume of the upstream Sobradinho Reservoir are satisfied [65]. However, the management strategy of the two axes is still under discussion. The Brazilian Ministry of National Integration reported that while affecting negatively the biotic environment, the water diversion project is expected to stimulate the local economy and increase water supply for the semi-arid regions, what is of great importance for the development of the country [19,43,64].

Riacho dos Mandantes is a small stream in a strategic location: next to the water diversion channel, to the intakes used for the irrigated lands and to the drainage system for irrigation agriculture. The tributary itself is dry most of the year, but reaches significant discharges during rainy periods (i.e. up to 100 m^3/s). During rare but intense rain events, large amounts of nutrients are likely to enter water bodies by erosion, wash-out, leaching and run-off (e.g. from tributaries and drainage systems). In the case of bays with low exchange rates such Icó-Mandantes, most vulnerable to eutrophication processes, such effects must be considered and effectively managed, to prevent water quality deterioration and associated health risks for drinking and irrigation water.

3.4 Material and methods

The modeling system

The modeling system was already presented in Matta et al. [67] (section 2.3 of the thesis); therefore, we report hereafter only the most important related information. The hydrodynamic software applied to the Icó-Mandantes Bay is TELEMAC-2D, a module of the open TELEMAC-MASCARET system, a powerful integrated modeling tool for free-surface flows, that solves the two-dimensional shallow water and transport equations with complex algorithms based on the Finite Element Method, computing the water depth, the two velocity components and the concentration at each point of the mesh and at each time step [77]. The two-dimensional depth averaged shallow water and transport equations are reported in Equation 2.1 to 2.4 of section 2.3. The constant viscosity model was adopted for turbulence, where the turbulent viscosity ν_t and the turbulent diffusivity were both set equal to 10^{-4} m^2/s [77,82]. The bottom and the surface friction (i.e. wind), presented on the right-hand side of Equation 2.2 and 2.3, are respectively determined by the empirical laws of Strickler [77] and Flather [104]. The first depends in particular on the flow field and on a roughness coefficient [$m^{0.33}$/s], chosen equal to 30, according to values calibrated by Cirilo [25] for the same reach and comparable flow discharges. The friction at the surface is function of the wind speed at 10 m high and a dimensionless wind coefficient, variable with wind magnitude and direction [77]. In Matta et al. [54], a statistical analysis of meteorological data of a 12 years' time span was conducted, obtaining a mean wind velocity and direction of respectively 5.5 m/s and 140° (Southeast wind). The above-mentioned values of bottom roughness, wind intensity and direction, have been set for each scenarios presented in this work as constant forcing conditions.

The computational domain chosen to conduct simulations in the bay has an area of around 100 km^2: it covers the Icó-Mandantes Bay itself and it includes a part of reservoir main stream, in order to assess water exchange, enabling inflow and outflow for the bay (Figure 3.1). For the open boundaries we set Neumann and Dirichlet boundary condition respectively imposing velocities and water levels at the inflow and the outflow. The conditions are explained in detail for each scenario in the correspondent paragraph.

The bathymetry of the model was set up using measured data mapping, conducted by echo sounder profiling during different water quality field campaigns, performed by project partners between 2012 and 2014. These data were imported and elaborated in Janet (Smile Consult GmbH), a powerful and efficient pre-processor tool for mesh generation. Different high-resolution unstructured grids with triangular elements were created in order to consider different scenarios: one is for low water level cases and another one is for mean and high water level cases, with a maximum bottom elevation of 299.5 m a.s.l. and 302.8 m a.s.l., respectively, and around 20,000 triangular cells, characterized by an averaged cell length of 150 m [55]. The mesh used for wet scenarios is shown in Fig. 3.1 (*right*).

Hydrological data

Daily values provided by the Hydroelectric Company of the São Francisco River [63] were used as reference database for the principal inflow and outflow boundaries, where the water elevation is the mean at the Luiz Gonzaga dam and the discharge is controlled by the dam and by the upstream Sobradinho Reservoir. Consequently to the prolonged drought affecting the region, in the last years, CHESF was forced to gradually reduce the mean operating discharge of 2,060 m^3/s up to values lower than the planned minimum of 1,300 m^3/s. In order to reflect the extremes emerging by climate change, we chose low and high operating conditions in the reservoir to simulate some of our scenarios. The values at the boundaries for the low (LWL) and high water level (HWL) cases were set in agreement with project partners and stakeholders as standard LWL and HWL conditions, in agreement with CHESF.

The WATCH Era-40 data [105] were used for the simulations of the eco-hydrological model SWIM [32,59], in order to obtain runoff values [Q, m^3/s] for the intermittent tributary Riacho dos Mandantes. SWIM results for Riacho dos Mandantes were computed on a daily basis and for a period of 30 years (1981-2010). Its daily flow rates were statistically analyzed and a discharge with a return period of 10 years (HQ_{10}) was determined using the Pearson Type III distribution. We obtained a value equal to 40.2 m^3/s, which was chosen as the peak of the simulated event, set 3 days long. This is an extreme event for the small tributary; thus, we will refer to it as a *flood*.

Data regarding the expected withdrawal from the eastern channel of the water diversion project were available by ANA 411/05 [65]: 10 m^3/s for normal operation and 28 m^3/s as maximum intake.

Simulation scenarios, initial and boundary conditions

The scenarios developed in this work are reflecting specific project partners (e.g. water quality group) and stakeholders (e.g. AGB Peixe Vivo, Belo Horizonte, Brazil) requests:

i. LWL and HWL: reference cases under steady state low and high water level- and flow-operating conditions, respectively;

ii. Q_OC and Q_MC: respectively operative and maximum withdrawal from the eastern channel of the water diversion project with the reservoir under steady state LWL-operating conditions;

iii. F_LWL and F_HWL: flood event from the intermittent tributary, with the reservoir respectively under steady state LWL- and HWL-operating conditions;

iv. RT_LWL, RT_HWL and RT_VWL: water residence times-simulations with the reservoir respectively under steady state LWL- and HWL-operating conditions, as well as time-variable (VWL).

A zero initial velocity and zero tracer concentration were the initial conditions for each scenario. Initial water elevation was set equal to the prescribed elevation at the outflow boundary, varying depending on the case and described in detail hereafter.

Boundary conditions after Neumann and Dirichlet at the inflow and outflow of the domain (Figure 3.1) were given for the reference cases (i.) respectively imposing a constant discharge and a constant water elevation of 300 m a.s.l. and 800 m^3/s for LWL, while 304 m a.s.l. and 8,000 m^3/s for HWL, values according to project partners and stakeholders. Reference cases have been run until steady state conditions (i.e. few days).

Since the severe drought affecting Northeast Brazil from approximately end of 2012 is increasing the concern about the water diversion project, for the scenarios ii. we considered LWL conditions to simulate the impacts of the eastern channel (abbreviated EC_T) on water hydrodynamics (i.e. water depths, velocities and water volumes). In addition to the principal inflow and outflow (Figure 3.1), it was necessary to implement a third open boundary in the mesh, in the location of the intake, with a width approximately equal to an averaged element length (approx. 100 – 150 m). Since TELEMAC needs minimum three nodes along an open boundary, the grid was refined in the surroundings of the new boundary with a mean length of about 30 m, obtaining 5 nodes at EC_T's boundary (Figure 3.2, *left*). Here the foreseen withdrawals (negative values) of 10 m^3/s for Q_OC and 28 m^3/s for Q_MC (ANA 2005) were imposed. The duration of the simulations was set to 10 days.

In order to simulate the impacts of a flash flood from the small tributary Riacho dos Mandantes, we followed an analog procedure as for the EC_T, implementing a third open boundary in the meshes used for both scenarios iii. and refining the grid in the near surroundings. The minimal edge length for this case was around 26 m. A typical hydrograph was imposed at the open boundary of the tributary, using the Neumann condition with a discharge variable in time and characterized by a peak of 40.2 m^3/s (HQ_{10}), which was reached 1.5 days after the start of the event, which had a total duration of 3 days. Concerning transport, a mass-conservative passive tracer was set at the same boundary with a concentration of 1 [-], kept constant for the entire duration of the event, in order to reproduce a constant contamination flowing within the flood curve. The results were controlled each 0.5 day before, during and up to one week after the simulated event; afterwards, each month until one year of computation.

Finally, modeling analyses for water residence time estimations were conducted. In general, residence time for a natural straight river flow (one-dimensional approach) can be rather simple, as described by Chapra [106]. In particular, the hydraulic residence time τ [s] is defined as the ratio of the considered volume V [m^3] to the stream outflow rate Q [m^3/s], as reported in Equation (3.1):

$$\tau = \frac{V}{Q} \tag{3.1}$$

Using the formula in Equation (3.1), we obtained a value of about two months for Itaparica Reservoir, considering the mean water level of 302.8 m a.s.l. prescribed at the outflow and the mean dam-controlled discharge of 2,060 m^3/s at the inflow boundary. In more complex cases where bays are present, as in this study area, no constant flow through is ensured and, consequently, Equation (5) is not applicable, since the flow is highly 2D (s. Figure 3.2, *right*). Several methods can be used, such as Lagrangian Particle Tracking [107].

In this study, an alternative method was implemented: a mass-conservative passive tracer with concentration equal to 10 [-] was set as initial condition (t = 0) in the whole bay, while zero concentration in the rest of the domain. The value of 10 [-] was assigned to each point of the mesh, higher than a specific horizontal coordinate (Figure 4, *left*). This limitation (i.e. x-coordinate > 560,157 m = approx. 560 Km) was used as well to distinguish the results related solely to the bay. In order to provide an approximated value of residence time for each scenario (iv), the results were divided into different intervals: a code was implemented, starting at t = 0 with c = 10 and counting after each saved time step how many nodes fit to a certain concentration interval including the extremes, i.e. concentration higher than 9, between 8 and 9, between 7 and 8, between 6 and 7, etc. The time at which all points of the bay belong to the latter interval (c < 1), was arbitrarily defined as the approximated water residence time, i.e. when all points of the bay have a concentration lower than 10% of the initial value.

These scenarios were calculated considering steady state conditions in the domain (LWL- and HWL-operating reservoir) and for time-variable conditions (VWL). For VWL, we considered a variable water level (Dirichlet boundary condition at the outflow, variable in time) chosen over the year 2012, in order to observe the influence of variable water levels and discharges on residence time estimations, taking into account the water level fluctuations of the reservoir due to HPP. We used daily water levels (m a.s.l.) at the Luiz Gonzaga dam [63], between 2012 and 2015. We chose the time span between January 17, 2012 and January 16, 2013, characterized by 3 m of yearly water level variation (i.e. 300.8 - 304.0 m a.s.l.). The discharge was kept constant to the mean 2,060 m^3/s for the entire computation, in order to check the only water level impacts on tracer evolution.

Further investigations were conducted assuming constant water elevations of 300 and 304 m a.s.l. combined with a time-variable discharge over the same time span, as well as time-variable discharges together with time-variable water levels. The results obtained are analog to the RT_VWL scenario; therefore, those are not presented in this paper.

3.5 Results and discussion

Reference cases

LWL and HWL scenarios intend to reproduce the reservoir under dry and wet conditions, respectively. To give an idea about the range of the mean flow velocities in the system [m/s], we report the respective values for LWL and HWL: 0.013 and 0.064 considering the entire computational domain, 0.015 and 0.083 in the reservoir main stream only, while 0.001 and 0.007 in the bay. Comparing the values in the bay and in the main stream, we notice that the velocities diverge more than one order of magnitude. The mean water depths [m] differ less than 1 m comparing LWL and HWL, being approx. 11 to 13 m in the main stream and 4 to 5 m in the bay. Looking at the resulting flow field, the bay is much more isolated by the reservoir main stream under wet (HWL) conditions, given to the much higher inflowing discharge (8,000 m^3/s to 800 m^3/s), which tend to separate the systems even more.

Eastern channel of the water diversion project

In this section, the results of Q_OC and Q_MC are presented, considering the effects of the EC_T on the hydrodynamics of the bay in 2D (i.e. changes in velocities, water depths and water volumes). Figure 3.2 (*right*) shows the flow field for LWL under steady state conditions, completely reached after around 5 days. The flow velocities obtained in the entire computational domain for the scenarios Q_OC and Q_MC are both 0.015 m/s, while respectively 0.007 and 0.010 m/s in the bay area. The averaged velocities of the entire domain increase with deltas lower than 10%, while more relevant changes up to 60 - 70% were observed in the bay, stimulated by the intake. Nevertheless, velocities remained low (order of cm/s).

The results were further analyzed in four points, Their values were extracted at the end of the simulation, under steady state conditions: one in the reservoir main stream and three inside the bay (Figure 3.2 *left*). Table 3.1 shows the impacts of the EC_T on the flow field inside the bay: the higher is the discharge withdrawn, the higher is the increase of the velocities inside the bay. The influence of the EC_T is also depending on the distance of the analyzed point from the intake: the lower is the impact, the longer is the distance (the effect decreases from point 8747 to point 8327). The point 4296 in the reservoir main stream was not influenced by the withdrawal.

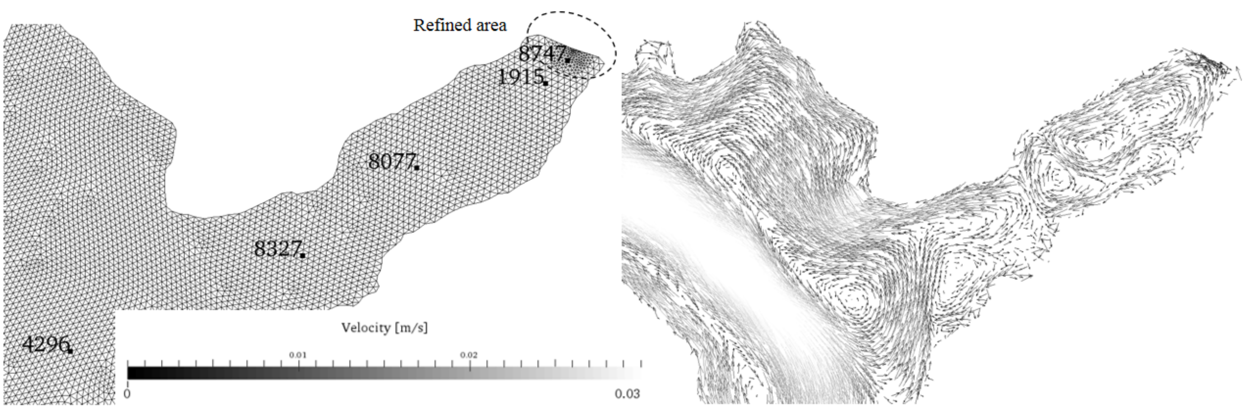

Figure 3.2 Detail of the LWL model used for Q_OC and Q_MC scenarios, where (*left*) the selected points (in the main stream: 4296; in the bay: 1915, 8077, 8327), the refinement near the channel open boundary of the triangular unstructured grid and (*right*) the flow field for LWL under steady state conditions are shown.

Table 3.1 Flow velocities in the selected points in the bay (1915, 8077, 8327) and in the mainstream (4296), for scenarios LWL, Q_OC and Q_MC, which respectively indicate the cases considering the operative and the maximum withdrawal from the eastern channel of the water diversion project, with the reservoir under steady state LWL-operating conditions as reference.

	Velocity [m/s]			Increase of velocities [%]		
Points ID	LWL	Q_OC	Q_MC	Δ (Q_OC/LWL)	Δ (Q_MC/LWL)	Δ (Q_MC/Q_OC)
8747	0.005	0.015	0.035	206	638	141
1915	0.007	0.008	0.012	23	83	39
8077	0.011	0.012	0.012	16	15	-1
8327	0.006	0.007	0.008	14	34	18
4296	0.033	0.033	0.033	0	0	0

The results reported here were analyzed exclusively in regards of hydrodynamics and relative changes due to the eastern axis in action, showing small effects, except for the near field of the withdrawal. Regarding another issue - water quality, Rossiter et al. [108] conducted a study on heavy metals levels at the future intake of the channel. According to a data collection between January 2012 and September 2014 and to CONAMA 357/05 [109], water quality was evaluated as *good* for public supply. Only copper showed median values greater than the legislation limit only in the dry season. Nevertheless, Gunkel et al. [110] reported high peaks e.g. of Chlorophyll a up to 70 μg/L in the inner bay. Studying water quality will be a necessity for the system. Additionally, regular monitoring of water quality is vital, due to the low water depths, the high evaporation rates and the low velocities inside Icó-Mandantes Bay, which do not facilitate exchange nor recirculation with the reservoir main stream.

Intermittent tributary Riacho dos Mandantes: impacts of a flood and tracer transport

Analyzing the results in different observation points, the flow velocities in the reservoir main stream were not influenced by the flood event, except for a slight increase of 001 to 0.002 m/s near the outflow boundary, not relevant compared to the mean velocities registered in the same location in the reference cases (i.e. 0.033 and 0.241 m/s, respectively for LWL and HWL). On the other hand, inside the bay the effects of the flood were large and were analyzed in two specific points: 8077 and 8327, same as shown in Figure 3.2 (*left*). There, velocities decreased in both scenarios, because the water flowing from the small tributary enters a distinct current along the northern shore and changes the circulation patterns in the inner bay, slowing them down. The highest impact was in 8077, which is nearer to the tributary boundary, for the F_LWL case (i.e. Δ = 0.006 m/s compared to a velocity of 0.009 m/s for LWL, while Δ = 0.003 m/s compared to a velocity of 0.012 m/s for HWL). Approximately 3 to 4 days after the end of the event, the velocities inside the bay reached the steady state conditions again (Figure 3.3, *left*). Such results are expectable concerning hydrodynamics, since the imposed discharges of 800 or 8,000 m^3/s at the main inflow boundary are predominant in the flow field, compared to a secondary inflow of maximum 40.2 m^3/s. Nevertheless, it confirms the isolated condition of the bay from the main river.

Regarding tracer transport, higher values of concentration were reached for F_LWL, but on the other hand, the tracer was retained longer for F_HWL. Analyzing the results in the selected points of

Figure 3.2 (*left*), the maximum concentrations of 38.2% and 0.38% were reached four and six days after the end of the flood event in the center of the bay (point 8077) respectively for F_LWL and F_HWL (Figure 3.3, *right*). The spreading process was much faster under drought conditions; in fact, the concentrations in 8077 were almost a third of the peak value already one week after the event, while in F_HWL the tracer concentrations reached after one month merely 2.8% and 0.33% at the observation points 8077 and 8327, respectively. In this case, the tracer moved much slower, because of the larger water volume to be mobilized and of the dominant inflow of 8,000 m^3/s, clearly separated by the bay. Tracer values started to be lower than 0.1% four months after the flood for F_LWL, while after six months for F_HWL.

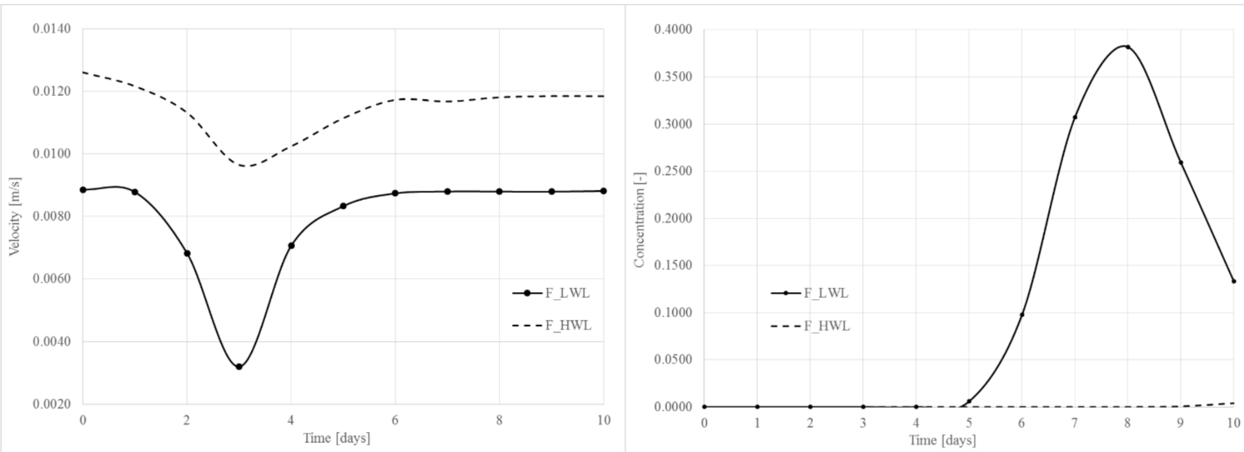

Figure 3.3 Flow velocity vs. time (*left*) and tracer concentration vs. time (*right*) registered in the center of the bay (point ID 8077) during the flood event for F_LWL and F_HWL scenarios. The flood event takes place between day 1 and day 4.

