Daddy Fell Into The Duck Pond

Everyone grumbled. The sky was grey.
We had nothing to do and nothing to say.
We were nearing the end of a dismal day.
And there seemed to be nothing beyond,
Then
Daddy fell into the pond!

And everyone's face grew merry and bright,
And Timothy danced for sheer delight
"Give me the camera, quick, oh quick!
He's crawling out of the duckweed!
Click!

Then the gardener suddenly slapped his knee,
and doubled up, shaking silently,
And the ducks all quacked as if they were daft,
And it sounded as if the old drake laughed.
Oh! there wasn't a thing that didn't respond
When
Daddy fell into the pond!

Alfred Noyes
Modelling the Water Quality of the Patos Lagoon, Brazil

Deborah Ann Tyrrell

Abstract

A two-dimensional depth integrated finite element modelling suite comprising the flow model TELEMAC-2D and the water quality model WQFLOW-2D has been calibrated to simulate the physics and chemistry of the Patos Lagoon and Estuary system in southern Brazil for the investigation of nutrients, primary production and faecal bacteria. The model has been evaluated for use as a predictive tool to aid the decision making process for the rehabilitation and management of the shallow embayment of Saco da Mangueira adjacent to the city of Rio Grande in the lower Patos Estuary. This bay is one of several shallow areas bordering the city which suffers from the water quality pollution problems associated with eutrophication due to the influence of multiple and conflicting human impacts including the disposal of waste water from domestic and industrial sources such as the fertiliser industry, fish processing, and petroleum refining.

The validated flow model indicated a very weak circulation in the Saco da Mangueira with velocities an order of magnitude lower than in the estuary. Simulations conducted to evaluate transport and mixing time scales demonstrated limited water exchange between the bay and the estuary principally controlled by wind direction and duration, with e-folding flushing times between 21 and 45 days using observed wind and river flow data.

The water quality modelling undertaken in this research represents the first reported application of WQFLOW-2D to the Patos lagoon and estuary system, and the first water quality modelling exercise of any kind reported to date for the Saco da Mangueira. Calibration and validation processes demonstrated that WQFLOW-2D could simulate annual average observed concentrations of water quality variables consistently and confirmed the eutrophic nature of the waters within the Saco da Mangueira. The model was used as a comparative tool to evaluate the predicted performance of hypothetical engineering schemes designed to improve the water quality within the bay and water exchange at the mouth. A number of recommendations were made including an imperative requirement for the collection of pollutant input and process data to reduce the level of uncertainty associated with the water quality model.
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Publications


Presentations and Conferences Attended

Modelling conference “Estuarine Modelling, Use or Abuse”, Westlakes Research Institute, Cumbria, UK, 6th – 7th September 2001.

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Modelling the Water Quality of the Patos Lagoon, Brazil

by

Deborah Ann Tyrrell
Chapter 1

Introduction

Multi-dimensional mathematical modelling of water quality is a challenging interdisciplinary art demanding the integration of the physical, chemical and biological components and processes affecting aquatic environments. The ability to quantify and predict the response of such environments to both natural and man-made perturbation can be achieved to a measurable level of confidence when the model is well designed, calibrated, and applied within its limitations. If this is successfully accomplished, the model has potential as an extremely useful tool for both understanding and extending the knowledge of complex environmental systems, and for supporting the environmental management process, through which regulatory authorities aim to determine the best solution to practical problems such as control of pollution and the protection of species and habitats considered under threat or in decline. The Patos lagoon and estuary is an aquatic system with complicated geography, conflicting water uses and pollution issues; it follows that managers and researchers may draw benefit from a water quality modelling tool.

1.1 The Study Area

The Patos Lagoon (‘Duck Pond’) is the largest choked coastal lagoon on earth and is located in the state of Rio Grande do Sul on the southern coast of Brazil between 30° to 32°S and 50° to 52°W (Figure 1.1). The region has a sub-tropical climate, and the system extends more than 250km NE to SW, with average width and depth of 40 km and 5m respectively. The tides are mixed and predominantly diurnal, with a microtidal mean range of just 0.47m, therefore, the dominant factors influencing the circulation of water are non-tidal, viz. winds, river flow, rainfall and evaporation.
Figure 1.1 The Patos Lagoon and Estuary System (maps from Agência Nacional de Águas (ANA) www.ana.gov.br)
Chapter I - Introduction

The Patos lagoon and estuary system is of major importance to the communities of the Rio Grande do Sul State, and is consequently subject to the influence of multiple and conflicting human impacts, many of which have the potential for pollution. Such activities include recreation and tourism; abstraction of drinking water and the disposal of domestic waste water; the industries of fertiliser production, fish processing, and petroleum refining; artisanal fisheries and aquaculture; agriculture; and navigation.

Within the boundaries of the estuary are several shallow embayments or “sacos”, which are biologically highly productive areas providing nursery grounds for important local species, but are degraded environments, especially the Saco da Mangueira, which suffers from eutrophication, algal blooms, and blooms of potentially toxic blue-green algae (*Microcystis aeruginosa*), owing to the input of effluents and refuse from industry, slums and large commercial and real estate enterprises, which have expanded along the shoreline for the last two decades (Tagliani & Saint Pastous Madureira, 2001). Increasing population and unregulated growth continues to exacerbate these problems; therefore, there is an immediate need for tools to assist managers and stakeholders in making appropriate long-term decisions to protect and repair the environment.

1.2 Aims and Objectives

The main aims of this research are to extend the knowledge of transport and dispersion processes gained from previous numerical simulations of the lagoon and estuarine hydrodynamics, and to evaluate a water quality model in terms of its ability to represent the involved processes and utility as predictive management tool. Specific objectives are as follows:
Chapter 1 - Introduction

- To collect and collate observations of the most relevant magnitudes relating to hydrodynamics, suspended matter, nutrients and pollutants in the southern most part of the Patos Lagoon Estuary and Saco da Mangueira;
- To interpret the data to gain an increased understanding of the physical, chemical and biological processes involved in the pollution of the Saco da Mangueira and surrounding area;
- To calibrate and validate modules of the numerical modelling suite TELEMAC for hydrodynamics, dispersion and water quality;
- To apply a hydrodynamic model to the study of transport and mixing time scales of the Saco da Mangueira;
- To apply the water quality model to a set of water quality management scenarios and evaluate its use as a predictive management tool;

1.3 Outline of the Thesis

Chapter 2 presents a review of the literature relating to the physical and chemical characteristics of the Patos Lagoon System. A detailed account of the data used in this research for the hydrodynamic and water quality modelling is provided in Chapter 3, including a description of recent site specific field studies undertaken, instrumentation and data processing.

Chapter 4 gives an introduction to hydrodynamic and water quality models in general, and describes in detail the TELEMAC modelling suite, with the emphasis on the 2-dimensional flow model (TELEMAC-2D) and the water quality module (WQFLOW-2D).
The calibration and validation of the hydrodynamic model are presented in Chapter 5, and simulations investigating flushing characteristics of the lagoon and estuary with a particular focus on the transport and mixing times scales in the Saco da Mangueira, are reported in Chapter 6.

Chapter 7 presents the calibration and validation of the water quality model, and the results of a number of model scenarios designed to investigate the changes in the quality of water under various environmental and pollutant input conditions are described and discussed in Chapter 8.

Chapter 9 presents the conclusions of this research together with recommendations for future work.
Chapter 2

Reviewing the Literature

2.1 Introduction

This review provides an overview of the Patos lagoon and estuary system and adjacent continental shelf area, in terms of the physical and biogeochemical processes and characteristics. Physical features such as geomorphology and regional climate are initially described, followed by a review of the literature relating to hydrodynamics, water and sediment chemistry including: nutrients and suspended matter; primary productivity; bacteria and other pollutants; metals and trace elements. Finally, a summary of the Brazilian and other international legislation relating to water quality is given in order to give context to the biochemistry of the system.