In the context of climate change, water multi-functionality and conservation of environmental resources, the outcomes of this particular application intend to enhance a more sustainable watershed management in the Icó-Mandantes Bay, and thus in the reservoir. Considering the findings in relation to the locations of the existent intakes for irrigation agriculture and water supply, we can affirm the following. For both applications investigated, we observed small effects regarding hydrodynamics, except for the local impacts (near the tributary/intake boundary). On the other hand, the changes were more relevant regarding transport. Looking at Figure 3.1, an occasional intense flow from the usually dry Riacho dos Mandantes must be considered by the water users. Concentrations reached high values (80 - 100% of the initial) for both wet and dry scenarios (F_HWL, F_LWL) in the northern tip of the bay on the short term (up to one week after the flood), where the eastern channel and the pumps EB-04 and EB-05 are located. There, the values remained higher than 10% for F_HWL until one month of computation, while for F_LWL the concentrations decreased of 90% already few days after the extreme event, reaching concentrations of approx. 1 to 2%. Near the intakes EB-02 and EB-03 maximum values of around 2% are reached after one month for F_HWL, while for F_LWL 5%. Near EB-01, we obtained values lower than 0.5% for both scenarios and for the whole computation time.

Water residence time estimations in the Icó-Mandantes Bay

Since the exchange processes between the reservoir main stream and the bay are very slow, it was necessary to compute long-term simulations up to 2 years. The purpose was to assess the time range of those exchange processes in the system, as described in the methods: the so-called residence times in this work are the times at which all cells gain a concentration lower than 10% of the initial value (arbitrary concentration limit, which could be set looser or stricter).

Figure 3.4 (*right*) shows the spreading of the passive tracer inside the bay after six months: the concentration retained in the bay after this period is respectively 40% and 60% for RT_LWL and RT_HWL, compared to the initial value (Figure 4, *left*). Likewise, RT_VWL results showed that the residence times is very high (> 1 year) and they are overall in accordance to the RT_LWL case (Figure 3.5). Thus, time-variable water level does not relevantly encourage water exchange between the bay and the main stream. Indeed, retention graphs of Figure 3.5 show that concentrations lower than 10% are reached the earliest after one year. After about 1.5 years, the RT_LWL and RT_VWL curves overlap. The estimated residence times were defined equal to 725 days for RT_HWL, 545 days for RT_LWL and RT_VWL. Looking back at Equation (3.1), the computed residence times for the bay are substantially longer than the reservoir's (about two months).

Comparing the results of the F_LWL and F_HWL scenarios, the tracer spreads faster in this latter case, because the flood from the tributary stimulates the hydrodynamics of the bay, usually almost stagnant. Thus, the ideal situation to sustain the bay's water quality would be to have a continuous inflow of water from the northeastern tip, stimulating the exchange between the reservoir main stream and the bay. E.g., the water flow withdrawn by the eastern diversion channel could be inverted, in the case of alarming nutrient overloads and high amount of algae in the shallow stagnant areas of the bay. Moreover, the results of this study showed that the water level and discharge variations did not stimulate significantly this exchange; on the contrary, the high water levels and strong discharges (e.g. higher than 3,000 m^3/s) contributed to the isolation of the bay. Furthermore, high water level fluctuations are known to stimulate the development of harmful algae blooms and greenhouse gases emissions [48,110]. The findings and suggestions proposed should be considered and discussed with the water users of the Luiz Gonzaga dam (CHESF), to reduce such risks and carry out further studies to properly plan sustainable operation measures.

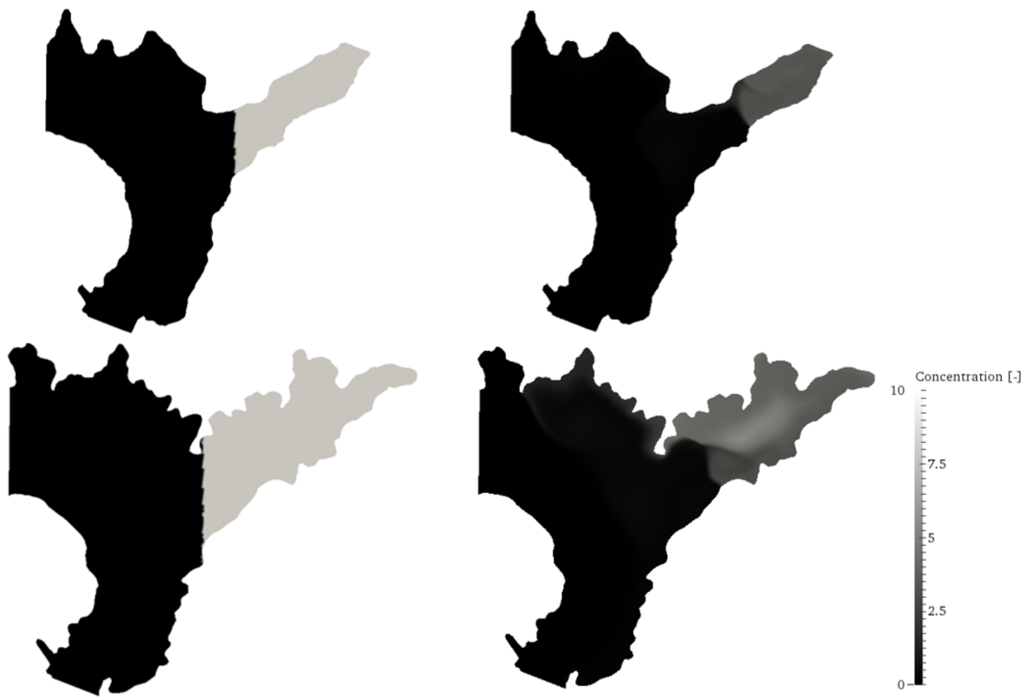

Figure 3.4 Spreading of the mass-conservative passive tracer concentration at zero time (*left*) and after 6-months simulation (*right*) for steady state scenarios RT_LWL (*upper*) and RT_ HWL (*bottom*).

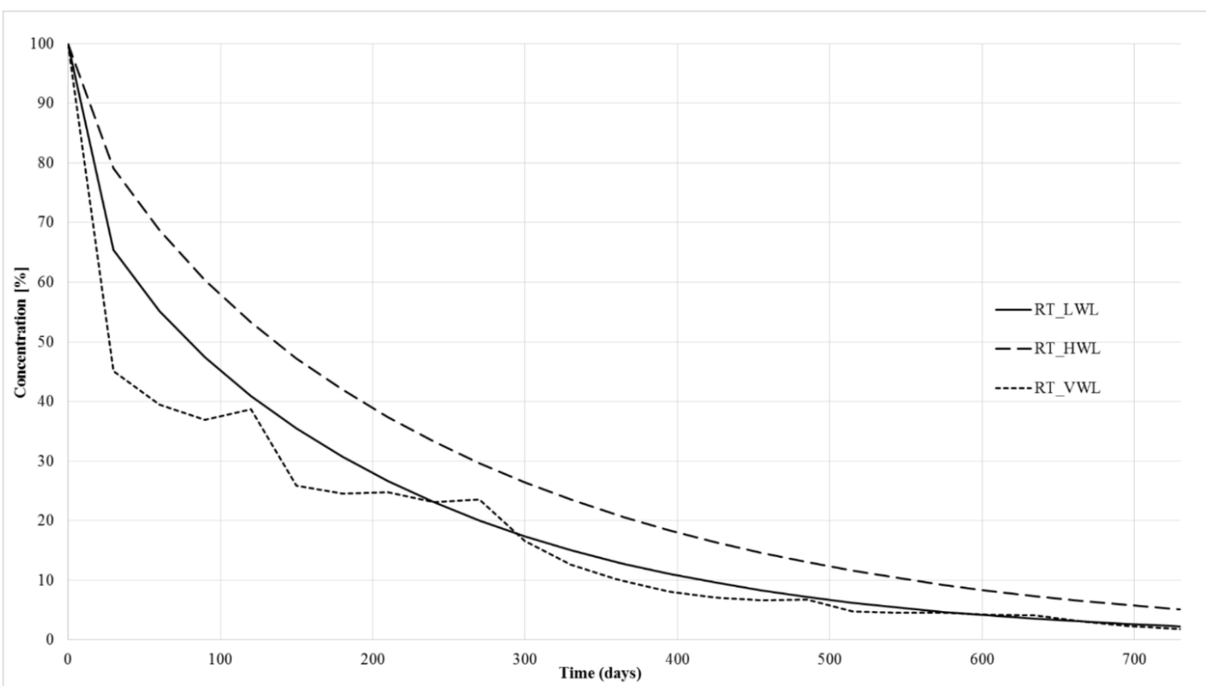

Figure 3.5 Evolution of the mean tracer concentration inside the bay vs. time.

Finally, in other first exploratory scenarios for the estimation of the bay's residence times, the intake of the water diversion channel was additionally taken into account. The results showed that the residence time of the bay was significantly reduced, up to around 50%, suggesting that the water withdrawal from the Icó-Mandantes Bay might affect the mixing of water at the local scale and be a positive side effect on water quality, as pollution will get diluted faster. Model scenarios investigating the impacts of water diversion channels, to improve lakes' dynamics and thus water quality, can be found e.g. in Li et al. [111] and specifically for Itaparica Reservoir in Melo et al. [43]. Further studies in this direction are needed and must be adapted to each specific case.

3.6 Conclusions

The object of this study was the Icó-Mandantes Bay, a branch of the Itaparica Reservoir, located along the Sub-Middle São Francisco River. Given to the prolonged drought affecting Northeast Brazil, the new water diversion project and the physical complexity of the system, managing the multiple uses of water in the bay is becoming more and more challenging. The aim of this research was to provide a first modeling tool for the region, capable of simulating 2D flow and transport scenarios.

The impacts of the eastern channel of the water diversion project and of a flood with mass-conservative transport from the intermittent tributary Riacho dos Mandantes were investigated, considering the reservoir operating under variable conditions, to take into account the water level variations due to HPP. The results showed that the 2D effects of the intake and the tributary on the hydrodynamics are negligible, except for the near field. In the case of intense rain events, the management of the intakes for irrigation agriculture and of the water diversion needs to be adapted. In the northeastern tip of the bay, high concentrations and long residence times were observed: higher values on the shorter term for drought scenarios and longer tracer retention for the high flow scenarios. Furthermore, an alternative method for estimation of water residence times of the bay was developed and tested. The results indicated high tracer retention times (> 1 year), alarming for the long-term stagnation of contaminants. First exploratory studies showed that the withdrawal by the eastern channel of the water diversion is able to reduce significantly water residence times of the bay and thus potentially improve water quality. Nevertheless, further investigations in this direction are needed.

The 2D hydrodynamic and transport modeling framework developed for Icó-Mandantes Bay and described in this paper is of highest importance for the water committee (i.e. CBHSF), managers (i.e. CHESF), as well as smallholders and universities (e.g. UFPE). It can be applied for local studies and applications, in order to support and improve the water management. The methodology and the outcomes of this work can be transferred to other reservoirs in semi-arid areas facing similar issues, where peripheral bays are isolated and used for multiple purposes. Water quality issues such as the development of harmful algae blooms in the lentic areas, their interactions with the reservoir main stream and the water withdrawals should be assessed in future research, coupling the existent model with a water quality module.

Chapter 4

4. Three-dimensional modeling of wind- and temperature-induced flows

Published as:
[112] Matta, E.; Selge, F.; Gunkel, G.; Hinkelmann, R. Three-dimensional modeling of wind- and temperature-induced flows in the Icó-Mandantes Bay, Itaparica Reservoir, NE Brazil. *Water (Switzerland)* **2017**, 9(10), 772; doi:10.3390/w9100772. Postprint.

4.1 Abstract

The Icó-Mandantes Bay is one of the major branches of the Itaparica Reservoir (Sub-Middle São Francisco River, Northeast Brazil) and focus of this study. Besides the harmful algae blooms (HAB) and the severe prolonged drought, the bay has a strategic importance, e.g. the eastern channel of the newly built water diversion will withdraw water from it (drinking water). This article presents the implementation of a three-dimensional (3D) numerical model, pioneer for the region, using TELEMAC-3D. The aim was to investigate the 3D flows induced by moderate or extreme winds as well as by heating of the water surface. The findings showed that a windstorm increased the flow velocities (at least one order of magnitude, i.e. up to $10^{-1} – 10^{-2}$ m/s) without altering significantly the circulation patterns; this occurred substantially for the heating scenario, which had in contrast a lower effect on velocities. In terms of the bay's management, the main implications are: (1) the withdrawals for drinking water and irrigation agriculture should stop working during windstorms and at least three days afterwards; (2) a heating of the water surface would likely increase the risk of development of HAB in the shallow areas, so that further assessments with a water quality module are needed to support advanced remediation measures; (3) the 3D model proves to be a necessary tool to identify high risk contamination areas e.g. for installation of new aquaculture systems.

4.2 Introduction

Managing reservoirs in the semi-arid region of the Brazilian Northeast is becoming dramatically challenging. The severe drought affecting the area since 2012 increased the conflicts among the multiple uses of water and it demands urgently more efficient communication and coordination between the different water users [3,66]. The prolonged dry periods predicted by climate change models are expected to reduce the dilution of nutrients and contaminants and affect the ecosystem by increasing water temperatures and reducing oxygen saturation levels; therefore, more eutrophic conditions are expected in lakes [16]. Phenomena such as droughts and the occurrence of harmful algae blooms (HAB) are increasingly affecting water bodies, especially those located in semi-arid areas [110,113]. Additionally, climate change effects influence the trophic level of lakes through many processes such as water heating, enhanced primary production and promotion of cyanobacteria by a high radiation input and intensification of bioremediation with decreased oxygen concentrations. In the region, further ecosystem impacts are generally attributed to the intensive and increasing aquaculture production, by the insufficient treatment of sewage from agricultural villages and by the untreated drainage water from irrigation [110]. Due to the decreasing inflows and the warming climate, the number of reservoirs with water quality problems is likely to increase in semi-arid regions of the world [76]. The high nutrient and sediment loads due to human activities and wastes, enhanced by soil leaching and wash-out during tributaries's flash floods, lead to more extensive and/or rapid eutrophication in reservoirs, compared to natural lakes [76,114,115].

Finding climate change-adaptive solutions to manage multiple uses of water through innovative technologies, as well as stakeholder procedures, will promote sustainable economic development in Brazil. This was the general aim of the INNOVATE project, to which this work belongs. The binational and interdisciplinary research project provided scientific research in the São Francisco River Basin and improved opportunities transferable to other hydropower reservoirs in semi-arid areas [66]. Adaptive management measures must be developed to mitigate the environmental impacts on reservoirs, primarily greenhouse gas emissions, eutrophication and water level fluctuations, among others [59,66,110].

Computational Fluid Dynamics (CFD) models are widely used to simulate complex hydrodynamics and transport (e.g. sediment) in various natural systems. Such models also allow to examine the effects of particular factors, and thus, identify research needs [68]. Models can be powerful tools to conceptualize complex interactions in natural resource management and to develop appropriated policies, supporting a systematic, integrative and multidisciplinary assessment at various scales [70]. Understanding and communicating the causal connections between fate and effects is fundamental for public acceptance of legislative steering to responsibly compromise between the use of water resources and the conservation of their ecological status; hence, advanced numerical tools are required [10].

For instance, Fenocchi et al. [72] investigated the effects of wind and complex bathymetry, comparing a 2D shallow water solver and a 3D Reynolds-averaged Navier-Stokes one, for the Superior Lake of Mantua, a shallow fluvial lake in Northern Italy. De Marchis et al. [73,96] used the 3D finite volume model PANORMUS [97], to assess wind- and tide-induced currents in the Stagnone di Marsala Lagoon and in the Augusta Bay in South Italy. The thermal stratification patterns using hydrodynamic modeling tools for water bodies in semi-arid areas were investigated by Abeysinghe et al. [40] with the aim to prevent algae blooms and eutrophication processes in the Kotmale Reservoir, Sri Lanka. They used a self-developed one-dimensional numerical model, called DYRESM, to predict the distribution of temperatures in response to metereological forcing, inflow and outflow. Liebe et al. [38] focused their work on some small reservoirs located in Africa (Ghana, Burkina Faso, Zimbabwe) and in Brazil, with the aim to assess their impacts on the rural communities, and thus, stimulate the improvement of water availability and economic development through proper planning, maintenance and operation. Abbasi et al. [42] assessed the heat exchange processes and the temperature dynamics between water and air in the small Lake Binaba in Ghana, as a tool to identify the impacts on water quality, enabling biological and environmental predictions.

Two- (depth-averaged) and three-dimensional (2D and 3D, respectively) models are usually preferred for lakes and reservoir management and the choice between them depends on whether the vertical variability of velocities, tracer profiles and stratification are significant or not. Nevertheless, one-dimensional (vertical) numerical models are also often applied for lakes, with the main purpose to assess eventual stratification patterns and temperature profiles over the water depth. For instance, Ladwig et al. [94] coupled the 1D-vertical General Lake Model (GLM) with the water quality AED2 to study wind-induced flow and nutrients spreading in the Lake Tegel in Berlin. In general, physical forces induce 3D effects on the flow field; forces applied on the free surface of a water body are transferred at depth by turbulence in the vertical plane; thus, the depth-averaged approximation is generally more limiting for wind-driven flows than for gravity-driven ones, such as straight rivers [72]. Wind in the first place, but also temperature changes affect hydrodynamics and water quality [42]. In particular, local scale analyses are connected to macrophytes and wind mixing, as well as to the transport of nutrients and pollutants across reservoirs [69,116]. The usefulness of 2D models is restricted to processes associated to the horizontal circulation, disregarding precise advection time scales and flow paths at specific depths [72]. In the case of large lakes, the assumption of horizontal uniformity is rarely valid, hence the application of 3D hydrodynamic models is required for proper calculations, as pointed out by many researchers even for very shallow depths (e.g. [42,73]).

In the framework of the above-mentioned INNOVATE project, this study focuses on the Icó-Mandantes Bay, one of the major branches of the Itaparica Reservoir (Pernambuco, NE Brazil). Although in many regions, small inland water bodies act as multi-purpose water sources, being extremely important for economic development, improving smallholder livelihoods and food security, hydrological impact assessments are rarely carried out [38]. In the study area, no modeling studies were found in literature and urgent questions have been raised in the last years by water managers, such as the effects of the newly built water diversion project on water quantity [19] or the impacts on water quality of the net-cage-based aquaculture systems, increasingly developing in the reservoir[44]. To answer to such stakeholders- and issues- oriented demands, in previous research [12,54,67], a 2D model capable to simulate hydrodynamics and tracer transport was setup and tested for several scenarios, using the open-source software TELEMAC-MASCARET [77]. The main hydraulic outcomes were that the water exchange between the Icó-Mandantes Bay and the reservoir main stream was hardly occurring, since the water in the bay is almost stagnant, in absence of external forces such as wind or flood events. Therefore, the same water body can be characterized by different flow (and vertical eddy viscosity) regimes [52,54].

Important management suggestions have been given in that context, for example in regards to the urge of assessing the spreading of contaminants in the domain, introduced for instance by the harmful flash floods occurring from the intermittent tributary Riacho dos Mandantes, located next to the withdrawals for water supply [12].

So far, the vertical flows (3D effects) induced by wind and temperature have not yet been taken into account in the Icó-Mandantes Bay. Only a limited number of CFD simulations for temperature distribution in shallow and small inland water bodies in semi-arid areas can be generally found [42]. As addressed by numerous experts [10,42,76,96], weather conditions (wind, temperature) influence currents and stratification in reservoirs, whose hydrodynamic processes and thermal state are the main drivers of their ecosystem. The classification of lakes according to their circulation patterns has proven to be very useful for limnology assessments [10,117]. Moreover, the vertical resolutions of the measured temperature profiles are often not sufficient for assessing small-scale turbulence effects or investigating variations of water temperature induced by wind velocity and heating in shallow waters [42]. Therefore, research is needed to deepen the knowledge of such complex processes in areas already challenged by climate change, water multiple uses and lack of advanced modeling techniques. In this article, the setup of a 3D model for the Icó-Mandantes Bay is presented, as well as the implementation of scenarios investigating hydrodynamics, wind- and density-induced flows. The study focuses on the 3D effects caused by wind and temperature changes over the vertical water column, addressing the following research questions:

- Since wind is considered responsible of hydrodynamic mixing in water bodies and of the relevant increase of flow velocities during storms in shallow lakes [72,96], does the wind (moderate wind, windstorms) significantly influence the three-dimensional flow circulations also in the Icó-Mandantes Bay and in which way? How do the flow velocities change and to which extent?
- Density differences are known to drive currents [10,42,69,76]: how does heating of the water surface due to warmer air temperature alter the hydraulics in the bay and how (e.g. velocity profiles, intensities)? Which are the consequent three-dimensional effects (e.g. stratification, flow circulation)?
- In the revised literature, the implications of the numerical results for appropriate environmental policy and management are often not explored and the focus of discussion is strictly limited on the hydrodynamic findings. In contrast, we intend to additionally address in this work: how do the outcomes of this research influence management of the bay (sustainability of aquatic ecosystem services)? Which are the recommendations and the adaptive measures to be embraced?

The results of this work deepen the knowledge of the complex hydrodynamics of this bay or similar behaving small water bodies in semi-arid areas, being particularly useful for future modeling studies, for stakeholders and water managers, in order to save time and resources.

4.3 Governing equations

The hydrodynamics and transport simulated in the Icó-Mandantes Bay are solved through the three-dimensional shallow waters equations at each time step and in each point of the mesh [77]. For this case study, a free surface changing in time, an incompressible fluid, the hydrostatic pressure hypothesis and the Boussinesq approximation for the momentum were assumed [71,77]. The governing equations in regards to the flow are the continuity equation, i.e. the conservation of the fluid mass, and the momentum equations in x-, y- and z-directions. The latter consists in the simplified equation for the vertical velocity w, given to the hydrostatic pressure hypothesis, which considers the pressure at one point depending on the atmospheric pressure on the surface and on the weight of the column of water above it.

The wind shear stresses ($f_{x,wind}$ and $f_{y,wind}$, in x- and y-direction, respectively) were determined in function of the wind speed at 10 m height (v_{wind} [m/s]), the density of the air (ρ_{air} [kg/m^3]) and a dimensionless empirical coefficient (a_{wind}), calculated according to the formula used by the Institute of Oceanographic Sciences (United Kingdom) [77], reported in Eq. 4.1 and 4.2:

$$f_{x,wind} = \frac{\rho_{air}}{\rho_0} a_{wind} v_{wind,x} \sqrt{v_{wind,x}^2 + v_{wind,y}^2}$$
$$f_{y,wind} = \frac{\rho_{air}}{\rho_0} a_{wind} v_{wind,y} \sqrt{v_{wind,x}^2 + v_{wind,y}^2} \tag{4.1}$$

$$a_{wind} = 0.565\ 10^{-3}\ if\ v_{wind} < 5\ m/s$$
$$a_{wind} = (-0.12 + 0.137\ v_{wind})\ 10^{-3}\ if\ 5 \leq v_{wind} \leq 19.22\ m/s \tag{4.2}$$
$$a_{wind} = 2.513\ 10^{-3}\ if\ v_{wind} > 19.22\ m/s$$

where $v_{wind,x}$ and $v_{wind,y}$ [m/s] are the components of wind velocity in x- and y-directions. The information about wind values used in the simulations are given in Section 4.2.

No flow measurements were available in the study area; thus, a proper calibration and validation for velocities, concentrations and temperatures could not be conducted. Values calibrated in previous work for the same reach under study and for similar flow discharges [25] have been used for the Strickler coefficient to evaluate the bottom friction, assuming it equal to 30 m$^{0.33}$/s. Additionally, values of bottom friction were varied in the range between 25 and 35 m$^{0.33}$/s and the results showed very small differences. Such values for friction are standard values for the type of soil and system of the bay under study.

Simple turbulence models were applied for the horizontal and vertical directions, which are respectively the constant viscosity and the mixing length Prandtl model [71,77], giving nearly same results as more complex models (e.g. k-ε) computed for a defined reference case under same conditions (e.g. checking mass conservation, velocities and water depths). Additionally, when running the k-ε model for the simulations, TELEMAC computes the turbulent viscosity coefficient for the specific scenario (horizontal and vertical). The results of the sensitivity studies conducted concerning the turbulent viscosity (between $10^{-2} \div 10^{-6}$ m^2/s; the latter is the TELEMAC default value) did not show high sensitivity to such parameters. Thus, the horizontal viscosity $\nu_{t,th}$ was assumed equal to 10^{-4} m^2/s for each case, which is in the range of literature values and of the results obtained with the k-ε model.

The governing equation in regards to the tracer transport is reported in Eq. 4.3, which consists in the heat transport equation, where the turbulent diffusivity was set equal to the turbulent viscosity of the momentum equations [77,82].

$$\frac{\partial(\rho T)}{\partial t} + u\frac{\partial(\rho T)}{\partial x} + v\frac{\partial(\rho T)}{\partial y} + w\frac{\partial(\rho T)}{\partial z} = \nu_{t,th}\frac{\partial(\rho T)}{\partial x} + \nu_{t,th}\frac{\partial(\rho T)}{\partial y} + \nu_{t,tv}\frac{\partial(\rho T)}{\partial z} \tag{4.3}$$

where T [°C], ρ [kg/m^3] are respectively the water temperature and the water density calculated by the model; $\nu_{t,th}$, $\nu_{t,tv}$ [m^2/s] are the horizontal and vertical turbulent thermal diffusivity.

The density-induced flow computed by the equation of state established by UNESCO [77] is:

$$\rho = \rho_0\{1 - \left[7\left(T - T_{ref}\right)^2 10^{-6}\right]\} \tag{4.4}$$

where ρ_0 [kg/m^3] is the reference water density and T_{ref} [°C] is the reference water temperature. The water density ρ [kg/m^3] is function of the water temperature T, assuming here that it is in the range of 0 to 40 °C.

According to Hervouet [77] and Sweers [118], the boundary condition at the water surface is:

$$\nu_{t,tv}\frac{\partial T}{\partial z} = -\frac{A}{\rho C_p}(T - T_{atm}) \tag{4.5}$$

where T_{atm} [°C] is the atmospheric temperature; C_p [J/kg/°C] is the specific heat equal to 4.18 and A [W/m^2/°C] is the so-called exchange coefficient. Eq. 4.5 assumes that the thermal power exchanged between water and atmosphere per surface unit is proportional to the temperature gradients between water and air by the exchange coefficient A [W/m^2/°C]:

$$A = (4.48 + 0.049\,T) + 2021.5\,b\,(1 + v_{wind})\,(1.12 + 0.018\,T + 0.00158\,T^2) \tag{4.6}$$

where the parameter b [-] depends on the location of the study area: 0.0025 was chosen, average suggested by [77] for regions near the Atlantic shores. The exchange coefficient A is the result of the nomogram developed by Sweers [30], which relates A at the water-air interface to the wind speed and the surface temperature, approximating the phenomena like radiation, convection of air in contact with water and latent heat produced by water evaporation.

4.4 Study region

The area of interest is the Icó-Mandantes Bay, one of the major off-stream branches of the Itaparica Reservoir, located in the semi-arid state of Pernambuco, NE Brazil (Figure 4.1). The reservoir is formed by the Luiz Gonzaga dam, built in the late 80s, in the Sub-Middle São Francisco River. The mean water discharge is 2,060 m^3/s, regulated by the upstream Sobradinho Reservoir, and the mean water elevation 302.8 m a.s.l., with a maximum annual water level fluctuation of maximum 5 m [63]. The average and the maximum water level of the reservoir are respectively 13 and 42 m [2].

The morphometric, chemical and limnological characteristics of the Icó-Mandantes Bay have been presented in detail in [44,48,50,55]. The study area has high air temperatures and strong winds concentrated in some hours of the day. The bay is vertically mixed, it has low water conductivity and low nutrients loads, which increase significantly during flash floods from the tributaries. The mean annual precipitations of ~ 475 mm/y are usually occurring between January and April during rare intense events. Between 2012 and 2015, the median water quality of the Itaparica Reservoir is characterized by low conductivity (71 µS/L) and low nutrient concentrations (dissolved inorganic nitrogen = 98 µg/L, total phosphorus = 20 µg/L), a transparency of 2.3 m Secchi disk depth and Chlorophyll a = 1.7 µg/L; thus, the reservoir was classified as mesotrophic. The water quality in the Icó-Mandantes Bay is depleted by an intermittent river inflow (called Riacho dos Mandantes) with high short-term nutrient input during the rainy season and by the drainage channels of the irrigated agriculture areas, located in the southeastern part of the bay. After such strong rain events, the median nutrient concentrations changes relevantly, with dissolved inorganic nitrogen = 77 µg/L, total phosphorus = 34 µg/L, a transparency of 0.9 m Secchi depth, and Chlorophyll a = 38 µg/L [49]. Nearly 35 to 45% of the bay area is covered by a submerged weed, namely *Egeria densa*. Due to the water level fluctuations cause by hydropower use, in particular when the surface elevation decreases, these dense vegetation mats are another significant source of nutrient input for the bay, after desiccation and mineralization [48,50]. Among others, such undesired effect due to declining lake levels was observed as well by Zamani in the Abolabbas Reservoir, Iran [76].

Nowadays the uses of the Itaparica Reservoir are multiple: besides the water storage and energy generation, it is also used for irrigation agriculture and aquaculture production, human and animal water consumption, navigation, recreation and fisheries. In particular, the Icó-Mandantes Bay is strategic for the local water management for numerous reasons. The eventual future development of new aquaculture systems in the bay of the reservoir may increase the phosphorus contents and the potential for eutrophication [44,67]. Water withdrawals for human and animal supply, as well as for irrigation agriculture, occur in the bay, where also the newly built water diversion channel (Figure 4.2) will operate with the aim to divert water to into the even drier northern watersheds [12].

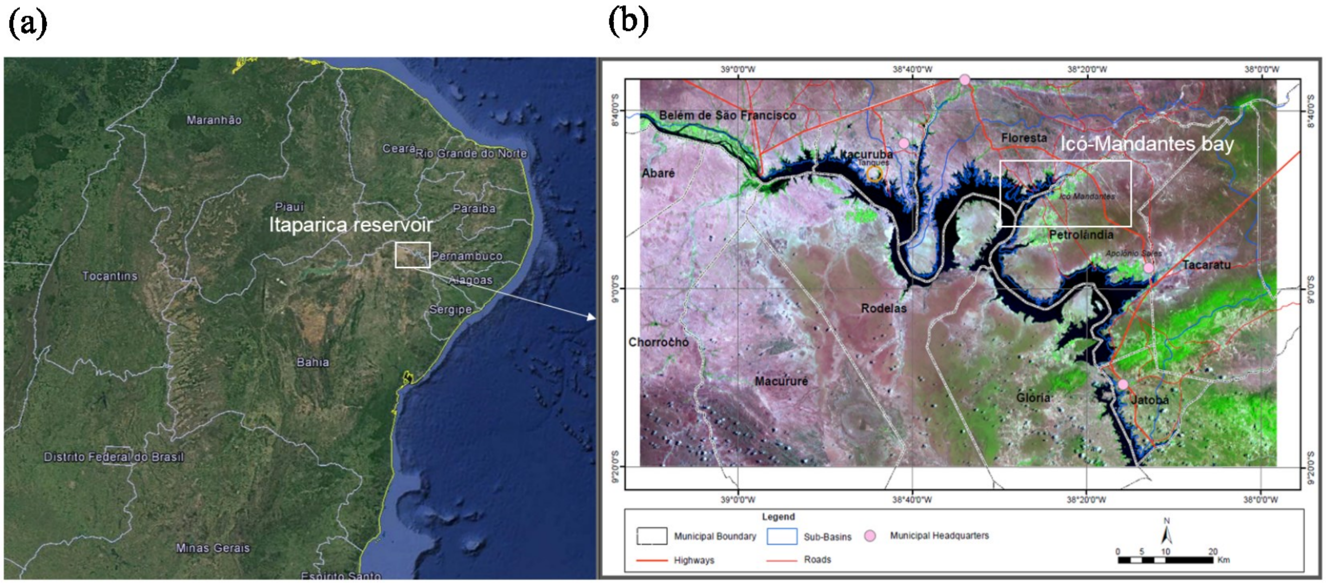

Figure 4.1 Location of the study area: Northeast Brazil (a), and capture of Itaparica Reservoir and Icó-Mandantes Bay (b). Adapted by the author from Google Earth (2016) and Lopes et al. [46].

4.5 Setup of the model and the scenarios

Computational domain and processing tools

A three-dimensional (3D) model of Icó-Mandantes Bay was set up with the open TELEMAC-MASCARET modeling system, using the unstructured triangular grid created in [67] with the software Janet (Smile Consult GmbH). The domain covers the whole bay and part of the Itaparica Reservoir, the so-called *main stream*, in order to allow the water exchange between the two water bodies, as well as a realistic inflow and outflow to the system (Figure 4.2).

The 3D grid consists of 14 layers. The resulting mesh consists of 13 prisms with variable height, depending on water depth d[m]. The layers are equidistant in the whole vertical direction (10% of d), except for the refinements near the bottom (1% of d) and near the surface (2% and 6% of d), for catching the effects of the correspondent friction stresses in higher detail. The final unstructured grid counts in total 162,932 nodes and 295,958 triangular elements, which are variable in length (range of 50 to 200 m). The surface area of the computational domain is around 128 km^2, while the maximum lengths of the domain in x- and y-direction are respectively around 18 km and 16 km.

The simulations were conducted with a time step of 30 s for each case investigated, through parallel computing on the HLRN system (North German Association for the Promotion of High and Maximum Performance Calculation) [74], using 24 processors. This enabled the simulations to be very fast; e.g. running the wind-induced flow scenarios for 10 days took between 2 and 5 minutes.

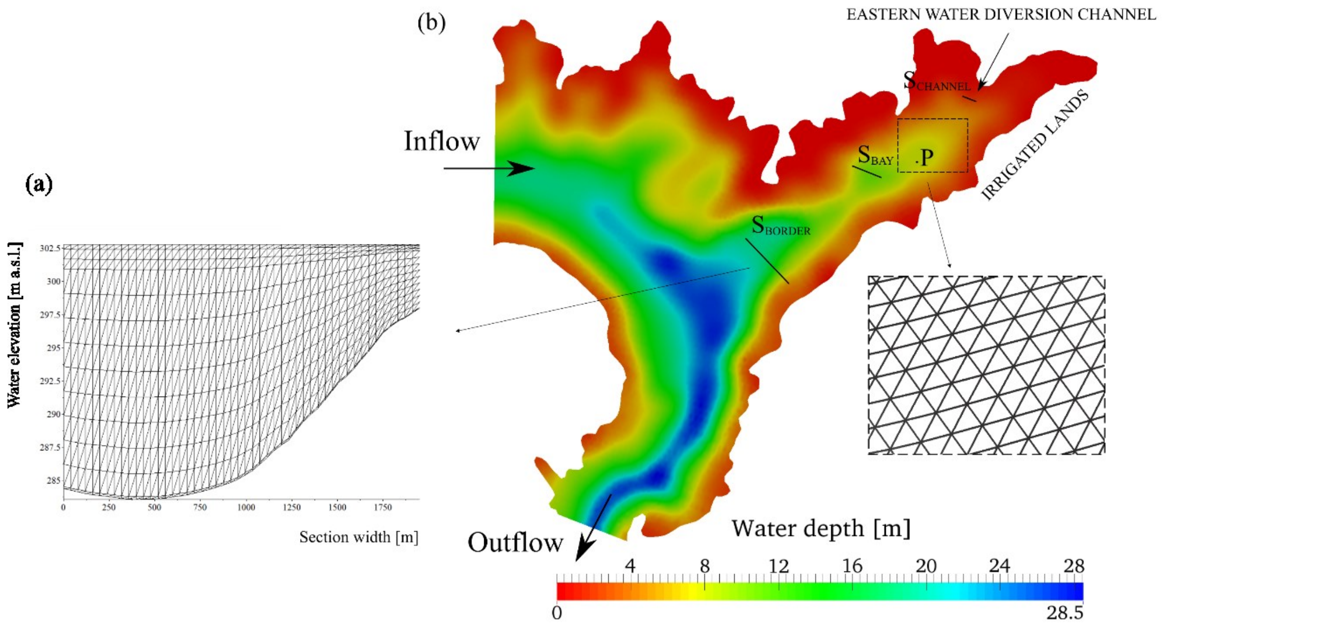

Figure 4.2 Computational domain, the inflow and the outflow boundaries, the water depth, a zoom of the horizontal mesh and the cross-sections selected for a later analysis of the results are shown (SBORDER, SBAY and SCHANNEL), as well as the location of the irrigated lands, the eastern channel of the water diversion project and the point of measurement P, which representes the position of the thermal data logger chains (b). The 14 horizontal layers and the refinement of the mesh over the water depth are reported for section SBORDER (a).

Wind and temperature data

Meteorological data is available since year 2002 on the database SINDA [119], a Brazilian integrated system of environmental data. Data of wind and temperature were recorded every three hours at the nearest weather station available located in Floresta (PE), a municipality about 25 – 30 km distant from the Icó-Mandantes Bay.

Wind data has been statistically analyzed in previous work [54]. The magnitude range of the entire sample comprises values between 0 and 15 m/s, with maximum 10% of values between 15 and 20 m/s. The predominant wind direction is 140° (from SE to NW) and the mean speed is 5.5 m/s, according to the normal Gauss distribution.

Air temperature was recorded as well between 2002 and 2016. The annual average is ~ 26 °C [110], with a high daily variability (ΔT) of about 10 to 20 °C/d, characterized by increasing values over the day (9 am – 6 pm) up to a maximum of 38 – 40 °C and decreasing over the night (6 pm – 9 am) until a minimum of 17 – 22 °C. Regarding water temperatures, Selge et al. [55] reported mean values of 24.8 °C and 27.7 °C, respectively for dry and rainy periods. During the rainy periods, the water temperatures increase and do not allow a stable thermal stratification, due to night cooling and convective currents, known as atelomixis [120,121]. This partial mixing down to the hypolimnion occurs with a frequency of a few days. Dry periods are characterized by stronger winds, higher cloud cover and high evaporation rates, resulting in lower water temperature and no stable thermal stratification, too. In order to have an idea of the stratification in the inner bay, we reported in Figure 4.3 the water temperatures over the depth for the period between October 2013 and October 2014 [49].

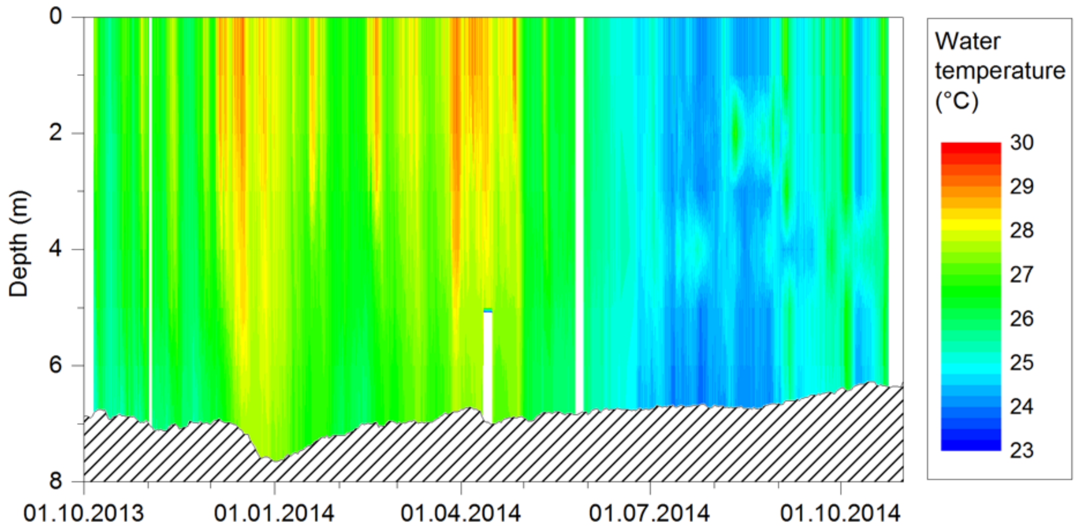

Figure 4.3 Contour plot of the vertical temperature profile in the center of the bay (S8°49'18" W38°24'32"), shown in point P of Figure 4.2, measured in a 1 m interval every 10 minutes. The structured area represents the changing water column height due to water level changes (Figure from [49]).

Simulation scenarios

The scenarios presented in this article are:

- REF (reference): application of constant mean wind on normal reservoir-operating conditions;
- WIND: simulation of a windstorm event, i.e. imposing 6 h of extreme wind, starting from REF;
- HEAT: simplified approach to simulate the effects of water heating, applying a constant temperature change (ΔT) between water and air equal to 10 °C, starting from REF;

The same boundary conditions concerning the flow were set up for the three scenarios (REF, WIND and HEAT). In detail, a constant water discharge of 2,060 m^3/s (mean value for the Itaparica Reservoir under normal operating conditions) was assumed at the inflow boundary, while at the outflow boundary a constant water level of 302.8 m a.s.l. (mean value at the Luiz Gonzaga dam [63]). The remaining lateral boundaries were set as closed walls with slip condition (i.e. the tangential velocity is different from zero).