2.2 Characteristics of the Patos Lagoon and Estuary

The Patos lagoon and estuary system is located in the state of Rio Grande do Sul on the southern coast of Brazil approximately 2,000 km south of Rio de Janeiro between 30 to 32°S and 50 to 52°W (Figure 2.1). The lagoon has a warm temperate climate influenced by the St Helena sub-tropical anticyclone in the South Atlantic, with an average of 223 days/y. sunshine (Klein, 1997), and average rainfall of 1750 mm/y. (Knoppers & Kjerfve, 1999). The southern Brazilian coastal region has a microtidal regime with a mean amplitude of just 0.47m due to the proximity of an amphidromic point for the M₂ constituent (Möller & Castaing, 1999). Tides are predominantly mixed-diurnal in nature.
with an F-parameter of 2.42, and the principal component ($O_1 = 25.8h$) has an amplitude of 10.8 cm (Garcia, 1997).

The Patos Lagoon is known as the largest choked coastal lagoon in the world, and was formed by flooding during the Holocene sea-level rise, and exposed during the late Quaternary (Knoppers & Kjerfve, 1999). The system extends more than 250 km NE to SW (main axis of the lagoon 180 km), with an average width of 40 km (maximum 59.8 km); an area of 10,360 km$^2$ (Kjerfve, 1994; Calliari 1997; Knoppers & Kjerfve, 1999); and an average depth of only 5m. Asmus (1997) divided the Patos lagoon into five biological units: Guaiba Bay (the major freshwater tributary at the northern end); Tapes Bay;
Chapter 2 - Reviewing the Literature

Casamento Lagoon; the central lagoon body comprising 4 elliptic cells (80% of lagoon); and the Patos estuary (10% of lagoon). The bathymetry of the lagoon is highly variable and characterised by natural and artificial channels with depth of 8 – 9m, large adjacent areas of less than 5m, and very shallow marginal bays (Calliari 1997, Fernandes, 2001).

The total Patos system watershed is 201,626 km² (including 51,194 km² from the Mirim lagoon), of which 75% discharges into the northern end of the Patos lagoon from the Guaiba river (Calliari, 1997, Windom et al. 1999, Niencheski et al., 1999). To the south of the Patos lagoon lies the Mirim lagoon (3,749 km²), and the two are connected by the 70 km long São Gonçalo Channel which has a mean fluvial discharge to the Patos estuary of 700 m³/s (Niencheski et al., 1999). The waters of the Mirim lagoon are used extensively for agricultural irrigation; therefore, there are a number of locks in the São Gonçalo Channel, which prevent saline water entering from the Patos estuary, and also reduce the freshwater flow into the estuary (Seeliger & Costa, 1997).

At the southern end of the lagoon lies the Patos estuary, which is bar-built and has an area of 971 km². The width of the upper estuary is 30 km, which reduces over a distance of 50 km from the tidal limit at Ponta da Feitoria to the southern Atlantic Ocean, where contact is through a single tidal inlet 22 km long, 2 km wide and 12m deep at the southern end of the system (Möller & Castaing 1996, Calliari, 1997). The bottom topography of the estuary is dominated by shoals of 1 – 5m, with an overall average depth of 3m (Knoppers & Kjerfve, 1999), though 80% is <2m and 50% is <1m (Niencheski et al., 1999). The maximum depth of the entire system is only 18m, found in the 700m wide inlet channel at the mouth of the estuary (Calliari, 1997, Niencheski et al., 1999).
There are a number of shallow embayments located in the southern region of the estuary surrounding the city of Rio Grande, namely Saco da Mangueira, Saco do Martins, Saco do Justino, Saco do Rio Grande, and Saco do Arraial. The shallow semi-enclosed bay of Saco da Mangueira is situated to the south of Rio Grande. It is oval in shape, with an area of 27.2 km$^2$ and a maximum depth of just 1.5m (Baumgarten et al., 1995). It is the hydrodynamics and water quality of this bay that will be receiving significant attention during this research.

The main cities and ports of the Patos system are located at Porto Alegre (population ~1,500,000) at the north of the Lagoon, Pelotas (population ~300,000) in the upper region of the estuary, and Rio Grande (population ~200,000) in the southern region of the estuary (Niencheski et al., 1999). The Patos system is of major importance to the communities of the Rio Grande do Sul State, and is consequently under the influence of multiple human impacts. The lagoon and estuarine waters are used for navigation; recreation and tourism; the abstraction of drinking water; industry (fertiliser and fish processing, petroleum refining); fisheries; agriculture (principally irrigated rice cultivation); and a number of food production industries (soya oil, wheat meal, canned products, etc.). In particular, nursery grounds for commercial fish and shrimp are provided in sheltered areas, which sustain a fishery that produces an average of 182 kg/ha/yr (Möller & Castaing, 1999).

The main impacts on water quality arising from human interactions were identified by Seeliger & Costa (1997):

- water demand for irrigation which reduces the freshwater flow into the system and results in modifications to flushing, salinity and nutrient balance, which ultimately affects the life cycles of commercially important fish and crustaceans;
inputs of nutrients from agriculture (phosphate 2-3 μM (0.06-0.09 mg/l); nitrogen >40 μM (>0.56 mg/l)), leading to eutrophication, algal blooms, and blooms of potentially toxic bluegreen alga (*Microcystis aeruginosa*);

- inputs of domestic effluent from approximately 3.5 million inhabitants;

- inputs of hazardous materials such as dissolved trace metals (Cu and Pb) from industrial effluents and mining activities, agrotoxins from pesticides, and hydrocarbons discharged by vessels through washing of tanks;

- modifications to water depths leading to changes in circulation patterns, resulting from inputs of suspended sediments, and shifting sediment deposition patterns from both natural and man-mediated processes including dredging activities in the navigation channel, and the construction of jetties at the mouth of the estuary.

An extensive study undertaken by Almeida *et al.*, (1993) between May 1991 and October 1992 identified the main effluents of waste waters in the vicinity of Rio Grande. A total of 76 effluent discharge points were detected, and of these, 18 discharges of domestic waste; 24 industrial wastes, 4 mixed effluents and 30 stormwater discharges.

Of particular relevance to this study is the industrial input of phosphates to Saco da Magueira from one of the largest fertiliser plants in S. America (~106 tons /year 1995) (Niencheski *et al.*, 1999).

^Eutrophication is “the enrichment of water by nutrients, especially compounds of nitrogen and phosphorus, causing an accelerated growth of algae and higher forms of plant life to produce an undesirable disturbance to the balance of organisms and the quality of the water concerned.”, (as defined by the European Commission Directive 91/271/EEC of 21 May 1991 concerning urban waste-water treatment).
Chapter 2 - Reviewing the Literature

2.3 Hydrodynamic Regime of the Patos Lagoon System

This section reviews the research conducted to date on the factors that affect water circulation in the Patos lagoon and estuary. The principal authors from the literature reviewed are O. O. Möller, J. P. Castello, and P. Castaing of the Federal University of Rio Grande (FURG). Some typical hydro-meteorological values for the Patos lagoon and estuary are summarised in Table 2.1.