The reference case REF was simulated until steady state was reached, considering the action of mean wind velocity and direction (i.e. 5.5 m/s, 140°). This scenario served as initial conditions, as well as a basis for comparison for the other scenarios (WIND and HEAT).

The WIND case represents a windstorm event, occurring for some hours during one day, disturbing the equilibrium conditions of REF. The extreme wind of 20 m/s (representing a gale, according to the Beaufort scale [122]) was applied for 6 hours between 9 am and 3 pm, the usual times of the day at which wind increases, within a total duration of simulation of 1 day (Table 4.1). Afterwards, the computation was continued for 5 days, in order to estimate the time needed by the system to return to equilibrium. The direction of the wind (140°) was kept constant to isolate the effects of wind's magnitude. For this scenario, the focus is exclusively on the hydrodynamics, i.e. on the wind-induced circulation patterns (horizontal and vertical) and on the local eddies caused by the wind's variation.

The HEAT case includes the transport of an active tracer; in particular, a constant temperature difference (ΔT) of 10 °C between water and air, respectively 26.5 °C and 36.5°C, was imposed to the system. A Dirichlet type condition for the water temperature at the inflow equal to 26.5 °C for HEAT and a Neumann type at the outflow were additionally prescribed for the tracer, imposing a zero gradient of temperature. The surface boundary condition, regulating the heating of the water surface, is reported and explained in Eq. 5 (and 6) of Section 2. This was chosen as a first approach, in order to verify whether heating the water surface by the atmosphere would affect the 3D flow field. If this is not the case (thus, the impact is minor), the simulation of a temperature's daily cycle would induce even lower changes.

Table 4.1 Simulated scenarios and selected parameters (REF, WIND and HEAT).

Scenarios	Simulation	Period of the day [h]	Wind velocity [m/s]	Wind direction [°]	Tracer transport
REF	10 days	00:00-24:00	5.5	140	Not included
WIND	1 day	00:00-09:00	5.5	140	Not included
		09:00-15:00	20.0		
		15:00-24:00	5.5		
HEAT	1 day, 1 week, 1 month	00:00-24:00	5.5	140	$\Delta T_{water-air}$= 10 °C

Observation points and sections

First, mass conservation was checked through the output of the initial and final water masses (volumes [m^3]), as well as the outflowing discharges at the correspondent boundaries at each time step. The 3D results were further analyzed over each horizontal layer and over time. In order to simplify the analysis, but still fully representing the results, the layers were chosen at the bottom (L_{BOTTOM}), at an intermediate level ($L_{INTERMEDIATE}$) and near the surface (L_{TOP}) (Figure 4). Afterwards, different vertical cross-sections have been chosen in some selected areas of the computational domain: S_{BORDER} at the border between the two different behaving systems (bay and reservoir main stream); S_{BAY} in the center of the bay and $S_{CHANNEL}$ next to the intake of the water diversion channel (Figure 2b). In Figure 2a, it is possible to observe the refinement of the mesh at the top and at the bottom for section S_{BORDER}.

4.6 Results

Reference case (REF)

The REF scenario is the reference case and represents the initial conditions for WIND and HEAT. Results show that the main stream is characterized by deeper waters (up to maximum 30 m water depth), while the bay is off-stream, with a maximum depth of ~ 20 m and large shallow areas along the shores lower than 3 m depth. The water in the bay is almost stagnant and the flow is mainly induced by the SE wind.

The REF results over the horizontal layers are shown in Figure 4. Looking at the variations along the water depth, it was possible to notice that the superficial levels are generally wind-oriented, while upwind (against the wind) the deeper ones (near the bed). We encountered the so-called *wind-induced return flows*: wind aligns with the flow at the surface, imposing return flow areas along the bottom [82]. Some eddies were detected near the bottom, also observable in the intermediate layers, but with higher frequency and horizontally dislocated.

The simulations were also conducted in absence of wind, in order to better observe the changes. When the wind was neglected, the vertical profiles of velocity resulted to be parabolic in the reservoir main stream part, characterized by maximum values near the surface, while in the bay quite linear with constant values very close to zero over the entire water column (stagnation areas). Otherwise, when the mean wind was considered (i.e. REF), the velocities decreased or increased in the superficial layers, respectively if the flow was upwind or in wind direction. For instance in section S_{BORDER} shown in Figure 2, the vertical magnitude of velocity (w) was comparable with the horizontal ones (u, v); thus, we incurred in some 3D effects (Figure 4.5b).

Windstorm case (WIND) and return to equilibrium condition

The results of this scenario were compared before, during and after the windstorm (20 m/s, 140°). The changes concerning the horizontal output of the flow field, as well as the variations over the vertical direction, can be observed in Figure 4.4b. The magnitude and the orientation of velocities were significantly influenced by the wind, but to different extents. The range of velocities increased at least of one order of magnitude during the windstorm: up to 10^{-1} m/s in the reservoir main stream and up to 10^{-2} m/s in the bay part.

During the storm i.e. at 12h (Figure 4.4b), the flow field is overall wind-oriented on the superficial layers, except for the main stream region, where a big horizontal clockwise circulation of approx. 2-km^2-area was formed. This horizontal pattern was still observable on the deeper intermediate and bottom layers, but rather shifted downstream, accompanied by an additional anticlockwise circulation of similar dimensions closer to the northern shore. On L_{BOTTOM} and $L_{INTERMEDIATE}$ in the bay, the flow field is weaker and more chaotic, compared to L_{TOP}. In areas where $d < 3$ m, the velocities are often wind-oriented over the entire water depth. Observing the results later on at 24h, the number of eddies increase in general over the superficial and intermediate layers, characterized by eddies of ~500 m to 1 km in diameter. This seems to be due to a sort of relaxation and readjustment of the flow field, attempting to return to initial equilibrium conditions. Velocities on L_{BOTTOM} are very close to zero. The variable and more irregular flow at this time step suggest the presence of 3D circulation.

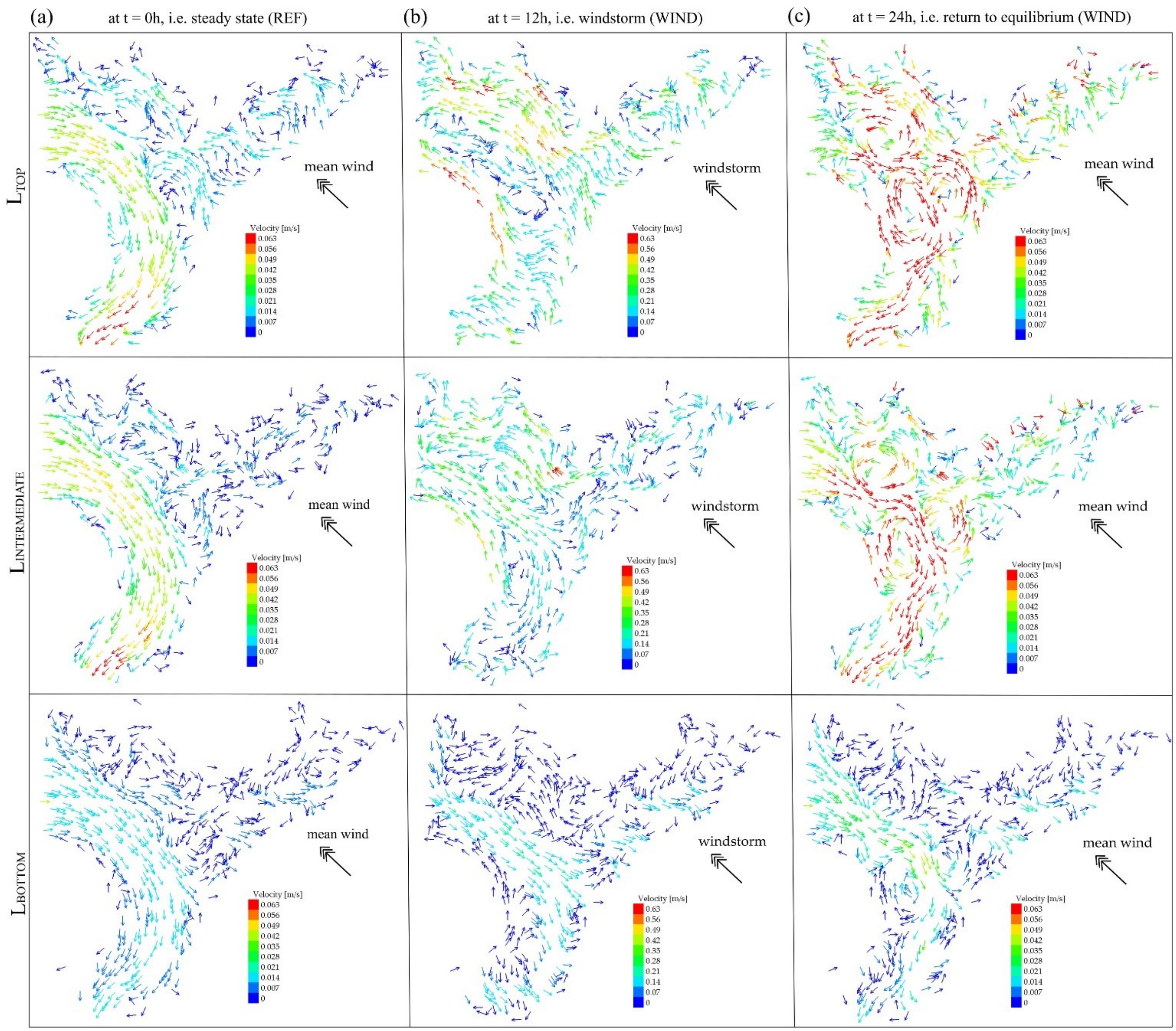

Figure 4.4 The horizontal layers at the surface (L_{TOP}), intermediate ($L_{INTERMEDIATE}$) and bottom (L_{BOTTOM}) are shown for WIND scenario at (a) t = 0h, i.e. steady state (REF), (b) t = 12h, i.e. windstorm and (c) t = 24h, i.e. return to equilibrium. The use of different scale was necessary for a clear display of the results, given to the different orders of magnitude. The relation between the intensities of velocities is 1:10 (a:b).

Looking at various cross-sections in the domain, different flow behaviors were observed. Along the reservoir main stream, where water is deeper, the velocity profiles have a parabolic shape, which is typical for open channels. There, the influence of the wind is evident through a deformation of the curve closer to the surface; the wind slows down the velocities near the surface, in the case of upwind flow, invoking the occurrence of return flows.

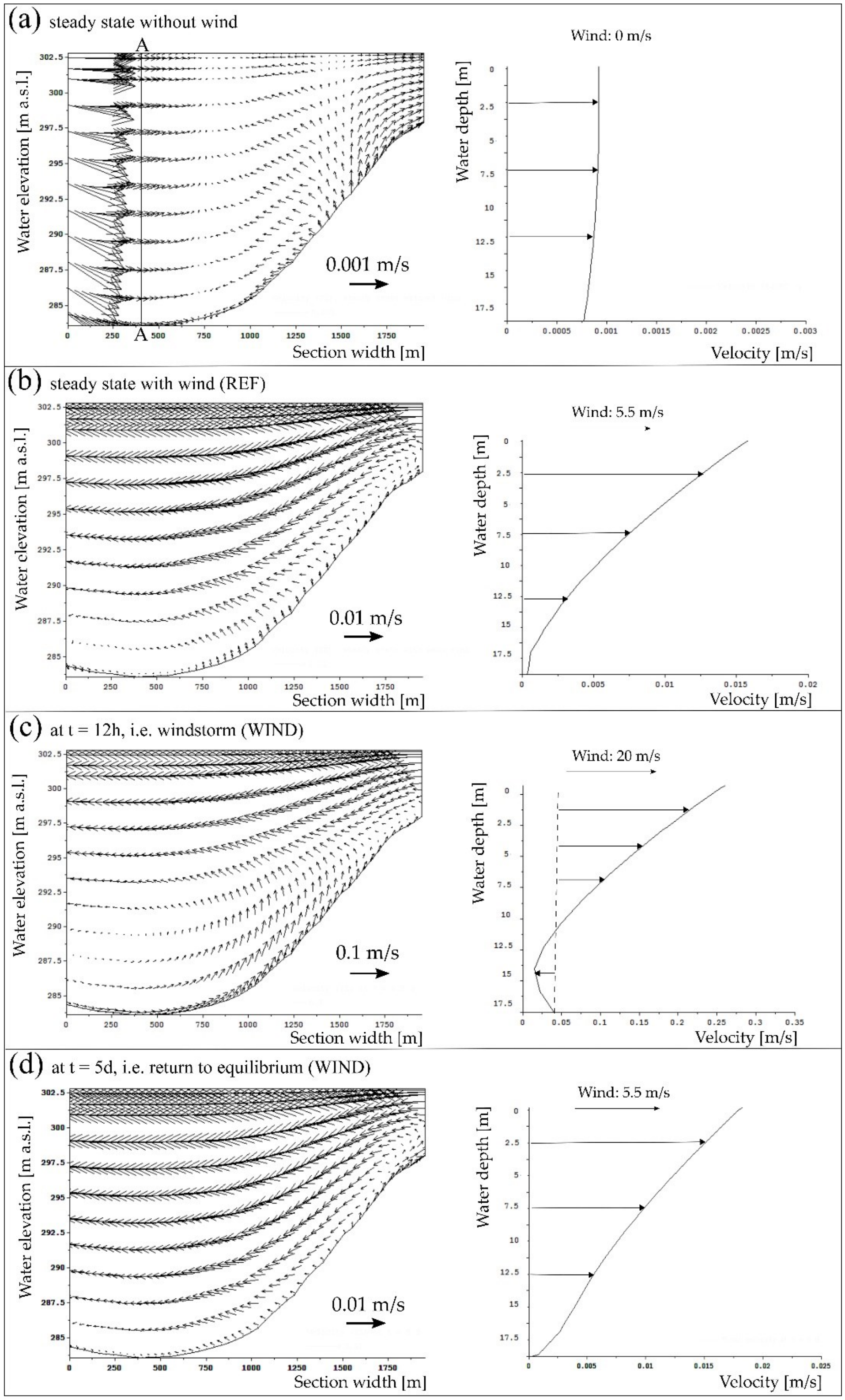

Figure 4.5 Vertical output of the velocities in section S_{BORDER} and profile in A-A for the different scenarios: in absence of wind (a), for REF (b), for WIND at t = 12h (c) and at t = 5 d after the windstorm (d).

Specifically in section S_{BORDER} (Figures 4.2 and 4.5), located at the imaginary border between the bay and the main stream, where mutual exchange processes take place, we observe water moving from the shores to the deeper inner parts (surface layers) and a weak upwelling for REF (Figure 4.5b), which becomes wider involving bigger part of the water depth during the windstorm, accompanied by a velocity's increase at least of one order of magnitude (at t = 12h, Figure 4.5c). In that region, the horizontal and vertical flow components are in a similar range.

Additionally, the behavior of the flow field in the center of the bay (namely S_{BAY} of Figure 4.2) is shown in Figure 4.6. Comparing REF and WIND (the latter during the windstorm, i.e. at 12h): the flow velocities are mostly wind-oriented in both cases in the vertical direction, with an increase of velocities of one order of magnitude for the latter (scale of 0.1 m/s). This flow pattern was rather maintained in time; therefore, the further steps are not reported. Finally, the WIND scenario was compared to REF also in the cross-section at the intake of the water diversion channel (namely $S_{CHANNEL}$ of Figure 4.2) and shown in Figure 4.7. In REF, the water velocities were <= 0.005 m/s, while during strong wind they increased by more than one order of magnitude (higher near to the bed), but they kept the same direction over the water depth. After around three days of simulation, the flow configuration became similar to pre-disturbance conditions, i.e. REF. In other shallow areas of the bay along the shores near the irrigated lands, the flow was mostly wind-oriented over the entire depth, both for REF and for WIND, because of the intensity of the wind, inducing movement in those shallow and stagnant waters.

Since steady state was not reached yet one day after the windstorm, the computation was continued for five additional days, under the same conditions as REF i.e. constant mean flow and mean wind. The changes observed at the end of this computation were lower than $1 \cdot 10^{-3}$ m/s, concerning mean velocities. Since the discharges at the outflow boundary reached the steady state already after four days, with differences < 0.1 m^3/s, and changes in the cross-sections and over the layers were no longer substantial, we can affirm that the flow field returned to equilibrium by that time. The water mass volumes V [m^3] were always conserved after each time step (ΔV lower than 0.01 %).

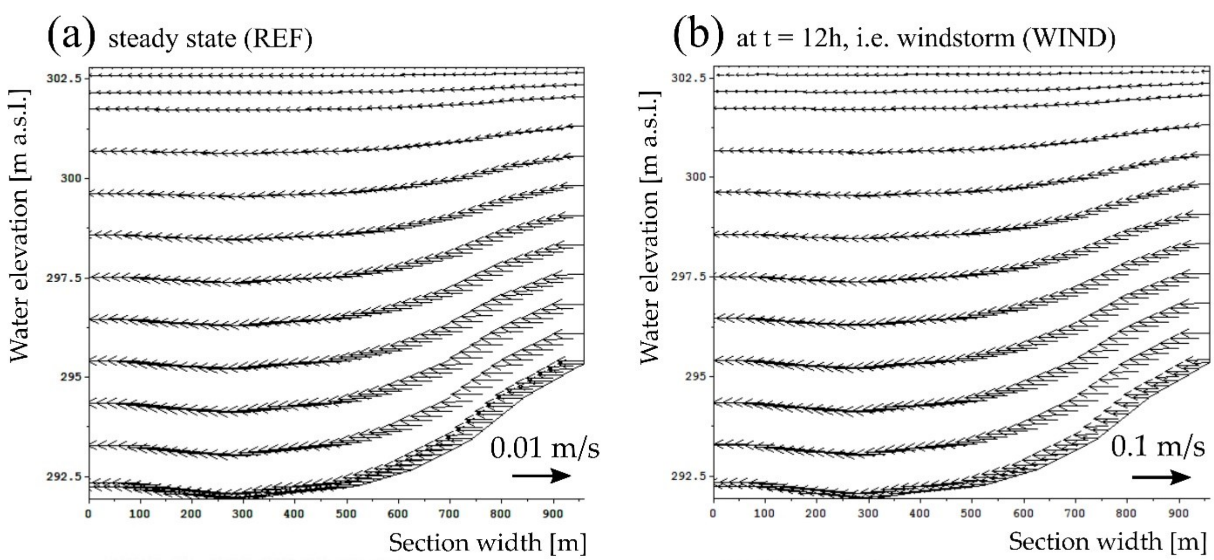

Figure 4.6 Vertical output of the velocities in section S_{BAY} for REF (a) and for WIND at t = 12h (b).

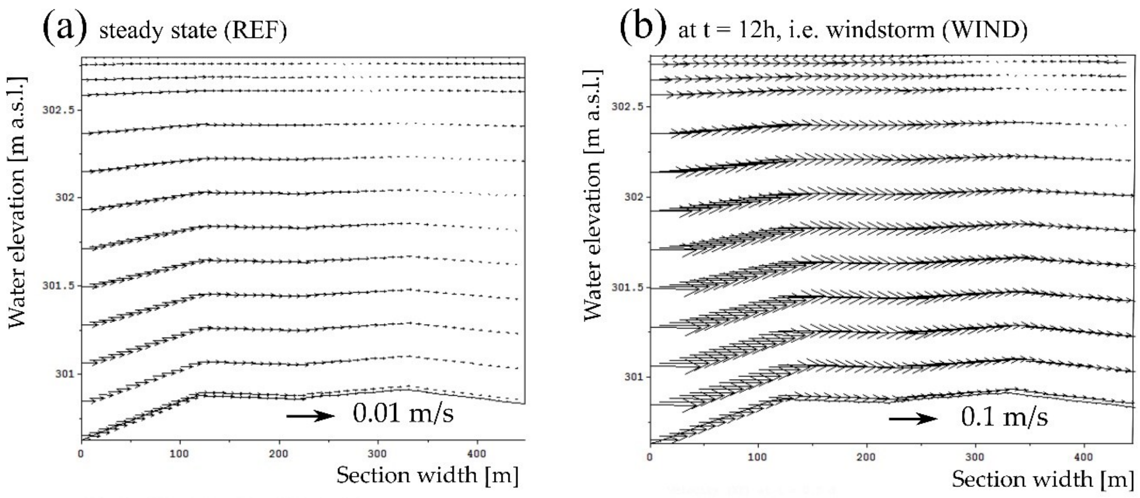

Figure 4.7 Vertical output of the velocities in section $S_{CHANNEL}$ for REF (a) and for WIND at t = 12h (b).

Simplified approach to simulate the effects of water heating (HEAT)

The results were analyzed at different time steps (i.e. after few hours and until one month), in order to identify the time needed by the entire system to shift to a new equilibrium under the imposed constant conditions (Section 4.3).

Looking at L_{BOTTOM}, already during the first three hours up to one day, the heating effects induced the velocity vectors to be oriented from the deeper areas in direction of the shores (Figure 4.8c). The flow velocities were higher near the inflow (shown in Figure 4.2), along the main stream nearer to the western shore and in the bay as well. The opposite behavior was noticed in the superficial layers: the flow field oriented from the shallower (and warmer) peripheral parts to the deeper (colder) ones (Figure 4.8a). As expected for smaller water depths, the shores were heated faster. The weakest velocities occurred at the intermediate levels, and, close to $L_{INTERMEDIATE}$, it was possible to observe a change in the flow configuration (bed- or surface-type). Figure 4.8 shows the outline of the temperatures and the flow field over the layers L_{BOTTOM}, $L_{INTERMEDIATE}$ and L_{TOP} after one day of simulation.

Continuing the calculations until one week, the velocities increased progressively in the entire domain: the flow configuration became rather stable after one day near the bottom, while in the upper layers (from $L_{INTERMEDIATE}$ to L_{TOP}) was still affected by slight changes. After one week, the water mass in the entire bay reached temperatures higher than 30 °C, and, after 2 weeks, no changes was observable in the flow field (neither circulation nor values).

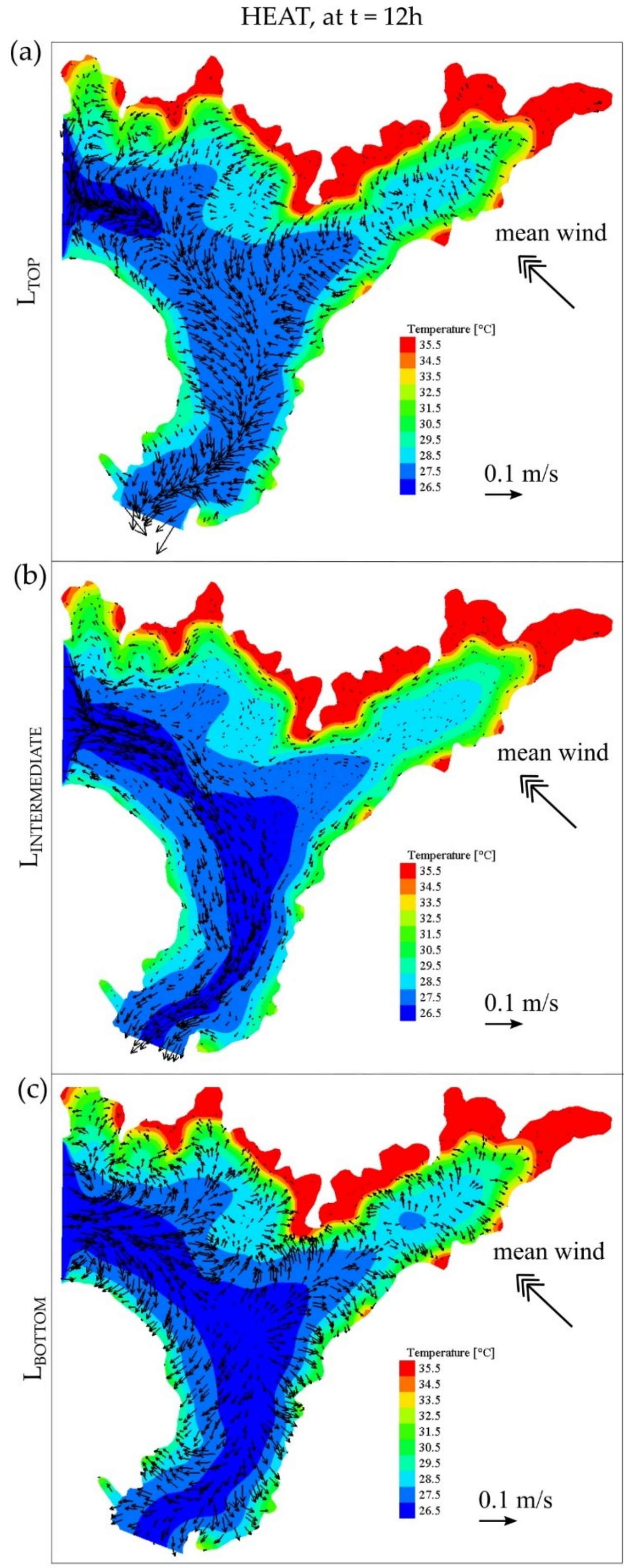

Figure 4.8 Results of the HEAT scenario after one day simulation. The horizontal layers at the surface (L_{TOP}), intermediate ($L_{INTERMEDIATE}$) and bottom (L_{BOTTOM}) are shown (respectively a, b, c).

Figure 4.9 reports the outline of the total velocities in S_{BORDER} (same of Figures 4.2 and 4.5). Comparing Figure 4.4a and 4.8, as well as Figure 4.5b and 4.9, the flow field changed for HEAT and the velocity vectors are oriented in opposite directions at the surface relative to closer to the bottom, suggesting an anticlockwise movement of the water mass from the warmer to the colder areas. The velocities' order of magnitude was in the same range as they were for the reference case REF (approx. 10^{-3} to 10^{-2} m/s), even if in the shallower part of the section the maximum values were at least doubled and the minimum were found in the central part of the section (approx. from 2 to $8 \cdot 10^{-3}$ m/s). A slight progressive increase of the flow field was registered until one week, while the vertical configuration remained constant in time. Between one week and two weeks, the maximum velocities raised still of ~ $3 \cdot 10^{-3}$ m/s and finally less than 1 mm/s between two weeks and one month. Looking at the temperature values in S_{BORDER}, the minimum and maximum values were respectively 26.8 and 28.4 °C after 12 hours, 27.5 and 29.5 °C after one day (Figure 4.9), 29.3 and 31.9 °C after three days, 30.6 and 33.5 after one week, 31.0 and 33.8 after one month. The maximum ΔT in water equal to maximum 2.5 to 3 °C reached after 3 days remained rather constant in time, while the overall values of temperature increased gradually until one week of simulation. Nevertheless, this did not occur over the vertical direction; thus, no stable stratification was observed. Additionally, the temperature gradient was formed between the shallow littoral areas and the center of the bay (Figure 4.9). In this case, the convective propagation of dense water intrusion occur after crossing temperature of maximum density, according to Boehrer and Schultze [10]. Afterwards, continuing the computation up to one month, no more changes were observed in the entire computational domain.

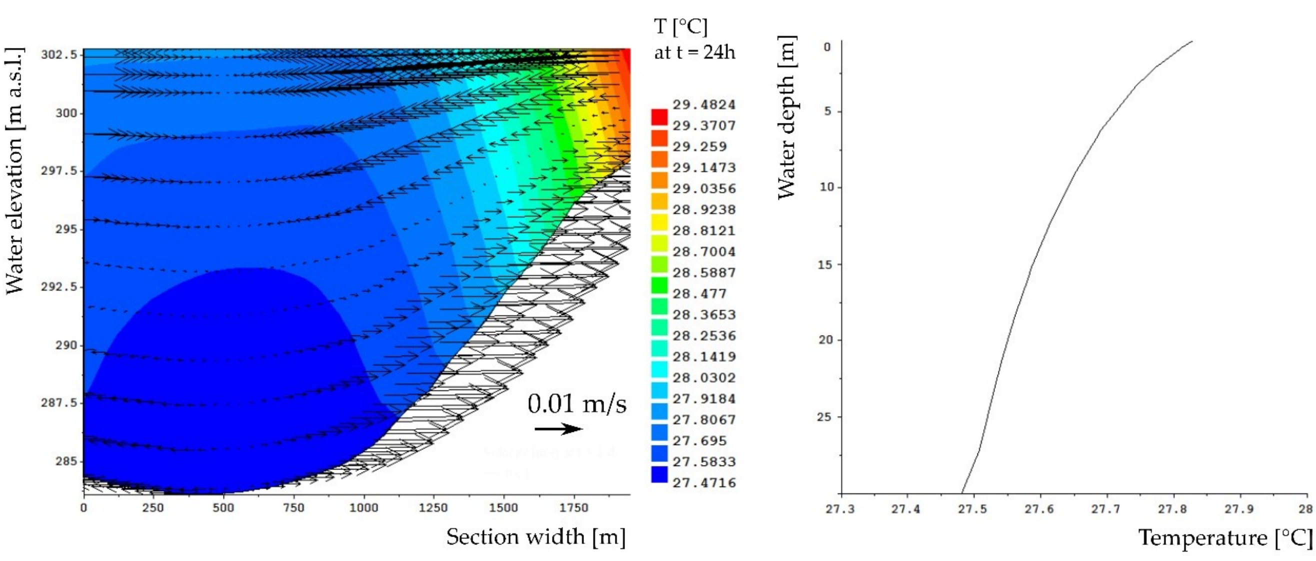

Figure 4.9 Results of the HEAT scenario after one day simulation in section S_{BORDER} (Figures 4.2 and 4.5), showing the vertical configuration of temperatures and velocities over the vertical section. The arrows represent the velocity intensities and orientations in the section (water mass) and it is observable how they were more intense near the contour of the section next to the shores.

In the center of the bay, the flow velocities had similar order of magnitudes compared to S_{BORDER}, even if with lower extremes. The temperatures had similar circulation patterns, but with higher vertical temperature gradient in S_{BAY} (i.e. <= 1 °C, Figure 4.10). For the section next to the water diversion channel, the velocities were approximately doubled and there was an impact on the currents as well. The temperature difference observed over the water depth was even smaller (< 0.5 °C, Figure 4.11).

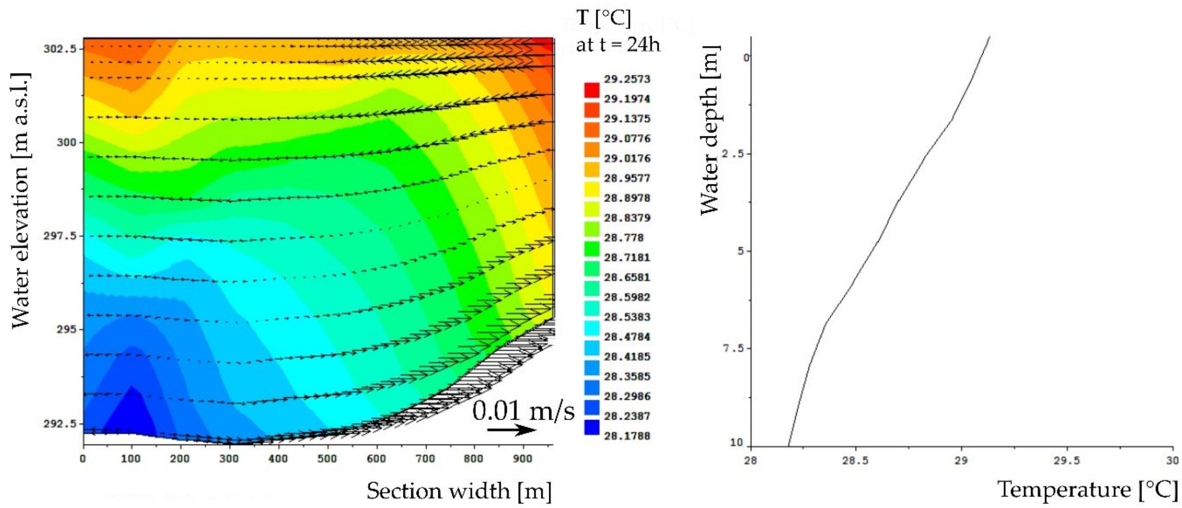

Figure 4.10 Results of the HEAT scenario after one day simulation in section S_{BAY} (Figures 4.2 and 4.6), showing the vertical configuration of temperatures and velocities over the vertical section. The arrows represent the velocity intensities and orientations in the section (water mass).

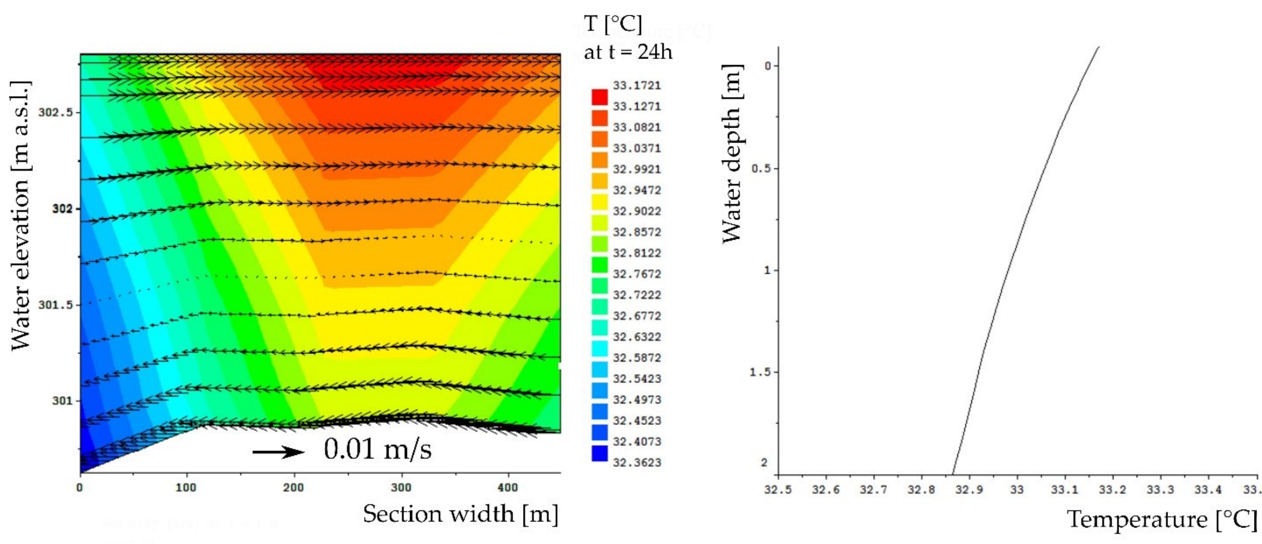

Figure 4.11 Results of the HEAT scenario after one day simulation in section $S_{CHANNEL}$ (Figures 4.2 and 4.7), showing the vertical configuration of temperatures and velocities over the vertical section. The arrows represent the velocity intensities and orientations in the section (water mass).

Synthesis of the modeling results

The results of the WIND and the HEAT scenarios, compared to the reference REF, showed that strong wind and density changes had an impact on the flow field, confirming a wide range of previous studies (e.g. [10,42,72,76,96]). On the one hand, while the configuration of the flow following the SE wind was rather maintained in time both horizontally and vertically, the imposed constant ΔT equal to 10 °C changed it substantially (e.g. the flow in the surface layers was induced from the shallow to the deeper waters). On the other hand, the wind had a much higher impact on the velocities, up to more than one order of magnitude. This is in agreement with De Marchis et al. [96] and Fenocchi et al. [72], who as well observed an increase of flow velocities of one order of magnitude in the case of wind and especially during storm events. For the density-induced flow, a velocity increase took place to a lower extend in some specific zones, e.g. on the bottom and superficial layers next to the lateral boundaries, while there was a general decrease at the intermediate water depths. According to Abbasi et al. [42], higher wind leads to higher return flows and shallow parts respond faster to air heating; the occurrence of these two phenomena are observable in our results, respectively in Figure 4.5-c, 4.8 and 4.9. Moreover, during the heating phase, temperatures increase especially in the top layers near the water surface [42], as noticed as well in Figures 4.10 and 4.11.

The vertical (w) and horizontal (u, v) components of velocities, as well as the water depths, were analyzed in detail for the cases investigated. The formers differed by at least two to three orders of magnitude (being u, v higher than w), except during the windstorm, when they reached a comparable range of values. The variation of the water depths have been analyzed in several observation points in the computational domain. They decreased in a range of 20 to 60 mm, comparing WIND to REF, due to the higher velocities, and increased in a range of 1 to 5 mm, comparing HEAT to REF, due to thermal expansion. Additionally, concerning the average values computed for the bay area, the water depths decreased by 7 mm, comparing WIND to REF, while they increased by 4 mm, comparing HEAT to REF. Thus, the variations of the water depths were considered absolutely minor (mm against means of at least 10 m).

Further summarizing the results, it can be mentioned that the flow field was able to return to equilibrium at least three days after a specific event (e.g. windstorm), as long as the disturbance (e.g. the wind) disappeared. Otherwise, it evolved until the achievement of a new steady state: few weeks were needed for the HEAT case.

Finally, a clear stable temperature stratification was not observable and the water column was well mixed over the entire computational time (up to one month). The ΔT in water over the vertical was generally lower than 0.5 °C (e.g. Figure 4.7), except for the most stagnant parts (e.g. Figure 4.10), where ΔT reached maximum 1 °C. Therefore, the water body is not classifiable as stratified (e.g., ΔT > 1 °C is one of the different criteria for stratification presented in [123]). This was considered a reasonable response of the system, in accordance with existing theories and limnological findings [10,49,110,121], due to the following reasons:

- the modeling showed that the 3D flow field was sensitive to the heating of water surface, inducing a vertical movement of the water mass and, thus, contributing to the vertical water mixing;

- the deeper reservoir main stream is characterized by a strong inflowing discharge from the upstream Sobradinho (here, approx. 2,000 m^3/s), which did not allow a stable stratification in the flow field concerning that part;
- large parts of the bay are shallow (see Figure 4.2) and highly influenced by the SE wind (usual ranges as for REF, with daily higher or lower peaks), contributing also to the vertical water mixing (in agreement with e.g. De Marchis et al. [96]);
- according to Boehrer and Schultze [10], stratification can be established in the warm season if the lake is sufficiently deep (which is not the case here). Additionally, lakes are found to behave like an epilimnion (to be well mixed), in response to strong temperature gradients between water and air (i.e. 10 °C in this case).

Concluding, the applicability and reliability of the presented model is retained acceptable, certainly with some constraints. This is mainly due to the extreme complexity of the processes studied, the lack of measurements of some parameters or their availability in only one point of the domain [39,42].

Recommendations for water management

Small inland water bodies are often neglected in hydrological and water resources management plans, principally because it is difficult and expensive to monitor them [38,39]. Nevertheless, they are of greatest importance for the regional economic development and for the maintainance of water quality standards. The implications between the important hydrodynamic findings of the numerical modeling for water management at the local scale are rarely explored, but need to be outlined. Currently, the water diversion channel is not yet in operation [124], while the withdrawals for irrigation agriculture are managed by CODEVASF (Development Company of the São Francisco and Parnaíba Valleys), outsourcing the engineering company PLENA Engenharia. The users are allowed to pump water for a few hours per day (usually 8-12h), with a maximum (hourly) withdrawal between 1.4 and 1.7 m^3/s [125].

In this work, we observed that the 3D effects on the flow field should be taken into account when managing the multiple water uses of the bay (addressed for instance in Arruda [47] and by the Ministry of National Integration [124]) deriving the following management suggestions and ideas for further investigations:

- The reservoir management needs a new approach, which requires first of all a differentiated analysis and evaluation for the reservoir main stream and its bays, characterized by different regimes (e.g. velocities), and where the 3D modeling is adopted as supporting tool;
- In particular, the withdrawals for drinking water and for irrigation agriculture, located in the tip of the bay and along the south-eastern shallow shores of the bay, should stop working during windstorms and at least three days afterwards, especially in case of rain after long droughts. In such event, two important facts would occur: (1) the mostly frequent wind from SE to NW induces the flow in a strong circulation current along the southeastern shore, where the irrigation lands are located, towards the tip of the bay; (2) the irrigation drainage systems would be overflowed and rich of nutrients and pollutants from the field, in case of rain, especially after long droughts. This implies that material

such as suspended sediments, nutrients and rubbish would be transported towards the tip of the bay, where the water diversion is located. To be able to prevent or at least reduce such issues, it is important as well to launch initiatives among the rural communities such as the cleaning up of the shores areas from undesired material and the implementation of waste-collection procedures, since there is no proper disposal of waste or emissions by various consumptions in the region;

- Water surface heating due to strong temperature gradients would induce the suspended material present in the surface layers to be transported to the center of the bay, where the water is more stagnant even during a windstorm. On the contrary, the substances, nutrients and sediments deposited in the bottom layers would be conducted towards the shores and to the upper layers, with the occurrence of upwelling near land. This may increase phenomena like the accumulation of sediments in the shallow areas, which dessiccate during the water level decrease due to hydropower operations, increasing the development of HAB. Further assessments using a water quality module are needed to support water management in this direction;
- The 3D model can then be used to identify high risk contamination areas in the Icó-Mandantes Bay, in order to plan promptly the necessary monitoring operations to ensure good standards of water quality for drinking water, as well as to control and regulate the development of further net cage aquaculture systems, in particular in the stagnant areas of the bay, next to the water intakes (water supply, irrigation).