<table>
<thead>
<tr>
<th>Location</th>
<th>Parameter</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lagoon/Estuary</td>
<td>Mean annual temp.</td>
<td>Between 13 °C (July) and 24 °C (January)</td>
<td>Klein, 1997</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Typical salinity</td>
<td>0 g/kg</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Estuary</td>
<td>Mean annual salinity</td>
<td>18 g/kg</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Estuary</td>
<td>Mean annual sal. range</td>
<td>3 - 34 g/kg</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Tidal Range</td>
<td>0 m in lagoon proper, 0.47 m in estuary</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Tidal regime</td>
<td>Mixed, mainly diurnal (F=2.42)</td>
<td>Garcia, 1997</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Principal harmonic</td>
<td>Q = 25.8 hr. 10.8cm</td>
<td>Garcia, 1997</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Sea level rise</td>
<td>1 m in 300 years</td>
<td>Calliari, 1997</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Maximum flushing currents</td>
<td>1.7 to 1.9 m/s</td>
<td>Garcia, 1997</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Freshwater Residence Time</td>
<td>5 months</td>
<td>Windom et al., 1999</td>
</tr>
<tr>
<td>Lagoon</td>
<td>Maximum lagoon velocity</td>
<td>0.3 m/s</td>
<td>Garcia, 1997</td>
</tr>
<tr>
<td>Lagoon</td>
<td>Flushing half life</td>
<td>82 days</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Lagoon</td>
<td>Transit time</td>
<td>20 days</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Estuary</td>
<td>Tidal flushing rate; half life</td>
<td>2013 m³/s; 3 days</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Dominant wind</td>
<td>NE winds (5 m/s), SW winds (8 m/s) during passage of cold fronts more common in Winter</td>
<td>Klein, 1997</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Local wind</td>
<td>Set up/set down mechanism of oscillation</td>
<td>Möller &amp; Castaing, 1999</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Mean summer winds (Sep to Apr)</td>
<td>3.6 to 5.1 m/s NE 22% of year</td>
<td>Garcia, 1997</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Mean winter winds (May to Oct)</td>
<td>5.7 to 8.2 m/s SW 12% of year</td>
<td>Garcia, 1997</td>
</tr>
<tr>
<td>Estuary</td>
<td>Mean monthly wind speed</td>
<td>5.12 m/s</td>
<td>Niencheski et al., 1999</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Total mean annual precipitation</td>
<td>12000 mm to 15000 mm. Most rainfall in Winter and Spring. Rainfall (132 cm) exceeds evaporation (~90 cm).</td>
<td>Klein, 1997, Niencheski et al., 1999</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Freshwater sources</td>
<td>Guaiba River (incl. Jacqui, Sinos, Cai, and Gravatai tributaries) 86%, Camaqua River most of remainder.</td>
<td>Niencheski et al., 1999</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Average Freshwater Discharge</td>
<td>3712 m³/s (700 m³/s from Mirim lagoon through São Gonçalo Channel)</td>
<td>Knoppers &amp; Kjerfve, 1999, Calliari, 1997</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Maximum Freshwater Discharge</td>
<td>Winter extreme 25,000 m³/s. Estuary surface plume can extend 40 km onto shelf</td>
<td>Niencheski et al., 1999</td>
</tr>
<tr>
<td>Lagoon/Estuary</td>
<td>Seawater intrusion</td>
<td>January to March 200 km into lagoon</td>
<td>Windom et al., 1999</td>
</tr>
<tr>
<td>Estuary</td>
<td>Inflowing seawater rate</td>
<td>1.3 m/s</td>
<td>Garcia, 1997</td>
</tr>
</tbody>
</table>

Table 2.1 Typical Values for Hydrography in the Patos Lagoon and Estuary
A number of field studies focusing on hydrographic and hydrodynamic measurements have been conducted in the Patos lagoon and estuary, and adjacent coastal waters between 1977 and 1998. Surveys have typically included the measurement of current speed and direction, water elevation, wind speed and direction, salinity, and temperature. The sampling locations for the survey data published to date are presented in Figure 2.2 and detailed in Table 2.2 below:

![Figure 2.2](image-url)
<table>
<thead>
<tr>
<th>Survey Period</th>
<th>Sampling Frequency/Season</th>
<th>Measurements and Survey Locations</th>
<th>Wind Velocity</th>
<th>River Flow</th>
<th>Other Measurements and Notes</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pre 1977</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10/87, 09/88, 02/90, 06/91</td>
<td>Spring, Summer, Autumn, Winter</td>
<td>55 stations in 10 cross shelf transects: surface, mid-depth and 20 cm above bed</td>
<td>Survey vessel &amp; Rio Grande (3 hourly intervals)</td>
<td>Temperature &amp; salinity (T/S at surface)</td>
<td>Castello &amp; Möller 1977</td>
<td></td>
</tr>
<tr>
<td>1988</td>
<td>12 monthly cruises</td>
<td>18 stations along the entire lagoon at 2m depth intervals</td>
<td>Survey vessel &amp; Rio Grande (3 hourly intervals)</td>
<td>Temperature &amp; salinity (T/S at surface)</td>
<td>Soares &amp; Möller 2001</td>
<td></td>
</tr>
<tr>
<td>12/02/88-28/03/88</td>
<td>Hourly</td>
<td>Rio Grande, Itapoa</td>
<td></td>
<td></td>
<td></td>
<td>Möller &amp; Castaing 1999</td>
</tr>
<tr>
<td>11-13/01/92</td>
<td>Hourly</td>
<td>Praticagem (Rio Grande Pilots)</td>
<td></td>
<td></td>
<td></td>
<td>Fernandes 2001</td>
</tr>
<tr>
<td>01-31/01/92</td>
<td>Hourly</td>
<td>Praticagem (DHN)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>06-11/04/92, 18-23/05/92, 22-27/06/92, 5-10/10/92</td>
<td>4 cruises total 110 hrs</td>
<td>Praticagem</td>
<td>Fixed station near Praticagem at 3, 6, &amp; 10m depths</td>
<td>Praticagem</td>
<td>T/S at 2m depth intervals from fixed station near Praticagem</td>
<td>Möller &amp; Castaing 1999</td>
</tr>
<tr>
<td>04/03/97-27/05/97</td>
<td>30 minutes</td>
<td>Mooring 125km off estuary on 48m isobath: current meters at 15m &amp; 43m below surface</td>
<td>Survey vessel &amp; Rio Grande</td>
<td>T/S</td>
<td>Soares &amp; Möller 2001</td>
<td></td>
</tr>
<tr>
<td>23/05-06/06/98</td>
<td>Hourly</td>
<td>Praticagem, Sao Jose do Norte (INPH)</td>
<td>Praticagem</td>
<td>During El Niño</td>
<td>Fernandes 2001</td>
<td></td>
</tr>
<tr>
<td>20-29/10/98</td>
<td></td>
<td>Estuary channel adjacent to Praticagem at hourly intervals</td>
<td>Estuary channel adjacent to Praticagem at 5 minute intervals</td>
<td>Praticagem</td>
<td>Vertical profiles (CTD), suspended matter, surface sediments &amp; sediment cores for organic matter, water content &amp; grain size</td>
<td></td>
</tr>
<tr>
<td>26-28/10/98</td>
<td>10 minutes</td>
<td>Feitoria</td>
<td>Feitoria</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>27-29/10/98</td>
<td>30-45 minutes</td>
<td>Praticagem, Marambaia, Feitoria</td>
<td>Praticagem, Marambaia, Feitoria: surface, middle &amp; 20cm above bed</td>
<td>Praticagem, Marambaia, Feitoria</td>
<td>Vertical profiles (CTD), suspended matter, surface sediments &amp; sediment cores for organic matter, water content &amp; grain size</td>
<td></td>
</tr>
<tr>
<td>05-06/11/98</td>
<td>30-45 minutes</td>
<td>Porto Rei</td>
<td>Porto Rei: surface, middle &amp; 20cm above bed</td>
<td>Porto Rei</td>
<td>Vertical profiles (CTD), suspended matter, surface sediments &amp; sediment cores for organic matter, water content &amp; grain size</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.2  Hydrographic and Hydrodynamic Fieldwork Conducted in the Patos Lagoon and Estuary
Most choked coastal lagoon systems are wind forced rather than tidally driven (Kjerve, 1986). The relative importance of winds, tides and river flow on the barotropic circulation of Patos lagoon were reviewed by Möller & Castaing (1996), and further studies conducted by Möller et al. (1996), and Möller (1996) demonstrated that the dominant factors influencing the circulation and residence time of water in the system are indeed non-tidal, i.e. winds, river flow, rainfall and evaporation. An important hydrological characteristic of the Patos lagoon estuary is considered to be its considerable range in salinity, which is responsible for both horizontal and vertical stratification (Kantin, 1982). Variation of salinity in the estuary results from seawater penetration and freshwater runoff mainly controlled by rainfall and wind, rather than tides.

Costa et al. (1988) conducted measurements of wind and surface water salinities for one year in the lower estuary and access channel, and showed that winter/spring winds from the north above 5 m/s induced oligohaline conditions in the access channel, and southerly winds above 13 m/s induced polyhaline conditions. During the dry months of summer and autumn even weak moderate south winds caused meso- and polyhaline salinities in both the access channel and the lower estuary. It was concluded that during periods of high river discharge in winter and spring, only very strong southerly winds would be able to force salt water into the lagoon. Further examination of the distribution of salinity in the lower estuary by Möller et al. (1991), showed a negative exponential relationship between monthly mean freshwater discharge and monthly mean surface salinity measured near the mouth of the estuary ($r = 0.79$). Mata & Möller (1993) applied the segmented tidal prism model by Dyer & Taylor (1973) to estimate the flushing time of Patos Lagoon estuary as a function of freshwater discharge and astronomical tide. Results demonstrated this model to be valid only when the estuarine circulation is not controlled by wind.
The main aspects of the summertime circulation and dynamics of the Patos Lagoon were described by Möller et al. (1996), through the analysis of time series of wind stress, water level and freshwater discharge, combined with the results of a barotropic circulation model (Princeton Ocean Model – POM). They verified that the longitudinal wind component is the main driving force, generating a set-up/set-down mechanism of oscillation with the nodal line in the deeper parts of the mid-lagoon area, and this coincides with the passages of frontal systems for the region. Sea breezes were observed to have a secondary effect in the northern part of the lagoon, and freshwater discharges caused variations in water level both seasonally and on a smaller time scale of 8-15 days.

The tidal signal was found to be important only near the estuary mouth, with significant signals from diurnal (T = 25.6h), semi-diurnal (T = 12.5h), and quarter-diurnal (T = 6.2h) tidal components. As is typical for choked lagoons, the tidal signal is strongly attenuated as the tidal wave advances through the estuary to the interior of the lagoon. Model results suggested that near the shore, the longitudinal momentum balance is mostly governed by friction, with the wind stress being balanced by the bottom friction. In the lateral direction, a geostrophic balance was verified in both regions. The wind forced circulation in summer was found to be characterised by downwind velocity near the shore, with upwind return flow occurring in the central lagoon areas, with maximum current velocities of ~0.3 m/s in the main body of the lagoon, and velocities reaching 1.7 – 1.9 m/s in the inlet following a prolonged period of heavy rainfall.

Möller & Castaing (1996) used time series of wind and water level records obtained along the lagoon for 1988 to assess the relative importance of winds, tides and river flow on the barotropic circulation of Patos Lagoon. They reported that during flood periods (late winter/ early spring), winds from the north-east are dominant, which enhance seaward
outflow from the lagoon. This situation becomes more dramatic during 'El Niño' periods when higher precipitation rates cause lagoon waters to remain fresh for several months. During low river discharge periods (summer, autumn and part of winter) south-westerly winds drive the circulation on time scales associated the passage of frequent frontal systems, from 3 to 16 days, and typical wind speeds are between 3 to 5 m/s (see Table 2.1).

The rivers flowing into the lagoon were reported to show typical mid-latitude flow patterns of high discharge in late winter and early spring followed by low to moderate discharge through summer and autumn, with total discharges varying from year to year. The average discharge of freshwater to the lagoon is 2000 m$^3$/s (Möller and Castaing, 1999), with monthly means ranging from 700 m$^3$/s during summer up to 3,000 m$^3$/s in spring. River discharge peaks of 20,000 and 12,000 m$^3$/s have been observed by Rochefort (1958) and Möller et al. (1991) respectively, with an extreme winter value of 25,000 m$^3$/s reported by Niencheski et al. (1999). Möller et al. (1991) have shown that for river flows in excess of 3,000 m$^3$/s, the estuarine/ coastal water mixing zone is transferred to the inner continental shelf and the inner limit of the salt water penetration is around Ponta da Feitoria. Conversely, during periods of low freshwater runoff seawater can penetrate up to 200 km into the lagoon (Windom et al., 1999). Owing to a total length of over 250 km, the residence time of freshwater during high discharge periods, was calculated to be about 5 months by Windom et al. (1999), which results in the salinity gradient being spread over most of the lagoon. The wind accounts for 65% of the circulation patterns so events some distance along the continental shelf will have an effect on the lagoon (Möller pers com.).

The relative importance of local and non-local winds on circulation described above were confirmed by Möller et al. (2001) by the use of time series analysis of wind, freshwater discharge, and water level records, and results from a 3D numerical model.
Fernandes (2001) completed a numerical modelling study involving calibration and application of the TELEMAC System in 2D and 3D modes, to study the hydrodynamics of the Patos lagoon. Measurements of wind velocities at 5 minute intervals and water levels at hourly intervals were made in the estuary channel adjacent to Praticagem between 20th and 29th October 1998, and current and wind velocities were recorded at 10 minute intervals in the estuary channel at Feitoria between 26th and 28th October 1998. Measurements of current velocities at surface, mid-depth and near-bed, and vertical profiles of salinity and temperature, together with water elevation, wind speed and direction, and samples of suspended matter, surface sediments and sediment cores for organic matter, water content and grain size, were also carried out at Praticagem, Marambaia and Feitoria between 27th and 29th October 1998. The measurements made between 27th and 29th October 1998 were repeated at a location in the estuary shallow area at Porto Rei between 5th and 6th November 1998 (during a strong El Niño event), and used as an independent data set for model validation.

Results of the study by Fernandes proved that the barotropic pressure gradients established between the lagoon and the coastal area as a result of local and remote wind combined with the freshwater discharge, are indeed the main forces controlling the sub-tidal circulation both within and outside of the lagoon. The results also confirmed previous studies by Möller, that the local winds dominate the lagoon circulation through the set-up/set-down mechanism of oscillation, whereas the non-local wind drives the circulation in the lower estuary, with the entrance channel acting as a filter that strongly reduces tidal and sub-tidal oscillations generated offshore.

The 3D TELEMAC simulations undertaken and reported by Fernandes (2001) showed that the wind drives the lateral flow in the shallow areas, whereas lateral pressure gradients
combined with channel curvature and geometry govern flows in the channel. Also, barotropic forces are the main mechanism controlling salt water penetration and salinity structure in the estuary. Significantly, the study concluded that the TELEMAC modelling system is a suitable tool to be used for future hydrodynamic, sediment transport and water quality studies in the Patos area.

2.4 Chemistry of the Waters of the Patos Lagoon System

It is clear from the previous section that the observed water circulation patterns are dominated by meteorological conditions and the geometry of the system. The temporal variations and spatial distributions of physico-chemical parameters throughout the Patos system have also been the subject of numerous studies undertaken over the past two decades by FURG. General patterns and trends result from the interactions between forcing factors, sediment characteristics and anthropogenic activities, many of which are related to the seasonal patterns of temperature, wind, and precipitation of the region. The shallow water depths and long residence times allow vertical mixing, resulting in significant interactions between sediments and the water column, leading to high biological productivity, which in turn affects water quality (Neincheski et al., 1999).