4.7 Conclusions

To study the dynamics of surface water bodies such as lakes and reservoirs, the use of three-dimensional (3D) models is often preferred, since external forces as wind play an important role, enhancing 3D effects in the flow field and being one of the main drivers of water movement. This occurs in particular in more isolated peripheral bays, where the velocities are usually very low and characterized by different hydraulic regimes compared to the reservoir main streams. The case of the Icó-Mandantes Bay, one of the major branches of the Itaparica Reservoir (Sub-Middle São Francisco River, NE Brazil) was presented in the article and a 3D model was set up using the open TELEMAC-MASCARET modeling system [77]. The impacts of wind and heating of the water surface on the hydraulics of the bay have been meticulously explored, in the horizontal and vertical direction, detecting the consequent 3D effects. In conclusion, an advanced reservoir management for multiple uses has to consider also the issue of water quality and, for this case study, to focus especially on the need to keep oligotrophic levels, because the Icó-Mandantes Bay is already overcharged [49]. Since the hydrodynamics of such a water body are highly linked with water quality complex processes ([69]; e.g., algae growth and sediment fluxes), in future work, the existent 3D model should be coupled with a water quality module (e.g. with TELEMAC's latest version 7.2 is currently feasible, using the WAQTEL module). In particular, further research should focus on (1) the risk of HAB development, mainly on their inoculation in the lentic bay areas and their interaction with the reservoir main stream, (2) the spreading of HAB and its impact on the withdrawals for drinking water or irrigation agriculture and (3) the adaptation of hydroelectric production to reduce water level fluctuations, in order to minimize the introduction of nutrients from the desiccated soils in the shallow areas and, thus, the greenhouse gases (GHG) emissions as well. Moreover, external forces such as the wind should be always included in the model, as well as the heating and cooling processes, since they have indeed complex and differentiated impacts of the hydraulics of water bodies such as the Icó-Mandantes Bay.

Chapter 5

5. Conclusions

In the framework of the bi-national, inter- and transdisciplinary INNOVATE project (e.g., [66]), this research focused on the Icó-Mandantes Bay, one of the major branches of the Itaparica Reservoir, located in the Sub-Middle São Francisco River Basin, Northeast Brazil. Two-dimensional (depth-averaged) and three-dimensional numerical models were set up with the open-source software TELEMAC-MASCARET [77], with the aim to assess the complex flow and transport processes in the water body, being stressed by multiple purposes (e.g. water supply) and dramatically affected by the impacts of climate change (e.g. extended drought).

Very few studies were previously conducted in the region and they mostly focused on the entire river basin or on the local scale, in order to respectively assess runoff discharges or limnologic parameters. So far, numerical modeling using hydrodynamic and transport models at the reservoir scale were not yet available in literature and the serious challenges that the water authorities, managers and smallholders have currently to face cried out for a tool, capable to predict the consequences of different (combined) scenarios and thus to support decision-making. Simulating several climate-, issues- and stakeholders-oriented scenarios, the models presented filled this gap and deepened the knowledge of a complex water system. Despite the lack of data and the impossibility to conduct hydraulic field campaigns during the course of the project, which would have been necessary for a proper calibration and validation, the models were tested in other ways, e.g. checking for mass conservation, carrying out sensitivity analyses and qualitatively comparing the results with similar studies in other parts of the world. The models are considered reliable with certain constraints. Moreover, the use of open-source modeling tools is considered an advantage of this study, pioneer for the region and ready to be further refined and improved, in order to be concretely taken into account and applied in future integrated water resource management plans.

This chapter synthetizes the main outcomes of the work done and the implications for water resource management in the Icó-Mandantes Bay, giving an outlook for future research studies.

5.1 Synthesis

This section synthesizes the scenarios investigated in Chapter 2 to 4, bringing together the specific scientific outcomes.

Synthesis of the outcomes of the two-dimensional modeling

The principal results of the 2D modeling (Chapter 2, 3) are reported in the following:

- Different unstructured grids with triangular cells were setup for the 2D simulations: one for the low water level (LWL) and one for the mean and high water level cases (MWL, HWL). This was done with the aim to analyze the results under both dry and wet conditions, varying initial and boundary conditions (constant or variable in time), concerning water elevations and discharges, according to the case to investigate. The meshes have approx. 20,000 triangular cells, with an averaged element length of around 120 m.
- The flow field results showed different behaviors for the part of the computational domain concerning the main stream of the Itaparica Reservoir and the one covering the Icó-Mandantes Bay. The first hydrodynamic simulations showed that the bay was clearly isolated from the reservoir main stream and the water in the bay was almost stagnant, in absence of external forces [52,54]. Since the wind is mostly present in the area, it was always taken into account in the numerical simulations. In particular, the reference cases presented in Chapter 2 to 4 took into account the mean wind (5.5 m/s) and the most frequent wind direction (140°, from Southeast towards Northwest), which were determined in previous unpublished work through a statistical analysis, together with an extreme wind velocity (20 m/s). The resulting mean flow velocities in the system, respectively for LWL and HWL scenarios, were 0.013 and 0.064 m/s, considering the entire area of the models, 0.015 and 0.083 m/s in the reservoir main stream only, while 0.001 and 0.007 m/s in the bay. Comparing the values in the bay and in the main stream, the velocities diverged more than one order of magnitude. The mean water depths (m), respectively computed for the LWL and the HWL cases, were around 11 and 13 m in the main stream, while 4 and 5 m in the bay. Under wet conditions (HWL cases) and, thus, for higher discharges and water levels, the bay was even more isolated from the main stream.
- The nutrient emissions of a net cage aquaculture system hypothetically located inside the bay, in a strategic location i.e. near the withdrawals for irrigation agriculture, were simulated on the short (1 day, 1 week) and on the longer term (1 month, 6 months), implementing a punctual tracer source and using data of dissolved nitrogen and phosphorus, measured in an aquaculture system already existent in the reservoir. The results showed that the increase e.g. of phosphorus already after one week simulation at the source of emissions was alarming (approx. 8 μg/L), considering the carrying capacity limits of the bay, and thus of the reservoir [44,55]. Moreover, the concentrations of nitrogen and phosphorus reached generally higher values for LWL and they spread

faster inside the bay, while for HWL were retained longer (56 % of the initial quantity left the domain after 6 months for LWL and only 36 % for HWL). Therefore, the study conducted suggested that installation of a net cage aquaculture system inside the Icò-Mandantes Bay would affect more the water quality under low water conditions on a shorter term, but under high water conditions on a longer term.

- The effects on the hydrodynamics due to the operation of the eastern channel of the water diversion project were investigated for a period of 10 days, considering dry conditions in the reservoir (worst scenario), as well as for the foreseen normal and maximum withdrawal (ANA 411, [65]). To do so, the unstructured grid set for LWL was used and an additional open boundary was implemented to enable the outflow, refining the grid in the surroundings of the new boundary. The flow field was not significantly influenced by the withdrawal concerning the water quantity, except for the increase of the flow velocities in the near-field of the channel's boundary. In detail, the mean flow velocities obtained for the operational and maximal withdrawal were both equal to 0.015 m/s (variation lower than 10 %), while respectively 0.007 and 0.010 m/s in the bay area (variation up to 60 to 70 %, although the velocities remained low in the order of cm/s). Observing the results in several points of the domain, they showed that the impact of the withdrawal was increasingly higher getting closer to the channel's boundary. The water depths and the water volume were not affected by the channel.
- The impacts of a flash flood from the intermittent tributary Riacho dos Mandantes was investigated together with tracer transport, since this small stream is considered one of the main sources of contaminants for the bay. A third boundary was opened at the location of the tributary and the grid was refined in the near surroundings. An hydrograph curve with a total duration of three days and with a peak of 40.2 m^3/s discharge (HQ_{10}) reached after 1.5 days was imposed at the new boundary, combined with a mass-conservative (passive) tracer, which was assumed to have a constant concentration, in order to reproduce a contamination through the flood curve. The scenario was conducted under dry and wet conditions, varying the respective water levels and inflow discharges flowing in the Itaparica Reservoir. The results showed that the flood had a very limited impact on the water dynamics in the main stream, while a much higher one in the bay. In the proximity of the tributary's inflow, the change in the flow velocities was around 0.006 m/s, compared to 0.009 m/s registered for the LWL reference case, while the variation was between 0.003 and 0.012 m/s for the HWL. The flow field returned to steady state approximately 3 to 4 days after the end of the flood event. Concerning the tracer transport, the concentrations reached high values (80 to 100% of the initial ones) for both wet and dry scenarios in the northern tip of the bay on the short term (up to one week after the flood), nearby the intakes of the water diversion channel and some pumps for irrigation agriculture. In that location, the values remained higher than 10% until one month of computation under wet conditions, while they decreased of 90% already few days after the extreme event for the drought scenario, reaching concentrations of approx. 1 to 2%. More south in the bay towards the reservoir main stream, the values of concen-

tration remained rather low during the entire computation time (lower than 5% in each case observed). Overall, the spreading of the tracer was much faster under drought conditions in the domain, while it was retained longer under wet conditions.

- In order to estimate the water residence time of the bay having no straight flow through, e.g. like a river, the classical one-dimensional methods could not be applied; therefore, it was necessary to implement an alternative approach. A mass-conservative (passive) tracer with a constant concentration was set as initial condition in the whole bay, while zero concentration in the rest of the domain. The results were organized into different intervals of concentration and the residence time was arbitrarily defined as the time at which all points of the bay belong to the latter interval, thus when the concentrations were lower than 10% of the initial value. Since the exchange processes between the reservoir main stream and the bay are very slow, it was necessary to compute long-term simulations up to 2 years. The simulations were conducted under constant as well as variable flow and water level conditions, while the southeastern mean wind was always taken into account. The results of the drought scenario (assuming a constant discharge and low water level) were found to be very similar to the ones which considered the daily variable water levels and flows, while they all differed relevantly by the results observed for the wet scenario (constant discharge and high water level). Thus, a time-variable water level did not relevantly encourage the water exchange between the bay and the main stream. As observed above for the Riacho dos Mandantes' case, the tracer concentrations were retained much longer in the bay for high water level conditions. E.g., after six months, approx. 40% and 60% of the initial quantity were still registered inside the bay, respectively for LWL and HWL conditions, and values lower than 10% were approached the soonest after one year. To conclude, the estimated residence times were defined equal to 725 days for the high water level case, while 545 days for the low and variable water levels and discharges. Besides, the computed residence times for the bay were much bigger than the reservoir's (approx. two months). Finally, the results of some exploratory studies (unpublished work) showed that the residence times were significantly reduced, when the eastern channel of the water diversion project was included in the model and simulated for the foreseen withdrawals, up to 50% for the maximum one. This is considered positive for the system, which is clearly characterized by very low exchange rates. This point will be discussed in more detail in the next section, concerning the management implications.

Synthesis of the outcomes of the three-dimensional modeling

The scenarios investigated using the 3D modeling and examined in Chapter 4, as well as the relative main outcomes, are reported in the following:

- A 3D model for the Icò-Mandantes Bay was set up, multiplying the unstructured grid created for the 2D scenarios over fourteen layers in the vertical direction, refined near the bottom and near the surface, in order to better assess the effects of the bottom and surface frictions, and choosing the 3D numerical settings, e.g. related to the turbulence models in the horizontal as well as in the vertical direction.

- The model was applied to simulate wind- and temperature-induced flows, in order to investigate the 3D effects on the flow field, in term of horizontal and vertical circulation patterns, flow velocities and water depths. Specifically, a mean wind case and a windstorm were investigated and analyzed over the horizontal layers as well as in different cross-sections, chosen in strategic locations. Besides, the heating of the water surface was simulated setting a constant temperature difference (ΔT equal to 10 °C) between the water and the atmosphere, under mean wind conditions. The results showed that strong wind and density changes had an impact on the flow field. On the one hand, the wind did not change the flow circulations neither horizontally nor vertically, but it had a much higher impact on the velocities in terms of intensity, up to more than one order of magnitude. On the other hand, the imposed constant ΔT lead to a much slighter increase of the velocities and only in some specific zones, e.g. on the bottom and superficial layers next to the lateral boundaries, while at the intermediate water depths the water became almost stagnant. Nevertheless, the density-induced flow changed the configuration of the flow, both horizontally and vertically (e.g. the flow in the surface layers was induced from the shallow warmer waters to the deeper colder ones).
- A clear stable temperature stratification was not observable and the water column was well mixed over the entire computational time (up to one month) and this was in accordance with the water quality analyses [49]. The ΔT over the vertical was generally lower than 0.5 °C, except comparing the water temperatures in the cross-section with the ones near the land shores (up to maximum 3 °C).
- The flow field returned to equilibrium at least a couple of days after a specific event simulated (e.g. a windstorm), as long as the disturbance (e.g. the wind) disappeared. Otherwise, it evolved until the achievement of a new steady state: a couple of weeks of simulation time was needed by the heating scenario.
- The vertical (w) and horizontal (u, v) components of velocities differed at least two to three orders of magnitude (being u, v higher than w), except during the windstorm, when they reached a comparable range of values. The water depths have been analyzed in several observation points of the domain and the variations were minor (order of mm against mean values of 10 m).

Conclusive remarks

To conclude, the use of the existent 2D model is suggested in case of absence or for moderate winds, as well as to assess only the water depths. For extreme wind scenarios and to simulate heating and cooling processes, the use of a 3D model is recommended, especially for specific research questions or management strategies. The observation of the results at specific depths, over different vertical cross-sections and profiles permits to refine the knowledge of the system, revealing certain circulation patterns and reaction to the imposed inputs. This becomes highly relevant for water management, e.g. the estimation of the time needed by a substance to reach the bottom and in which amount allows to evaluate the availability of nutrients, for the growth of algae or macrophytes and to understand the eutrophication potential in the bay. However, a scenario-oriented approach is needed for the Icó-Mandantes Bay, as well as many other water bodies around the world, stressed out by the impacts of climate change, water multiple uses and characterized by complex flow dynamics and processes, which are hard to be predicted a priori. Such systems require a ready-to-use tool, in order to properly assess the specific management questions. The models and the methodology presented in this work are a pioneer modeling approach for the region, which can be further investigated and refined, as well as applied in similar bay or reservoirs elsewhere in the world.

5.2 Recommendation for the future water management in the Icó-Mandantes Bay

Managing the multiple uses of water in the Icó-Mandantes Bay is becoming increasingly challenging; therefore, efficient technologies such as hydrodynamic and transport modeling tools should be applied, to assess the specific water quantity and quality issues. The following practical suggestions are the product of the scientific outcomes of this work:

- Concerning the aquaculture activities, fish (tilapia) production in the Itaparica Reservoir amounts to 20,000 tons per year. The Brazilian regulation (CONAMA 413/2009, [99]) allows 1% of the lake surface to host aquaculture, i.e. approx. 43,267 tons per year, but there are concerns about the sustainability of this regulation (e.g., [44]). Given to the low exchange rates between the reservoir and the Icò-Mandantes Bay and, consequently, the high risk of nutrient accumulation beneath the fish cages, it is advisable not to install an aquaculture system inside the bay. If this should not be feasible, since the aquaculture production is also responsible to stimulate the economic development of the region, it is suggested to locate the fish cages not in the stagnant areas where the water is too shallow (e.g., in the tip of the bay next to the eastern channel of the water diversion project), but to prefer deeper areas in order to guarantee enough space for translocation and dilution of organic material, avoiding an extreme increase of sediments beneath the cages. Furthermore, the 3D model can be used to identify high risk contamination areas in the bay, in order to consciously plan the location of eventual future aquaculture systems, taking into account the issue of harmful algae blooms and meteorological events (windstorms, flash floods, heat).
- The intermittent tributary Riacho dos Mandantes is considered one of the main sources of contamination for the bay, because this small stream is characterized by very low discharges (equal to zero almost the entire time of the year), which reach values up to 100 m^3/s during heavy rains, letting large amounts of nutrients to enter the bay by erosion, wash-out, leaching and run-off (e.g. from the nearby drainage systems). In the case of small dry streams and bays with low exchange rates, that are most vulnerable to eutrophication processes, such rain events must be considered and effectively managed, to prevent water quality deterioration and associated health risks for drinking and irrigation water. In

this specific case, since the mouth of the stream Riacho dos Mandantes is next to the intake of the eastern water diversion channel, it is highly recommended to monitor its withdrawal during the rainy period and especially after long droughts, e.g. stopping the operation of turbines and the pumping system during the heavy rains and at least for two days after the end of the rain. Similar monitoring procedures are meant as well for the drainage and the intakes for irrigation agriculture, located next to the small tributary. Finally, in regions such as the rural Brazilian Northeast next to municipalities of Petrolândia, there is no proper disposal of waste or emissions produced by various consumptions; e.g. the local people are used to leave the rubbish on the land, worsening the risk of contamination during flash floods. Therefore, management actions are not sufficient alone, but they must be combined with cultural, social and government measures, e.g. in schools and churches, in order to raise awareness regarding such issues and their consequences, taking hold especially of the young people. Moreover, the dry riverbeds and banks must be periodically cleaned up. Such cleaning operations can be organized by the communities or by the smallholders, involving for example kids and teenagers doing some volunteer work, as well as unemployed or retired people, eventually in return for a small reward. Out of these purposes, also media can be used, since they have high following rates in lower developed regions with a relevant percentage of illiterate population or, anyhow, with no high cultural standards.

- So far, the water quality studies at the intake or within the water diversion channel have not been yet conducted or not sufficiently to have a complete overview (e.g. not analyzing all the relevant parameters), but this is of high necessity to ensure acceptable quality standards for water supply. Additionally, monitoring the water quality in the channel is of vital importance, due to the low water depths, the high evaporation rates and the low velocities inside the Icó-Mandantes Bay, which do not facilitate exchange nor recirculation with the reservoir main stream.
- The estimation of the water residence times for the bay were conducted with the alternative experimental approach presented in Chapter 3. The criteria used to analyze the results, i.e. the residence time of water is arbitrarily chosen as the time at which all cells inside the bay have a lower concentration than 10%, can be stricter, lowering the concentration limit (e.g. 5% or 1%). This methodology can be applied for different scenarios, in order to assess specific issues, and to other similar bays, where the water dynamics and processes are complex and classical approaches cannot be used. In this sense, first exploratory scenarios were simulated (unpublished work), additionally taking into account the withdrawal from the water diversion channel and recalculating the water residence times, which were significantly reduced (approx. 50 %). The results suggest that the water withdrawal from the Icó-Mandantes Bay might affect the mixing of water at the local scale and be a potential positive side effect on water quality, as the pollution would get diluted faster. Model scenarios investigating the impacts of water diversion channels, to improve lakes' dynamics and thus water quality, can be found e.g. in Zhang et al. [126], Li et al. [98] and, specifically for Itaparica Reservoir in Melo et al. [43], as mentioned in Chapter 1.

- The simulation results of the transport of tracers in the domain showed that varying the discharges and the water levels at the inflow and outflow boundaries did not stimulate significantly the water exchange between the reservoir main stream and the bay. In addition, the high water levels and strong discharges (e.g. higher than 3,000 m^3/s) contributed to the isolation of the bay. This finding should be considered e.g. by CHESF, in regards of the management measures of the Luiz Gonzaga dam.
- Out of the studies conducted and the knowledge gained about the system, the ideal scenario for the Icó-Mandantes Bay to better ensure water quality standards would be to have a continuous inflow of water from the northeastern tip, because this would stimulate the exchange between the reservoir main stream and the bay. It was previously stated that the tributary Riacho dos Mandantes cannot contribute in this sense or at least not permanently, given to its dry riverbed and the long-lasting drought periods. Therefore, during periods of low wind, nutrients overload, high amount of algae blooms and/or particular contamination rates, one management measure can consist in the inversion of the water flow withdrawn by the eastern diversion channel, in case of necessity. Experimental studies can be conducted by the responsible water managers (tasked by the National Ministry of Integration, Brazil), in order to assess the consequences of this action, concerning the water quality. Certainly, such operation measures can be discussed with the stakeholders and further analyzed, checking for their feasibility.

In conclusion, the reservoir management needs innovative measures, which urge of differentiated analysis and evaluation for the reservoir main stream and its bays, characterized by different regimes (e.g. velocities), and where the 2D and 3D modeling can be adopted as supporting tools.