Field studies have been carried out in the coastal waters adjacent to the Patos lagoon, and the southern part of the Patos lagoon and estuary from 1979 onwards. Measurements have typically included physical profiling and the collection of water samples at various water depths for the determination of nutrients, suspended matter, primary productivity parameters, bacteria, and trace metals. The sampling locations for the survey data published to date are presented in Figure 2.3 and detailed in Table 2.3 below.
Figure 2.3  Water Quality Sampling Locations
## Survey Period | Sampling Freq. | Survey Locations | Depths | Parameters                                  | Reference |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Pre 1977</td>
<td></td>
<td>17 sediments from southern Patos Lagoon</td>
<td></td>
<td>grain size, statistical and morphoscopic analysis</td>
<td>Calliari et al., 1977</td>
</tr>
<tr>
<td>7/67-7/82</td>
<td></td>
<td>Patos Lagoon</td>
<td></td>
<td>N-NH₄⁺, N-NO₂⁻, and P-PO₄³⁻</td>
<td>Kantin et al., 1984</td>
</tr>
<tr>
<td>3/78-3/79</td>
<td>Monthly</td>
<td>Two areas surrounding Rio Grande</td>
<td></td>
<td>inorganic compounds, oil</td>
<td>Kantin et al., 1981</td>
</tr>
<tr>
<td>9/78-3/80</td>
<td>Monthly</td>
<td>Water from 7 estuary sites</td>
<td>Surface</td>
<td>T, S, P-PO₄³⁻, N-NO₃⁻, N-NH₄⁺, Si, seston</td>
<td>Kantin &amp; Baumgarten, 1982</td>
</tr>
<tr>
<td>4/79-3/80</td>
<td>13 x 2 day</td>
<td>Water from 17 estuary sites</td>
<td>Surface, bottom</td>
<td>TSM, T, S, transparency, wind, LANDSAT images</td>
<td>Calliari et al., 1982, &amp; Hartmann &amp; Calliari, 1982</td>
</tr>
<tr>
<td>18/4/79</td>
<td></td>
<td>Lower estuary</td>
<td></td>
<td>Enteromorpha</td>
<td>Seeliger &amp; Cordazzo, 1982</td>
</tr>
<tr>
<td>11/79-10/80</td>
<td>Monthly</td>
<td>Water from 5 estuary sites</td>
<td>Surface</td>
<td>Hg, TSM</td>
<td>Seeliger &amp; Braga Knak, 1982</td>
</tr>
<tr>
<td>11/79-6/81</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4/80-6/81</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8/81-7/82</td>
<td>Daily and</td>
<td>Water from 11 estuary sites</td>
<td>Surface</td>
<td>benthic algae (94 species), S, T, day length, light radiation</td>
<td>Coutinho &amp; Seeliger, 1984 &amp; 1986</td>
</tr>
<tr>
<td></td>
<td>Biweekly</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9/81-2/82</td>
<td>Monthly</td>
<td>Water from 10 sites from north of Rio Grande to estuary mouth</td>
<td>Surface at 10 sites, mid and bottom at 2 sites</td>
<td>T, S, DO, seston, N-NH₄⁺, P-PO₄³⁻, anionic detergents at 10 sites, BOD₅ and N-NO₂⁻ at 2 sites</td>
<td>Ameida et al., 1984, &amp; Kantin et al., 1982</td>
</tr>
<tr>
<td>Pre 1982</td>
<td></td>
<td>Water from Saco de Manguiera and Saco do Arraial</td>
<td></td>
<td>T, S, TSM, P-PO₄³⁻, N-NO₂⁻, N-NH₄⁺</td>
<td>Baumgarten et al., 1982</td>
</tr>
<tr>
<td>Pre 1982</td>
<td>Hourly in 24 hour periods</td>
<td>At the narrower point of the Canal do Norte</td>
<td>Surface, 8m and 16m</td>
<td>current speed and direction, water elevation, S, T, TSM, P-PO₄³⁻, N-NO₂⁻</td>
<td>Cruz et al., 1982</td>
</tr>
<tr>
<td>Pre 1982</td>
<td>Daily</td>
<td>Water from Pelotas city pollution sources</td>
<td></td>
<td>BOD₅, total coliform, faecal coliforms</td>
<td>Palm &amp; Cobalchini, 1982</td>
</tr>
<tr>
<td>16/7-21/82</td>
<td>Water at 91 sites from shelf and oceanic waters</td>
<td>Vertical profiles</td>
<td>T, S, N-NO₃⁻, N-NO₂⁻, P-PO₄³⁻, Si, N-NH₄⁺, Chl-a, secchi depth, photosynthetic rates</td>
<td>Pereira, 1990</td>
<td></td>
</tr>
<tr>
<td>19/2-26/3/83</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pre 1983</td>
<td></td>
<td></td>
<td></td>
<td>nutrients, surfactants, sulphides, oil, grease, coliforms</td>
<td>Kantin, 1983</td>
</tr>
<tr>
<td>10-28/10/87</td>
<td>Early spring</td>
<td>Water from 53 ocean sites off Rio Grande</td>
<td>Surface and through depth</td>
<td>T, S, Si, N-NO₃⁻, P-PO₄³⁻, Chl-a</td>
<td>Ciotti et al., 1995</td>
</tr>
<tr>
<td>7-15/9/88</td>
<td>Late winter</td>
<td>Sediment at 61 estuarine sites</td>
<td></td>
<td>Cu, Cr, Zn, Cd, and Pb</td>
<td>Baisch et al., 1988</td>
</tr>
<tr>
<td>3/89-3/90</td>
<td>Weekly</td>
<td>Water at 1 shallow estuary site</td>
<td>Surface</td>
<td>bacteria, flagellates, ciliates, Chl-a, N-NH₄⁺, N-NO₃⁻, N-NO₂⁻, P-PO₄³⁻, eston weight, POC, T, S, 14C uptake</td>
<td>Abreu et al., 1992 &amp; Abreu et al., 1994</td>
</tr>
<tr>
<td>6/6, 7/7, 12/8, 13/9, 2/12/89</td>
<td>5 x 1 day</td>
<td>Water from 19 longitudinal estuarine sites, and 4 transect sites</td>
<td>Surface, profiles every 1m</td>
<td>T, S, Secchi depth, Chl-a, N-NH₄⁺, N-NO₂⁻, N-NO₃⁻, P-PO₄³⁻</td>
<td>Abreu et al., 1995</td>
</tr>
<tr>
<td>Pre 1990</td>
<td>Estuary</td>
<td></td>
<td></td>
<td>shells and soft parts of Balanus improvisus (copper, lead, manganese), T, S, pH, TSM</td>
<td>Baumgarten &amp; Niencheski, 1990</td>
</tr>
</tbody>
</table>

**Table 2.3** Biogeochemical Fieldwork Conducted in the Patos Lagoon and Estuary
<table>
<thead>
<tr>
<th>Survey Period</th>
<th>Sampling Freq.</th>
<th>Survey Locations</th>
<th>Depths</th>
<th>Parameters</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>30/6/89, 30/8/89, 30/5/90, 30/6/90, 1/8/90, 30/8/90, 1/12/90, 22/4/91</td>
<td>8 x 1 day</td>
<td>Water from 20 estuary sites, 1 site in Sao Goncalo</td>
<td>Surface, bottom, vertical profiles every 1m</td>
<td>T, S, conductivity, N-NH$_4^+$, N-NO$_3^-$, N-NO$_2^-$, Si, P-PO$_4^{3-}$, TSM</td>
<td>Niencheki &amp; Windom, 1994</td>
</tr>
<tr>
<td>8/90 - 4/91</td>
<td>Weekly for 9 months</td>
<td>Water from 1 site in Saco da Mangueira and 1 site in Saco do Armaial</td>
<td>Surface</td>
<td>T, S, POC, seston, Chl-a, N-NH$_4^+$, N-NO$_3^-$, N-NO$_2^-$, P-PO$_4^{3-}$, Si, TSM, anionic detergent</td>
<td>Persich et al., 1996</td>
</tr>
<tr>
<td>1/8/90</td>
<td>High flow 5288 m$^3$/s</td>
<td>Water from 12 sites in the estuary</td>
<td>Surface, bottom, vertical profiles every 1m</td>
<td>T, S, conductivity, TSM, dissolved and particulate: Al, Fe, Ni, Cu, Zn, Cd, Pb, Li, P, V, Cr, As, Ag, Ba, Mn, POC</td>
<td>Niencheki et al., 1994</td>
</tr>
<tr>
<td>30/8/90</td>
<td>Low flow 1400 m$^3$/s</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22/4/92, 6/5/92, 22/5/92, 3/6/92, 23/9/92, 11/3/93, 18/3/93, 26/93, 8/7/93</td>
<td>9 ebb surveys</td>
<td>Water from 8 sites adjacent to Rio Grande main outfall</td>
<td>Surface</td>
<td>T, S, pH, TSM, P-PO$_4^{3-}$, N-NO$_3^-$, N-NO$_2^-$, N-NH$_4^+$, DO, BOD$_3$, COD, met</td>
<td>Baumgarten et al., 1998</td>
</tr>
<tr>
<td>2/12/92, 22/12/92, 26/3/93, 15/4/93, 22/4/93, 17/6/93</td>
<td>6 flood surveys</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pre 1994</td>
<td>During 1 year</td>
<td>Different points of the shallow area of Lagoon</td>
<td></td>
<td>Chl-a, POC</td>
<td>Procna et al., 1994</td>
</tr>
<tr>
<td>94 - 95</td>
<td>During 1 year</td>
<td>Estuary</td>
<td></td>
<td>Microcystis aeruginosa (cyanobacteria)</td>
<td>Matthiensen et al., 1999</td>
</tr>
<tr>
<td>2/94 - 1/96</td>
<td>24 x 1 or 2 days</td>
<td>Water at 6 lagoon sites and 7 estuarine bloom sites</td>
<td>Surface</td>
<td>Chl-a, cyanobacterii (m.aeruginosa) bloom composition</td>
<td>Yunes et al., 1996</td>
</tr>
<tr>
<td>14-15/12/95</td>
<td>Water from 22 estuary and lagoon sites</td>
<td>Mid-depth (2-4m below surface)</td>
<td>N, K, Mg, Ca, Si, P-PO$_4^{3-}$, N-NH$_4^+$, N-NO$_3^-$, N-NO$_2^-$, pH, DO, Al, Cd, Co, Ca, Fe, Mn, Ni, Pb, Zn, T, S</td>
<td>Windom et al., 1999</td>
<td></td>
</tr>
<tr>
<td>15/1, 22/1, 29/1, 5/2, 12/2, 19/2, 26/2/96</td>
<td>Weekly</td>
<td>Water from North of Rio Grande, Saco Mangueira mouth, West Jetty</td>
<td>Surface</td>
<td>T, S, Secchi depth, N-NH$_4^+$, P-PO$_4^{3-}$, N-NO$_3^-$, N-NO$_2^-$, pH, seston weight, Chl-a, DO, BOD$_3$, total and faecal coliforms</td>
<td>Santos et al., 1997</td>
</tr>
<tr>
<td>Pre 1999</td>
<td></td>
<td></td>
<td>Sedimentation rates</td>
<td></td>
<td>Toldo et al., 1999</td>
</tr>
</tbody>
</table>

Table 2.3 (cont) Biogeochemical Fieldwork Conducted in the Patos Lagoon and Estuary
Chapter 2 - Reviewing the Literature

The following sections review the water quality characteristics of the Patos Lagoon estuary and southern part of the Patos Lagoon, with reference to variation in the conservative physical properties of temperature and salinity, and of controlling variables such as pH, suspended solids and dissolved oxygen. Salinity is used as a reference to determine whether a substance is conservatively transported, removed or added to the system, but this is true only if values for minimum and maximum salinities (freshwater and marine end members) remain constant over the residence time (Neincheski et al., 1999).

2.4.1 Water Quality Variables

This section relates principally to suspended solids and the nutrient variables of nitrate, nitrite, ammonia, phosphate, and silicate. Nitrogen is generally monitored as nitrate, nitrite and ammonium concentrations which, when added together, produce total inorganic nitrogen (TIN) or dissolved available inorganic nitrogen (DAIN), an approximation of bioavailable nitrogen. Phosphorus is also present in the aquatic environment in both inorganic and organic forms, and the principal inorganic form is orthophosphate measured as dissolved orthophosphate (soluble reactive phosphate SRP, or dissolved available inorganic phosphate DAIP), or as total reactive phosphate (TRP) by measuring phosphate in unfiltered samples. The ratio of these principal nutrients in river water is generally 10:1 (Langston et al., 2003). Also reviewed here are the available literature relating to contamination in the lower Patos estuary from phenolic compounds and oils, anionic detergent, and bacteria. The principal authors for the Patos lagoon and estuary are: M. G. Baumgarten, R. Kantin, L. F. Niencheski, and H. L. Windom.

The biogeochemical cycle consists of nutrient uptake in seaward flowing water, sinking particulate material and remineralisation in landward flowing deep water (Niencheski and Windom, 1994). Nutrients and contaminants entering the system through human activity
affect water quality through the mixing processes of estuarine hydrodynamics, and physical/chemical exchange in both dissolved and particulate forms with sediments, water column, and biota (Neincheski et al., 1999).

According to Neincheski et al. (1999), freshwater inputs from the Guaiba River have a residence time of 20 days travelling 250 km through the lagoon to reach the Patos estuary, and will therefore have undergone biochemical changes that may reduce their original impact. The long transit time of the lagoon means that dissolved inorganic nitrogen and dissolved phosphate from the freshwater inputs appear to be removed from the water column of the southern part of the lagoon due to phytoplankton production in further north (Niencheski and Windom, 1994). Some typical nutrient concentrations for the Patos lagoon estuary are presented here in Table 2.4.

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>VALUE</th>
<th>SOURCE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sources of nutrients and suspended matter</td>
<td>86% from Guaiba river</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td></td>
<td>Anthropogenic from Porto Alegre, agricultural from Mirim though São Gonçalo Channel, sewage from Pelotas and industrial/port activities from Rio Grande</td>
<td>Niencheski et al., 1999</td>
</tr>
<tr>
<td>Average seston load</td>
<td>80 mg/l</td>
<td>Abreu et al., 1995</td>
</tr>
<tr>
<td>Maximum seston load</td>
<td>700 mg/l (in summer)</td>
<td>Abreu et al., 1995</td>
</tr>
<tr>
<td>Winter phosphate</td>
<td>$-0.5 , \mu M$ ($-0.016 , \text{mg/l}$)</td>
<td>Abreu et al., 1995</td>
</tr>
<tr>
<td>Maximum phosphate</td>
<td>4 $\mu M$ (0.124 mg/l) (in summer)</td>
<td>Abreu et al., 1995</td>
</tr>
<tr>
<td>Mean annual dissolved inorganic phosphate</td>
<td>0.2 $\mu M$ (0.006 mg/l)</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Mean annual dissolved inorganic phosphate range</td>
<td>0.0 - 0.6 $\mu M$ (0 - 0.019 mg/l)</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Maximum nitrate</td>
<td>70 $\mu M$ (0.980 mg/l) (end of winter early spring)</td>
<td>Abreu et al., 1995</td>
</tr>
<tr>
<td>Mean annual dissolved inorganic nitrate</td>
<td>4 $\mu M$ (0.056 mg/l)</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Mean annual dissolved inorganic nitrate range</td>
<td>0.0 - 7.0 $\mu M$ (0 - 0.098 mg/l)</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Maximum ammonium</td>
<td>10 $\mu M$ (0.140 mg/l) (end of winter early spring)</td>
<td>Abreu et al., 1995</td>
</tr>
<tr>
<td>N:P ratio</td>
<td>7:1</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
</tr>
<tr>
<td>Average silicate concentration</td>
<td>175 $\mu M$ (4.90 mg/l)</td>
<td>Niencheski et al., 1999</td>
</tr>
</tbody>
</table>