5.3 Outlook

In the next future, further research studies and water management can address the following points, learning from the goals reached within this work and trying to overcome its limitations.

- Since the last drought is lasting since approximately 2012, the bathymetry data and the physical boundaries, collected in 2013 and used to set up the grid of the models during the first phase of this work have most probably changed. No big variations in the results are expected updating the bathymetry with the newest measurements, but in case of further financial support and research in the region, such refinements as well as sensitivity analyses can be conducted, e.g. in order to assess their impact. However, while the data of bottom elevations were quite numerous for the bay itself, along the reservoir main stream as well as in the entire Itaparica Reservoir between Belém de São Francisco (South and West coordinates respectively 8°38'59.18" and 39° 4'15.07", in the reference system WGS84) and the Luiz Gonzaga dam were very scarce (around 90 in an area of approximately 828 km^2); thus, the model set up for the reservoir [53] was very course and needed significant interpolation efforts. When additional consistent bathymetry data should be available for the entire reservoir, the existent model can be refined and applied for future modeling scenarios.

- The two-dimensional and three-dimensional models set up during these years need to be properly calibrated and validated. For this reason, in case of further financial support and research in the region, field campaigns must be conducted, ideally in some specific periods of the year and under different conditions; e.g., several weekly campaigns, in different seasons such as dry and wet periods (whenever possible), during strong or weak wind. The kind of data needed are e.g. flow measurements such as velocities, to estimate the turbulent diffusivity and the bottom friction or to check the velocity profiles over the depth in strategic locations; still, the collection of temperature values and profiles, radiation, cloudiness, air humidity, wind intensities and directions, transparency or other water quality parameters can be precious for further analyses. Yet, tracer experiments should be conducted, e.g. to determine the most suitable approach to account for turbulent viscosity and diffusivity. A good tutoring during the field campaigns, as well as reliable and accurate measurement tools are necessary. Finally, after a statistical analysis of the data, these can be incorporated into the models to proper calibrate and validate them, as well as to define specific investigation cases.

- As clearly pointed out in the thesis, the important issue of water quality, as well of sediment transport and desiccation processes should be considered in future research, with the aim to keep oligotrophic levels and to support an advanced and differentiated management for the bay and the reservoir. Furthermore, the risk of development of harmful algae blooms in the lentic areas, their spreading and interaction with the reservoir main stream, together with their impact on the withdrawals for drinking water or irrigation agriculture should be assessed. To do so, the water quality of the Icó-Mandantes Bay can be assesses specifically, coupling the existent 3D model with a water quality one. Among other available tools, the TELEMAC-3D software up to version 7.1 is able to generate the appropriate files necessary to run the water quality simulations using the engine DELWAQ (Deltares, s. Chapter 1). Otherwise, the newest TELEMAC-MASCARET version (7.2) includes a separated water quality module, called WAQTEL. Information can be found in the related forum as well in the website, comprising a validation folder with five examples in 2D and five others in 3D; although, no complete tutorial or user manual is yet available. A further implementation of sediment transport and modeling of bed evolution can also be done using e.g. SISYPHE for 2D sediment transport or SEDI-3D for 3D suspended sediment transport, both part of the TELEMAC-MASCARET modeling system.

- As mentioned in the previous sections of this chapter, a water quality study at the intake and within the water diversion channel is of high importance, as well as a periodic monitoring, with the aim to ensure a good quality water supply to the regions involved in the project of the Brazilian Ministry of Integration, which are the States of Pernambuco, Ceará, Paraíba and Rio Grande do Norte. Additionally, the setting of new modeling scenarios should consider the withdrawal (normal and maximum) from the water diversion channel in operation. E.g., further investigations are needed to assess the impacts of this intake on the water residence times of the bay, as well as of the reservoir.

- Nowadays, there is much debates among water scientists, experts and managers concerning the so-called Integrated Water Resource Management (IWRM), defined by the Global Water Partnership (GWP) as *a process which promotes the coordinated development and management of water, land*

and related resources, in order to maximize the resultant economic and social welfare in an equitable manner without compromising the sustainability of vital ecosystems (e.g., [127]). The concepts of the IWRM have been accepted internationally as the way forward for an efficient, equitable and sustainable development and management of the world's limited water resources and for coping with conflicting demands [128,129]. A wide overview about the topic and its history is given e.g. in Stålnacke and Gooch [130]. In this context, it is of great importance to work towards an integrated water resource management, dealing with the specific water issues and technologies in a wider perspective and searching for holistic solutions to the challenges. This was one of the efforts successfully performed in this work as part of the INNOVATE project, merging the eco-hydrological modeling at the basin (larger) scale (e.g., [59]), directly linked with the global climate scenarios, with the local studies regarding the water quality assessments (e.g., [50,55,110]). Further integrated scenarios can be designed with the mentioned holistic approach, again including the interested third parts, such as the committee of the Sâo Francisco River (CBHSF), but at the same time punctually checking for the feasibility and the implications of the scenarios e.g. with the hydropower managers (CHESF).

- Additionally linked with the previous point, the new 10 years (2016-2025) management plan developed for the São Francisco River Basin by the Portuguese NEMUS company, designated by the agency AGB Peixe Vivo (Belo Horizonte, Brazil), is huge and rather dispersive, when it is approached to address specific issues at the smaller scale, e.g. in the interest of the smallholders such as the farmers and fishermen living in the communities nearby the Icó-Mandantes Bay. Concrete discussions and integrations between the different models currently available are necessary, with the goal to conduct a valuable research, giving concrete, reliable and feasible management suggestions, protecting in this way the precious and limited water resources.

- Carrying out a good quality research does not only imply the use of accurate data samples, high-resolution as well as integrated models, the development of innovative approaches to study the complex water issues or, yet, the simulation of different scenarios to support a sustainable water management, but also the collaboration between scientists and project partners, expert of different disciplines and stakeholders, sharing the respective field of expertise, points of strength and of weaknesses at the same time, asking for assistance, where the own capabilities are limited. A valuable research with concrete implications in the field is not possible in isolation, there is the need to interact not just between professionals, but with the local people as well, because their experience is extremely precious. Such ideas and concepts have been taken into account in the INNOVATE project to a certain extent, but need to be enhanced and supported increasingly also from the financial side, during the planning of new research projects, which must deal with the complex challenges around the world and comprise different disciplines. This focus should be considered as well when the project team members are recruited. Finally, the awareness-raising in form of lectures or talks, concerning the water quantity and quality issues, the knowledge transfer among the schools, the universities and the water companies interested or involved in the region are valuable and extremely necessary actions, that the INNOVATE project implemented rather successfully. This example can be followed in further research projects, together with the urge to be continuously improved. Still, important initiatives among the rural communities such as the cleaning up of dry riverbeds and the (differentiated) waste-collection, must be concretely stimulated, supported and launched.

Bibliography

1. World Bank, W. *Turn Down the Heat Why a 4°C Warmer World Must Be Avoided*; Washington D.C., 2012; ISBN 9781464800535.
2. Intergovernmental Panel on Climate Change (IPCC). *Field, C.B., Barros, V.R., Dokken, D.J. , Mach, K.J., Mastrandrea, M.D., Bilir, T.E., Chatterjee, M., Ebi, K.L., Estrada, Y.O., Genova, R.C., Girma, B., Kissel, E.S., Levy, A.N., MacCracken, S., Mastrandrea, P.R. and White, L.L. (eds.).*; 2014;
3. Marengo, J. A.; Torres, R. R.; Alves, L. M. Drought in Northeast Brazil—past, present, and future. *Theor. Appl. Climatol.* **2016**, 1–12, doi:10.1007/s00704-016-1840-8.
4. FAO *Review of world water resources by country*; Food and Agriculture Organization of the United Nations, 2003; ISBN 9251048991.
5. da Silva, V.; de Oliveira, S.; Hoekstra, A.; Dantas Neto, J.; Campos, J.; Braga, C.; de Araújo, L.; Aleixo, D.; de Brito, J.; de Souza, M.; de Holanda, R. Water Footprint and Virtual Water Trade of Brazil. *Water* **2016**, *8*, 517, doi:10.3390/w8110517.
6. Marengo, J. A. Vulnerabilidade, impactos e adaptação àmudança do clima no semi-árido do Brasil. *Parcerias Estratégicas* **2008**, *27*, 149–175.
7. Tundisi, J. G.; Matsumura-Tundisi, T. Integration of research and management in optimizing multiple uses of reservoirs: The experience in South America and Brazilian case studies. *Hydrobiologia* **2003**, *500*, 231–242, doi:10.1023/A:1024617102056.
8. Tundisi, J. G. Recursos hídricos no futuro: problemas e soluções. *Estud. avançados* **2008**, *22*.
9. Gunkel, G.; Sobral, M. C. *Reservoir and River Basin Management: Exchange and Experiences from Brazil, Portugal and Germany*; Univerlagtuberlin, Ed.; 2007;
10. Boehrer, B.; Schultze, M. Stratification of lakes. *Rev. Geophys.* **2008**, *46*, 1–27, doi:10.1029/2006RG000210.
11. de Araújo, J. C.; Döll, P.; Güntner, A.; Krol, M.; Abreu, C. B. R.; Hauschild, M.; Mendiondo, E. M. Water Scarcity Under Scenarios for Global Climate Change and Regional Development in Semiarid Northeastern Brazil. *Water Int.* **2004**, *29*, 209–220, doi:10.1080/02508060408691770.
12. Matta, E.; Koch, H.; Selge, F.; Simshäuser, M. N.; Rossiter, K.; Nogueira da Silva, G. M.; Gunkel, G.; Hinkelmann, R. Modeling the impacts of climate extremes and multiple water uses to support water management in the Icó-Mandantes Bay, Northeast Brazil. *J. Water Clim. Chang.* **2017**, *subm.*
13. Bond, N. R.; Lake, P. S.; Arthington, A. H. The impacts of drought on freshwater ecosystems: an Australian perspective. *Hydrobiologia* **2008**, doi:10.1007/s10750-008-9326-z.
14. Gophen, M. Lake Management Perspectives in Arid, Semi-Arid, Sub-Tropical and Tropical Dry climate. In *Proceedings of Taal2007: The 12th World Lake Conference*; 2008; pp. 1338–1348.

15. Sousa Júnior, W.; Baldwin, C.; Camkin, J.; Fidelman, P.; Silva, O.; Neto, S.; Smith, T. F. Water: Drought, Crisis and Governance in Australia and Brazil., doi:10.3390/w8110493.

16. Gunkel, G.; Sobral, M. do C. Re-oligotrophication as a challenge for a tropical reservoir management with reference to Itaparica Reseroir, São Francisco, Brazil. *Water Sci. Technol.* **2013**, *67*, 708–714.

17. Gunkel, G., Selge, F., Keitel, J., Lima, D., Calado, S., Sobral, M., Rodriguez, M., Matta, E., Hinkelmann, R., Casper, P., Hupfer, M. Impacts of water management on aquatic ecosystem services of a tropical reservoir (Itaparica, São Francisco, Brazil) and development of advanced reservoir management tools. *Reg. Environ. Chang.* **2018**, doi:10.1007/s10113-018-1324-8.

18. Cirilo, J. A. Public Water Resources Policy for the semi-arid Region. *Estud. Avançados* **2008**, *22*, 61–82, doi:10.1590/S0103-40142008000200005.

19. Castro, C. N. D. C. *Transposição Do Rio São Francisco: Análise De Oportunidade Do Projeto*; 2011;

20. Rogers, P. California drought: Plan advances to enlarge major reservoir. Available online: http://www.mercurynews.com/2017/07/03/california-drought-plans-to-enlarge-major-bay-area-reservoir-move-forward/ (accessed on Aug 7, 2017).

21. Martin, B.; Ding, L.; Hannoun, I. A.; List, E. J. Predicting effects of reservoir expansion with three-dimensional modeling: Case study of Los Vaqueros Reservoir. *Lake Reserv. Manag.* **2013**, *29*, 217–232, doi:10.1080/10402381.2013.837565.

22. CR (Construction Review Online) Kenya constructs largest water project in semi arid area Available online: https://constructionreviewonline.com/2016/02/kenya-constructs-largest-water-project-in-semi-arid-area/ (accessed on Aug 10, 2017).

23. Jadhav, M. V; Shaikh, E.; Gite, E.; Yadav, E. Sand Dam Reservoir – Need Of Semi Arid Areas. *Int. J. Eng. Res. Appl. www.ijera.com* **2012**, *2*.

24. Elshemy, M. M. Water quality modeling of large reservoirs in semi-arid regions under climate change – Example Lake Nasser (Egypt), Technischen Universität Carolo-Wilhelmina zu Braunschweig, Germany, 2010.

25. Cirilo, J. A. Análise dos processos hidrológico – Hydrodinâmicos na bacía do Rio São Francisco, UFPE, Recife, 1991.

26. Güntner, A. Large-scale hydrological modelling in the semi-arid north-east of Brazil, 2002.

27. Ferreira Junior, M. G. Uso de modelagem na avaliação da capacidade de suporte de reservatórios com projetos de aquicultura, tendo o fósforo como fator limitante. Modeling usage in the reservoir support capacity evaluation with aquaculture projects, having phosphorus as a limit, UFRJ, Rio de Janeiro, Brazil, 2011.

28. Kwon, H. H.; de Assis de Souza Filho, F.; Block, P.; Sun, L.; Lall, U.; Reis, D. S. Uncertainty assessment of hydrologic and climate forecast models in Northeastern Brazil. *Hydrol. Process.* **2012**, *26*, 3875–3885, doi:10.1002/hyp.8433.

29. Ramon, J.; Cantalice, B.; Filho, C.; Stosic, B. D.; Piscoya, V. C.; Guerra, S. M. S.; Singh, V. P.;

Filho, M. C. Hydrological Sciences Journal Relationship between bedload and suspended sediment in the sand-bed Exu River, in the semi- arid region of Brazil Relationship between bedload and suspended sediment in the sand-bed Exu River, in the semi-arid region of Brazil. *Hydrol. Sci. J. – J. des Sci. Hydrol.* **1789**, *58*, doi:10.1080/02626667.2013.839875.

30. Marengo, M. P. S. P. and F. J. and A. C. M. M. and H. B. and J.; Pereira, M. P. S.; Justino, F.; Malhado, A. C. M.; Barbosa, H.; Marengo, J. The influence of oceanic basins on drought and ecosystem dynamics in Northeast Brazil. *Environ. Res. Lett.* **2014**, *9*, 124013, doi:10.1088/1748-9326/9/12/124013.

31. Koch, H.; Biewald, A.; Liersch, S.; De Azevedo, J.R.G.; Da Silva, G.S.; Kölling, K.; Fischer, P.; Koch, R.; Hattermann, F. F. Scenarios of climate and land-use change, water demand and water availability for the São Francisco River Basin. **2015**, *36*, 96–114, doi:10.5327/Z2176-947820151007.

32. Krysanova, V.; Hattermann, F.; Huang, S.; Hesse, C.; Vetter, T.; Liersch, S.; Koch, H.; Kundzewicz, Z. W. Modelling climate and land-use change impacts with SWIM: lessons learnt from multiple applications. *Hydrol. Sci. J.* **2015**, *60*, 606–635, doi:10.1080/02626667.2014.925560.

33. Oliveira De Assis, J. M.; Meira De Souza, W. Climate analysis of the rainfall on sub medium part of the São Francisco River Basin based on the rain anomaly index. *RBCIAMB* **2015**, *36*, 115–127, doi:10.5327/Z2176-947820151012.

34. Silva, E. A.; Pedrosa, M. M.; Azevedo, S. C.; Cardim, G. P.; Carvalho, F. P. S. Assessment of surface water at the Sobradinho reservoir under the effects of drought using multi-temporal landsat images. In *The International Archives of the Photogrammetry, Remote Sensing and Spatial Information Sciences. XXIII ISPRS Congress*; Prague, Czech Republic, 2016; p. Volume XLI-B8.

35. Farias, A. A. de; Sousa, F. de A. S. de; Alves, T. L. B.; Souza, J. T. A. Temporal analysis of events of drought in the municipalities of Caraúbas and Monteiro - PB. *J. Hyperspectral Remote Sens.* **2016**, *6*, 82–90, doi:10.5935/2237-2202.20160010.

36. Santos, J. C. N. dos; Andrade, E. M. de; Araújo Neto, J. R.; Meireles, A. C. M.; Palácio, H. A. de Q. Land use and trophic state dynamics in a tropical semi-arid reservoir. *Rev. Ciência Agronômica* **2014**, *45*, 35–44.

37. Paredes-Trejo, F.; Barbosa, H. Evaluation of the SMOS-derived soil water deficit index as agricultural drought index in Northeast of Brazil. *Water (Switzerland)* **2017**, *9*, doi:10.3390/w9060377.

38. Liebe, J. R.; Andreini, M.; Giesen, N. van de; Steenhuis, T. S. The small reservoirs project: Research to improve water availability and economic development in rural semi-arid areas. In *The hydropolitics of Africa: A contemporary challenge.*; Kittisou, M., Ndulo, M., Nagel, M. and Grieco, M. (eds. ., Ed.; Cambridge Scholars Publishing: Newcastle, United Kingdom, 2007.

39. Abbasi, A. Energy Balance and Heat Storage of Small Shallow Water Bodies in Semi-arid Areas, TU Delft, Delft, Nederlands, 2016.

40. Abeysinghe, K. G. A. M. C. S.; Nandalal, K. D. W.; Piyasiri, S. Prediction of thermal stratification of the Kotmale reservoir using a hydrodynamic model. *J. Natl. Sci. Found. Sri Lanka* **2005**, *33*, 25–36.

41. Chitata, T.; Mugabe, F. T.; Kashaigili, J. J. Estimation of Small Reservoir Sedimentation in Semi-Arid Southern Zimbabwe. *J. Water Resour. Prot.* **2000**, *6*, 1017–1028, doi:10.4236/jwarp.2014.611096.

42. Abbasi, A.; Annor, F.; van de Giesen, N. Investigation of Temperature Dynamics in Small and Shallow Reservoirs, Case Study: Lake Binaba, Upper East Region of Ghana. *Water* **2016**, *8*, 84, doi:10.3390/w8030084.

43. Melo, G.; Morais, M.; Sobral, M. C.; Gunkel, G.; Carvalho, R. Influência de Variáveis Ambientais na Comunidade Fitoplanctônica nos Reservatórios Receptores do Projeto de Integração do Rio São Francisco. (The Influence of Environmental Variables on Phytoplankton Community of the Receptors Reservoirs by the São Franci. *Rev. Bras. Geogr. Física* **2012**, *6*, 1300–1316.

44. Gunkel, G.; Matta, E.; Selge, F.; Silva, G. M. N. da; Sobral, M. do C. Carrying capacity limits of net cage aquaculture in brazilian reservoirs. *Rev. Bras. Ciências Ambient.* **2015**, 128–144, doi:10.5327/Z2176-947820151008.

45. Rodorff, V.; Siegmund-Schultze, M.; Gottwald, S.; Sobral, M. C.; Köppel, J. Eficácia de programas de acompanhamento (follow-up) – 25 anos após a construção do reservatório de Itaparica no Nordeste brasileiro. In *Governança e recursos hídricos: Experiências nacionais e internacionais de gestão.*; Theodoro HD, M. F. [Eds], Ed.; Belo Horizonte, 2015; pp. 199–218 ISBN 9788584250851.

46. Lopes, F. B.; Andrade, E. M. de; Meireles, A. C. M.; Becker, H.; Batista, A. A. Assessment of the water quality in a large reservoir in semiarid region of Brazil. *Rev. Bras. Eng. Agrícola e Ambient.* **2014**, *18*, 437–445, doi:10.1590/S1415-43662014000400012.

47. Arruda, N. O. de Controle do aporte de fósforo no reservatório de Itaparica localizado no semiárido nordestino, Federal University of Pernambuco (UFPE), Recife, Brazil, 2015.

48. Keitel, J.; Zak, D.; Hupfer, M. Water level fluctuations in a tropical reservoir: the impact of sediment drying, aquatic macrophyte dieback, and oxygen availability on phosphorus mobilization. *Environ. Sci. Pollut. Res.* **2015**, doi:10.1007/s11356-015-5915-3.

49. Selge, F. *Aquatic ecosystem functions and oligotrophication potential of the Itaparica reservoir, São Francisco river, in the semi-arid Northeast Brazil*; ITU Schriftenreihe Nr. 33, Papierflieger Verlag Clausthal-Zellerfeld, 2017; ISBN 978-3-86948-580-5.

50. Lima, D. The role of water level fluctuations in the promotion of phytoplankton and macrophyte pioneer species in a tropical reservoir in the Brazilian semiarid, Technische Universität Berlin, 2017.