Table 2.4 Typical Values for Nutrients in the Patos Lagoon Estuary
Chapter 2 - Reviewing the Literature

Castello and Möller (1977) described the seasonal variation in temperature, salinity, dissolved oxygen, phosphate and nitrate in surface water samples from the shelf and offshore area between 20°S and 38°S using data obtained from the 'Banco Nacional de Dados Oceanográficos do Brasil'. The paper discussed the instability of the western margin of the subtropical convergence zone where the Brazil and Falkland Currents interact, and showed that frequent ascension of the Antarctic Intermediate Water along the continental slope occurs. In winter, freshwater from the La Plata River and Patos Lagoon significantly influences the salinity and nutrient distribution on the Uruguayan and Brazilian shelf.

The first reported hydrographic measurements for the Patos lagoon estuary were conducted by Calliari et al. (1982), and Hartmann and Calliari (1982) who reported on a survey campaign of monthly measurements from surface and bottom water of suspended matter, salinity, temperature, transparency and wind at seventeen locations in the estuary, during thirteen cruises of two days duration each between April 1979 and March 1980. The cruises coincided with the passage of the LANDSAT satellite (18-day orbit). The suspended matter concentrations increased with depth and also towards the lagoon's mouth, with a lateral gradient that increased from the east margin towards the west margin. At surface and bottom, the suspended matter ranged from 6.91 mg/l in summer to 78.18 mg/l in winter. The organic fraction was generally 60% of the total. These results give some indication of the processes of settling velocity and turbulence in the estuary. The results for salinity gave a bi-seasonal alternating trend with high values in spring and autumn, and low values in winter and summer. The surface water temperature varied from 13 °C in winter to 25 °C in summer.
Kantin et al. (1982) and Almeida et al. (1984) reported on studies conducted to evaluate the concentrations of polluting organic compounds in the Patos lagoon estuary. Monthly measurements of temperature, salinity, dissolved oxygen, seston, ammonia, phosphate, and anionic detergents from surface water samples were taken at ten sampling stations located from the north of the city of Rio Grande to the mouth of the estuary, between September 1981 and February 1982. Monthly mid- and bottom water samples at two stations were also analysed for nitrate and biochemical oxygen demand (BOD). Salinity ranged from 0 to 35 g/kg, and was positively correlated with detergents, phosphates, nitrates, and BOD. At the stations near to Rio Grande the mean concentration of dissolved oxygen was 5.25 ± 0.17 mg/l; 24.2 ± 10.59 μM (0.339 ± 0.148 mg/l) for nitrates; 2.25 ± 0.64 μM (0.070 ± 0.020 mg/l) for phosphates; and 8.72 ± 1.69 μM (0.122 ± 0.024 mg/l) for ammonia. The mean concentrations reported for stations further north of Rio Grande were 5.65 ± 0.16 mg/l for dissolved oxygen; 20.70 ± 10.18 μM (0.290 ± 0.143 mg/l) for nitrates; 1.24 ± 0.27 μM (0.038 ± 0.008 mg/l) for phosphates; and 7.81 ± 2.17 μM (0.109 ± 0.030 mg/l) for ammonia. The results showed that the area close to Rio Grande presented significantly higher mean concentrations of phosphates and seston, and lower concentrations of dissolved oxygen than those of the area further north. A negative correlation was apparent between dissolved oxygen and detergents, phosphates, nitrates and ammonia, which suggested that the more polluted areas were associated with low dissolved oxygen and high salinity. Eutrophication was more intense for the area close to Rio Grande.

Kantin and Baumgarten (1982) reported on observations made from monthly measurements of temperature, salinity, phosphate, nitrate, ammonia, silicate, and seston in surface water samples from 7 sites in the Patos Lagoon estuary between September 1978 and March 1980. Results showed that under calm weather conditions, vertical
homogeneity was the principal hydrographic characteristic, and fluctuations in salinity controlled the behaviour of nutrients. Non-conservative behaviour was observed for inorganic nitrogen, soluble reactive phosphorus, and silica (but less apparent), suggesting trapping of these nutrients by the sediments. In contrast, the highest values were likely to have resulted from mineralising processes and contamination by domestic sewage.

Paim & Cobalchini (1982) reported a study on water pollution around Pelotas city (situated adjacent to the São Gonçalo channel) from both domestic and industrial waste inputs. The parameters measured were BOD, total and faecal coliforms, and comparisons were made with the Patos lagoon, São Gonçalo channel and Mirim lagoon. The study concluded that reduction of pollution from Pelotas was necessary as well as more extensive studies on water quality.

Kantin (1982) reported high concentrations of nitrogenated nutrients in the estuary during the winter and summer. Concentrations of phosphate $>3 \mu M (>0.093 \text{ mg/l})$ were found in summer and $<1 \mu M (0.031 \text{ mg/l})$ in other seasons, which was considered to be due to the trapping of phosphates in sediments. The ratios of nitrate (N-NO$_3$) to phosphate (P-PO$_4$) were less than 10, which is typical of a lagoon environment. Sampling stations near the entrance of the Patos lagoon showed large fluctuations of salinity and nutrients during a 24-hour period, with salinities ranging from 0 to 25 g/kg in the shallow bays, and from 0 to 33 g/kg in the estuary. In subsequent studies Kantin (1983) and Kantin et al. (1984) reported on levels of ammonia, nitrate, phosphate, surfactants, sulphides, oil and grease, and coliforms, which were measured from 1978 to 1982 in the Patos Lagoon. Eutrophication processes were observed and the most polluted areas were found to be located near the wastewater outfalls of Rio Grande.
Niencheski and Windom (1994) described the transport of nutrients between the Patos estuary and Mirim lagoon using a mass balance approach to evaluate the annual nutrient budget. Vertical profiles of temperature, salinity, and conductivity at 1m intervals, together with surface and near-bed water samples for the analysis of ammonia, nitrate, nitrite, silicate, phosphate, total suspended matter were collected from 20 sites within the estuary, and 1 site in the São Gonçalo Channel during eight 1 day cruises conducted on 30th June and 30th August 1989, 30th May, 30th June, 1st August, 30th August, and 1st December 1990, and 22nd April 1991. Results indicated that the system had more dissolved nitrogen (DIN), phosphorous (DIP) and silicate than could be explained by dissolved and particulate inputs associated with freshwater, which lead to the conclusion that the excesses were likely to originate from anthropogenic inputs mainly associated with fertiliser manufacture.

Niencheski et al. (1999) fully reviewed the behaviour of dissolved oxygen, dissolved nutrients and total suspended matter (TSM) from survey data collected between May 1990 and July 1991 by Niencheski & Windom (1994), and Baumgarten et al. (1995), in the southern Patos lagoon, estuary, and São Gonçalo Channel, Saco da Mangueira and Saco do Martins. Conclusions from the results of these studies are summarised as follows:

- **Saline stratification** (which favours the removal and storage of nutrients) was observed during summer conditions of low rainfall and SW winds, whereas during winter well-mixed conditions were observed with the dominance of fresh water.
  