51. Da Silva, G. M. N. *Zoneamento da pesca artesanal no reservatório de Itaparica, Rio São Francisco, Brasil*; Recife, Brazil, 2016;

52. Özgen, I.; Seemann, S.; Candeias, A. L.; Koch, H.; Simons, F.; Hinkelmann, R. Simulation of

hydraulic interaction between Icó-Mandantes bay and São Francisco river, Brazil. In *Sustainable Management of Water and Land in Semiarid Areas*; 2013; pp. 28–38 ISBN 9788541502597.

53. Broecker, T.; Özgen, I.; Matta, E.; Cabral, J.; Candeias, A. L.; Hinkelmann, R. Simulation of Flow and Transport Processes in a Brazilian Reservoir 2014.

54. Matta, E.; Özgen, I.; Cabral, J.; Candeias, A. L.; Hinkelmann, R. Simulation of Wind-induced Flow and Transport in a Brazilian bay. In *International Conference on Hydroscience & Engineering (ICHE)*; Lehfeldt, R. & Kopmann, R. (eds), Ed.; Bundesanstalt für Wasserbau ISBN 978-3-939230-32-8: Hamburg, Germany, 2014.

55. Selge, F.; Matta, E.; Hinkelmann, R.; Gunkel, G. Nutrient load concept-reservoir vs. bay impacts: A case study from a semi-arid watershed. *Water Sci. Technol.* **2016**, *74*, 1671–1679, doi:10.2166/wst.2016.342.

56. Matta, E.; Selge, F.; Gunkel, G.; Rossiter, K.; Jourieh, A.; Hinkelmann, R. Quantification of exchange processes between a bay and a river using a two-dimensional high-resolution transport model. In *IWA-DIPCON Conference*; 2015.

57. Matta, E.; Simshäuser, M. N.; Koch, H.; Selge, F.; Gunkel, G.; Rossiter, K.; Hinkelmann, R. Modeling the interaction of multiple uses, climate and land-use changes in a bay of Itaparica reservoir, São Francisco river. In *Proceedings XXI SBRH Conference, Brasilia, Brazil*; 2015.

58. Matta, E.; Silva, G. M. N.; Lorenz, R.; Gunkel, G.; Hinkelmann, R. Estimation of water residence time in Icò-Mandantes bay using the TELEMAC-2D modeling system. In *I SBHSF Conference, June 6-9, 2016, Juazeiro, Brazil.*; 2016.

59. Hattermann, F. F.; Koch, H.; Liersch, S.; Silva, A. L. L.; Azevedo, R.; Selge, F.; Silva, G. N. S. N. S.; Matta, E.; Hinkelmann, R.; Fischer, P.; Venohr, M.; Azevedo, J. . R.; Selge, F.; Silva, G. N. S. N. S.; Matta, E.; Hinkelmann, R.; Fischer, P.; Venohr, M. Climate and land use change impacts on the water-energy-food nexus in the semi-arid northeast of Brazil – scenario analysis and adaptation options. *Reg. Environ. Chang.* **2017**, *subm.*

60. Berger, V., Fan, F., Gabel, F., Galvão, P., Gies, M., Grabner, D., Langhans, S., Machado, A., Manzione, R., Matta, E., Andreu, A., de Moraes, M., Morihama, A., Macedo-Moura, P., de Paiva, A., Periotto, N., Porst, G., Rigotto, C., Roters, B., Schulz, S., S, C. *How Do We Want to Live Tomorrow? Perspectives on Water Management in Urban Regions*; 2017;

61. Siegmund-Schultze M (Ed) (2017) Interplay between multiple uses of water reservoirs via innovative coupling of aquatic and terrestrial ecosystems. Final Report of the INNOVATE Consortium (Verbundschlussbericht). January 2012 to March 2017. TU Berlin, Germany. dx.doi.org/10.2314/GBV:1011609282.

62. Hagel, H.; Hoffmann, C.; Doluschitz, R. Mathematical Programming Models to Increase Land and Water Use Efficiency in Semi-arid NE-Brazil. **2014**, *5*, 173–181.

63. CHESF, Companhia Hidro Elétrica do São Francisco. Sistemas de Geração: Luiz Gonzaga. Available online: https://www.chesf.gov.br/ (accessed on Jan 11, 2015).

64. Ministério da Integração National (Ministry of National Integration) Projeto de Integração do Rio São Francisco (Project of Integration of the São Francisco River) Available online:

http://www.integracao.gov.br/web/projeto-sao-francisco/entenda-os-detalhes (accessed on Aug 9, 2017).

65. Brazil. ANA, National Water Agency. Resolution 411 of the 22 September 2005.

66. Siegmund-Schultze, M. (Ed) Guidance manual – a compilation of actor-relevant content extracted from scientific results of the INNOVATE project. **2017**, 128.

67. Matta, E.; Selge, F.; Gunkel, G.; Rossiter, K.; Jourieh, A.; Hinkelmann, R. Simulations of nutrient emissions from a net cage aquaculture system in a Brazilian bay. *Water Sci. Technol.* **2016**, *73*, 2430–2435, doi:10.2166/wst.2016.092.

68. Falconer, R. A.; George, D. G.; Hall, P. Three dimensional numerical modeling of wind-driven circulation in a shallow homogeneous lake. *J. Hydrol.* **1991**, *124*, 59–79.

69. Ji, Z.-G. *Hydrodynamics and water quality: modeling rivers, lakes, and estuaries*; Wiley & Sons, Inc.: Hoboken, New Jersey, USA, 2008; ISBN 978-0-470-13543-3.

70. Hattermann, F. F.; Weiland, M.; Huang, S.; Krysanova, V.; Kundzewicz, Z. W. Model-Supported Impact Assessment for the Water Sector in Central Germany Under Climate Change—A Case Study. *Water Resour. Manag.* **2011**, *25*, 3113–3134, doi:10.1007/s11269-011-9848-4.

71. Hinkelmann, R. *Efficient Numerical Methods and Information-Processing Techniques in Environment Water*; Stuttgart, Germany, 2003; ISBN 3933761204.

72. Fenocchi, A.; Petaccia, G.; Sibilla, S. Modelling flows in shallow (fluvial) lakes with prevailing circulations in the horizontal plane: limits of 2D compared to 3D models. *J. Hydroinformatics* **2016**.

73. de Marchis, M.; Ciraolo, G.; Nasello, C.; Napoli, E. Wind- and tide-induced currents in the Stagnone lagoon (Sicily). *Environ. Fluid Mech.* **2012**, *12*, 81–100, doi:10.1007/s10652-011-9225-0.

74. HLRN (Norddeutsche Verbund für Hoch- und Höchst-leis-tungs-rech-nen) Available online: https://www.hlrn.de/home/view/Main/WebHome (accessed on Aug 8, 2017).

75. Özgen, I. Coarse Grid Approaches for the Shallow Water Model, TU Berlin, 2017.

76. Zamani, B.; Koch, M.; Hodges, B. R.; Fakheri-Fard, A. Pre-impoundment assessment of the limnological processes and eutrophication in a reservoir using three-dimensional modeling: Abolabbas reservoir, Iran. *J. Appl. Water Eng. Res.* **2016**, 1–14, doi:10.1080/23249676.2016.1209440.

77. Hervouet, J. M. *Hydrodynamics of Free Surface Flows. Modelling with the Finite Element Method*; 2007; ISBN 9780470035580.

78. Kanarska, Y.; Maderich, V. A non-hydrostatic numerical model for calculating free-surface stratified flows. *Ocean Dyn.* **2003**, *53*, 176–185, doi:10.1007/s10236-003-0039-6.

79. Mahgoub, M.; Hinkelmann, R. Three-dimensional non-hydrostatic simulation of gravity currents using TELEMAC3D and comparison of results to experimental data Mohamed Mahgoub * and

Reinhard Hinkelmann Michele La Rocca. *Prog. Comput. Fluid Dyn.* **2015**, *15*, 56–67.

80. Prandtl, L. Über die ausgebidete Turbulenz. *Zeitschrift für augewandte Math. und Mech.* **1925**, *5*, 136.

81. Smagorinski, J. General circulation experiments with the primitive equations. The basic experiment. *Mon. Weather Rev.* **1963**, *91*, 99–164.

82. Jourieh, A. Multi-dimensional Numerical Simulation of Hydrodynamics and Transport Processes in Surface Water Systems in Berlin, Technische Universität Berlin, 2015.

83. Ayachit, U. *The ParaView Guide: A Parallel Visualization Application*; Kitware, Inc.: USA, 2015; ISBN 1930934300, 9781930934306.

84. Kopmann, R.; Markofsky, M. Three-dimensional water quality modelling with TELEMAC-3D. *Hydrol. Process.* **2000**, *14*, 2279–2292, doi:10.1002/1099-1085(200009)14:13<2279::AID-HYP28>3.0.CO;2-7.

85. Sinha, J.; Manivanan, R.; Kanetkar, C. N.; Ghosh, L. K. Hydrodynamic simulation of deep reservoir by 3D model. *ISH J. Hydraul. Eng.* **2004**, *10*, 14–22, doi:10.1080/09715010.2004.10514750.

86. Morelissen, R.; Vlijm, R.; Hwang, I.; Doneker, R. L.; Ramachandran, A. S. Hydrodynamic modelling of large-scale cooling water outfalls with a dynamically coupled near-field–far-field modelling system. *J. Appl. Water Eng. Res.* **2016**, *4*, 138–151, doi:10.1080/23249676.2015.1099480.

87. Broecker, T.; Schaper, J.; El-Athman, F.; Gillefalk, M.; Hilt, S.; Hinkelmann, R. Surface water - groundwater interactions. In *37th IAHR World Congress, Kuala Lumpur, Malaysia*; Kuala Lumpur, Malaysia, 2017.

88. Teuber, K.; Grüneberger, M.; Despot, D.; Dietmar, S.; Barjenbruch, M.; Hinkelmann, R. Modeling and measuring of interfaces in sewer systems. In *37th IAHR World Congress, Kuala Lumpur, Malaysia*; Kuala Lumpur, Malaysia, 2017.

89. Lian, J.; Yao, Y.; Ma, C.; Guo, Q. Reservoir Operation Rules for Controlling Algal Blooms in a Tributary to the Impoundment of Three Gorges Dam. *Water* **2014**, *6*, 3200–3223, doi:10.3390/w6103200.

90. Hodges, B. R.; Imberger, J.; Laval, B.; Appt, J. Modeling the Hydrodynamics of Stratified Lakes. *Hydroinformatics* **2000**, 23–27.

91. Imberger, J. and J. C. P. A dynamic reservoir simulation model - DYRESM 5. *Transp. Model. Inl. Coast. Waters* **1981**, 310–361.

92. Herzfeld, M., & Hamilton, D. P. A computational aquatic ecosystem dynamics model of the Swan River, Western Australia. In *International Conference on Modelling and Simulation, University of Tasmania, Hobart.*; (Eds.), A. D. M. & M. M., Ed.; 1997.

93. Hein, B.; Viergutz, C.; Wyrwa, J.; Kirchesch, V.; Schöl, A. Impacts of climate change on the water quality of the Elbe Estuary (Germany). **2016**, 1–12, doi:10.1080/23249676.2016.1209438.

94. Ladwig, R., Kirillin, G., Hinkelmann, R., Hupfer, M.; Ladwig, R.; Kirillin, G.; Hinkelmann, R.; Hupfer, M. Lake on life support: Evaluating urban lake management measures by using a coupled 1D-modelling approach. In *EGU General Assembly 2017*; Copernicus GmbH, Göttingen, Germany: Vienna, Austria, 2017.

95. Wu, R.-S.; Liu, W.-C.; Hsieh, W.-H. Eutrophication Modeling in Shihmen Reservoir, Taiwan. *J. Environ. Sci. Heal. Part A* **2004**, *39*, 1455–1477, doi:10.1081/ESE-120037846.

96. de Marchis, M.; Freni, G.; Napoli, E. Three-dimensional numerical simulations on wind- and tide-induced currents: The case of Augusta Harbour (Italy). *Comput. Geosci.* **2014**, *72*, 65–75, doi:10.1016/j.cageo.2014.07.003.

97. Napoli, E, Armenio, V, De Marchis, M. The effect of the slope of irregularly distributed roughness elements on turbulent wall-bounded flows. *J Fluid Mech* **2008**, *613*, 385–394.

98. Li, Y.; Acharya, K.; Chen, D.; Stone, M. Modeling water ages and thermal structure of Lake Mead under changing water levels. *Lake Reserv. Manag.* **2011**, *26*, 258–272, doi:10.1080/07438141.2010.541326.

99. CONAMA (Conselho Nacional do Meio Ambiente) *Resolução no. 413, de 26 de Julho de 2009 (Law resolution no. 413 of the Brazilian Environment Council, published on the 26th of July, 2009).*; Brazilian Ministry of the Environment. http://www.mma.gov.br/port/conama/ legiabre.cfm?codlegi=608 (accessed 7 March 2016);

100. Gutiérrez, A. P. A.; Engle, N. L.; De Nys, E.; Molejón, C.; Martins, E. S. S.; Guti??rrez, A. P. A.; Engle, N. L.; De Nys, E.; Molej??n, C.; Martins, E. S. S. Drought preparedness in Brazil. *Weather Clim. Extrem.* **2014**, *3*, 95–106, doi:http://dx.doi.org/10.1016/j.wace.2013.12.001.

101. Marengo, J. A.; Bernasconi, M. Regional differences in aridity/drought conditions over Northeast Brazil: Present state and future projections. *Clim. Change* **2015**, *129*, 103–115.

102. Hirata, R.; Conicelli, B. P. Groundwater resources in Brazil: A review of possible impacts caused by climate change. *An. Acad. Bras. Cienc.* **2012**, *84*, 297–312, doi:10.1590/S0001-37652012005000037.

103. NEMUS São Francisco River Basin Management Plan 2016-2025, Brazil. Available online: http://www.nemus.pt/en/projects/water/ (accessed on Apr 6, 2017).

104. Flather, R. A. *Results from surge prediction model of the North-West European continental shelf for April November and December 1973, Report 24*; 1976;

105. Weedon G. P., Gomes S., Viterbo P., Shuttleworth W. J., Blyth E., Österle H., Adam J. C., Bellouin N., Boucher O., B. M. Creation of the WATCH Forcing Data and Its Use to Assess Global and Regional Reference Crop Evaporation over Land during the Twentieth Century. *J. Hydrometeorol.* **2011**, *12*, 823–848.

106. Chapra, S. *Surface Water Quality Modeling.*; McGraw-Hill, New York, USA, 1997;

107. Banas, N. S.; Hickey, B. M. Mapping exchange and residence time in a model of Willapa Bay, Washington, a branching, macrotidal estuary. *J. Geophys. Res. Ocean.* **2005**, *110*, 1–20, doi:10.1029/2005JC002950.

108. Rossiter, K. W. L.; Morais, M. M.; Calado, S. C. S.; Benachour, M.; Matta, E. Diagnóstico da Qualidade da Água ao longo de um Canal de concreto: Um estudo de caso do Canal do Sertão Alagoano. *Rev. Bras. Ciencias Ambient.* **2015**, 157–167, doi:10.5327/Z2176-947820151010.

109. CONAMA (Conselho Nacional do Meio Ambiente). Brazilian Ministry of the Environment. *Resolução no. 357, de 17 de Março de 2005 (Law resolution no. 357 of the Brazilian Environment Council, published on the 17th of March, 2005)*;

110. Gunkel, G.; Selge, F.; Keitel, J.; Lima, D.; Calado, S.; Sobral, M.; Rodriguez, M.; Matta, E.; Hinkelmann, R.; Casper, P.; Hupfer, M. Management of a tropical reservoir (Itaparica, São Francisco, Brazil): Multiple water uses, impact, and ecological sustainability. *Reg. Environm. Chang.* **2017**, *subm.*

111. Li, Y. P.; Tang, C. Y.; Wang, C.; Anim, D. O.; Yu, Z. B.; Acharya, K. Improved Yangtze River diversions: are they helping to solve algal bloom problems in Lake Taihu, China? *Ecol. Eng.* **2013**, *51*, 104–116.

112. Matta, E.; Selge, F.; Gunkel, G.; Hinkelmann, R. Three-dimensional modeling of wind- and temperature-induced flows in the Icó-Mandantes Bay, Itaparica Reservoir, NE Brazil. *Water (Switzerland)* **2017**, *9*, 772, doi:10.3390/w9100772.

113. Coutinho, R. M.; Kraenkel, R. A.; Prado, P. I.; Scheffer, M.; Guttal, V.; Ives, A. Catastrophic Regime Shift in Water Reservoirs and São Paulo Water Supply Crisis. *PLoS One* **2015**, *10*, e0138278, doi:10.1371/journal.pone.0138278.

114. Kennedy, R. H.; Thornton, K. W.; D.E., F. Characterization of the reservoir ecosystem. In *Microbial processes in reservoirs*; Gunnison D., E., Ed.; Junk: Boston, USA, 1985; pp. 27–38.

115. Smith, V. H.; Tilman, G. D.; Nekola, J. C. Eutrophication: impacts of excess nutrient inputs on freshwater, marine, and terrestrial ecosystems. *Environ. Pollut.* **1999**, *100*, 179–196.

116. Bednarz, T. P.; Lei, C.; Patterson, J. C. Unsteady natural convection induced by diurnal temperature changes in a reservoir with slowly varying bottom topography. *Int. J. Therm. Sci.* **2009**, *48*, 1932–1942, doi:10.1016/j.ijthermalsci.2009.02.011.

117. Hutchinson, G. E. *A Treatise on Limnology, vol. 1. Geography, Physics and Chemistry*; John Wiley: New York, USA, 1957;

118. Sweers, H. E. A nomogram to estimate the heat-exchange coefficient at the air-water interface as a function of wind speed and temperature; a critical survey of some literature. *J. Hydrol.* **1976**, *30*, 375–401, doi:10.1016/0022-1694(76)90120-7.

119. INPE Sistema Integrado de Dados Ambientais Available online: http://www.sinda.crn2.inpe.br/PCD/SITE/novo/site/index.php (accessed on Aug 8, 2017).

120. Gunkel, G.; Casallas, J. Limnology of an equatorial high mountain lake – Lago San Pablo, Ecuador: The significance of deep diurnal mixing for lake productivity. *Limnologica* **2002**, *32*, 33–43.

121. Selge, F.; Gunkel, G. Water Reservoirs: Worldwide distribution , morphometic characteristics and thermal stratification processes. In *Sustainable Management of Water and Land in Semiarid*

Areas; 2013; pp. 15–27 ISBN 9788541502597.

122. Beaufort wind force scale - Met Office Available online: http://www.metoffice.gov.uk/guide/weather/marine/beaufort-scale (accessed on Aug 8, 2017).

123. Engelhardt, C.; Kirillin, G. Criteria for the onset and breakup of summer lake stratification based on routine temperature measurements. *Fundam. Appl. Limnol. / Arch. für Hydrobiol.* **2014**, *184*, 183–194, doi:10.1127/1863-9135/2014/0582.

124. Ministério da Integraçao National (Ministry of National Integration) *Relatorio de Integração do Rio São Francisco com bacias hidrograficas do nordeste setentrional (Report of the Integration of the São Francisco River with Hydrographical Basins of the Northeast)*; 2004;

125. Projetos Públicos de Irrigação — Companhia de Desenvolvimento dos Vales do São Francisco e do Parnaíba, CODEVASF (Public Irrigation Projects - Development Company of the São Francisco and Parnaíba Valleys, CODEVASF) Available online: http://www.codevasf.gov.br/principal/perimetros-irrigados (accessed on Sep 26, 2017).

126. Zhang, X.; Zou, R.; Wang, Y.; Liu, Y.; Zhao, L.; Zhu, X.; Guo, H. Is water age a reliable indicator for evaluating water quality effectiveness of water diversion projects in eutrophic lakes? *J. Hydrol.* **2016**, *542*, 281–291, doi:10.1016/j.jhydrol.2016.09.002.

127. Global Water Partnership. *Integrated Water Resources Management Global Water Partnership Technical Advisory Committee (TAC)*; Stockholm, Sweden, 2000;

128. Food and Agriculture Organization of the United Nations. Land and Water Development Division. *Status Report on Integrated Water Resources Management and Water Efficiency Plans*; 2008;

129. Food and Agriculture Organization of the United Nations. Land and Water Development Division; Global Water Partnership. *Roadmapping for Advancing Integrated Water Resources Management (IWRM) Processes*; 2007;

130. Stålnacke, P.; Gooch, G. D. Integrated Water Resources Management. *Irrig. Drain. Syst.* **2010**, *24*, 155–159, doi:10.1007/s10795-010-9106-6.