  Thermal stratification was unusual except in the 12 m deep navigation channel.

- **Dissolved oxygen** values were all close to 100% saturation, due to shallow water depths and predominantly windy conditions.
- **Total suspended material** (TSM) increased towards the sea due to resuspension in the narrow access channel and inflow of saltwater, with average values of 50 mg/l observed in access channel and 30 mg/l in the shallows. Suspended particles from river inputs are primarily from the north and are desorbed by sediments in that region. Concentrations of TSM and phosphate generally increased with salinity, and decreased in freshwater.

- **Phosphate** is removed through adsorption and through primary production, resulting in low concentrations and perturbation of the phosphate buffer mechanism. Phosphate in the higher salinity region averages <2 μM (0.062 mg/l), which is typical of non impacted estuaries. Around Rio Grande the highest phosphate concentrations were in the summer and lowest in winter. The highest concentrations of phosphate were detected in Saco da Mangueira in all cruises, where phosphate concentrations depend on salinity versus phosphorus from the fertilizer plant. It was suggested that phosphate adsorption is depressed by increasing salinity due competition for ion exchange sites by other anions at higher salinities, or blocking of anion exchange sites by ions in seawater.

- **Nitrate** is produced in situ, particularly in upper estuary, and generally behaves conservatively with some remobilisation at higher salinities observed.

- High levels of ammonium observed in winter 1990 were considered to be due to inputs from Patos lagoon and São Gonçalo Channel, and further south from atmospheric input from Rio Grande's industrial area. Inputs from the São Gonçalo Channel are diluted by the Patos lagoon. Ammonium levels were enhanced in the estuarine zone by the penetration of bottom seawater promoting resuspension of sediments, and also sewage inputs from Pelotas. A mechanism of removed of ammonium in the upper estuary during times of high productivity,
subsequent remobilisation at higher salinities, is similar to that suggested for phosphate, nitrate, and nitrite. General levels of ammonium were higher in the shallow areas due to the proximity of anthropogenic inputs and organic sediment resuspension.

- **Silicate** generally decreases seaward in a conservative manner. Inputs from the Patos lagoon and São Gonçalo Channel meet the supply for phytoplankton uptake without significant depletion. Silicate never appears to be limiting in the estuary, leading to favourable conditions for diatom production supporting commercial fish populations.

### 2.4.2 Primary Production

The data collected to assess primary productivity include the following parameters: dissolved oxygen, biochemical oxygen demand, $^{14}$C uptake, benthic algae, chlorophyll-a, ciliates, cyanobacteria, day length, flagellates, light radiation, pH, particulate organic carbon, and Secchi depth. The principal authors for the Patos lagoon are: C. Odebrecht, U. Seeliger, and P.C. Abreu. Although data are limited for the Patos system, it has been shown that phytoplankton production and biomass have seasonal patterns (maximum in Spring/Summer, and minimum in Autumn/Winter) (Niencheski et al., 1999, Abreu et al., 1994). Some typical values for the Patos lagoon estuary are presented here in Table 2.5.

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>VALUE</th>
<th>SOURCE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chl-a winter level</td>
<td>10 $\mu$g/l</td>
<td>Yunes et al., 1996</td>
</tr>
<tr>
<td>Mean annual Chl-a</td>
<td>4 $\mu$g/l (range 1 - 11 $\mu$g/l)</td>
<td>Knoppers &amp; Kjerfve (1999)</td>
</tr>
<tr>
<td>Minimum biomass</td>
<td>&lt; 2 mg/l (Autumn/Winter)</td>
<td>Niencheski et al. (1999)</td>
</tr>
<tr>
<td>Maximum biomass</td>
<td>10.56 mg/l (Spring/Summer increased light, temp, dissolved inorganic nutrients)</td>
<td>Niencheski et al. (1999)</td>
</tr>
<tr>
<td>Phytoplankton uptake</td>
<td>phytoplankton based system</td>
<td>Knoppers &amp; Kjerfve (1999)</td>
</tr>
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<td>Phytoplankton uptake</td>
<td>&gt;8 mg Chl-a/l northern area, &lt;2.5 mg Chl-a/l estuary</td>
<td>Niencheski et al. (1999)</td>
</tr>
<tr>
<td>Net primary production</td>
<td>0.56 ± 0.68 gC/m$^2$/day</td>
<td>Knoppers &amp; Kjerfve (1999)</td>
</tr>
<tr>
<td>Primary producers</td>
<td>autotrophic flagellates, centric and pennate diatoms</td>
<td>Knoppers &amp; Kjerfve (1999)</td>
</tr>
</tbody>
</table>

Table 2.5 Typical Values for Primary Productivity in the Patos Lagoon Estuary
Abreu et al. (1992) measured values of bacteria, flagellates, ciliates, Chl-a, ammonia, nitrate, nitrite, phosphate, seston weight, particulate organic carbon, temperature, salinity, and \( ^{14}C \) uptake from weekly samples from a shallow region of the Patos lagoon estuary (32°07'S, 52°06'W) between March 1989 and March 1990. A study on bacterial dynamics from this survey data concluded that attached bacterial biomass dominated the bacterial community and enhanced nutrient quality. Biological factors such as primary production and protozoan grazing, rather than physico-chemical processes, were the main control on bacterial dynamics. Phytoplankton production stimulated the growth of bacterioplankton, and attached bacterial abundance was poorly correlated with the amount of seston. A reduction in bacterial cell volume concurrent with an increase in cell numbers was proposed as a possible response to counteract the effects of protozoan grazing.

Further work by Abreu et al. (1994) using the data collected from the surveys conducted between March 1989 and March 1990 showed that phytoplankton production varied seasonally, the lowest values occurring in the austral winter (June-August 1989) and the highest rates during spring and summer (March 1989; September 1989-March 1990). In general, primary production rates related to incident irradiance and water temperature, whilst high seston loads and low nitrate concentrations appeared to limit photosynthetic activity.

Proença et al. (1994) made measurements of chlorophyll-a and particulate organic carbon concentrations, at sites in the shallow area of the Patos lagoon over a one year period. Chlorophyll-a ranged from 0.3 to 49.4 \( \mu g/l \), and particulate organic carbon ranged from 0.1 to 4.3 mg/l, and highest concentrations for both parameters occurred in winter and summer.
Abreu et al. (1995) assessed information collected from vertical profiles of temperature, salinity and Secchi depth, and chlorophyll-a, ammonium, nitrate, nitrite, phosphate in surface water samples from 19 longitudinal estuarine sites, and 4 transect sites during 5 one day cruises conducted in 1989 on 6th June, 7th June, 7th July, 12th August, 13th September, and 2nd December. Results gave high concentrations of chlorophyll-a up to 16.72 μg/l, ammonium of up to 3.0 μM (0.042 mg/l), nitrate up to 13.0 μM (0.182 mg/l), and phosphate up to 3.0 μM (0.093 mg/l), in euhaline waters close to the mouth of the estuary. An additional period of weekly monitoring at a shallow fixed station between September and November 1989 showed that nutrient-rich saltwater entering the estuary coincided with peaks of phytoplankton production. The possible causes for the observed positive relationship between salinity and nutrients were reported to be sewage input, sediment resuspension and return of previously exported estuarine water to the lagoon.

Yunes et al. (1996) conducted research to evaluate the occurrence and toxicity to mice and shrimp, of blooms of the cyanobacteria Microcystis aeruginosa (M. aeruginosa), during 24 cruises of 1 to 2 days duration between February 1994 and January 1996. Samples were collected for the analysis of chlorophyll-a and bloom composition, from surface waters at 6 sites in southern Patos lagoon, and 7 other estuarine stations associated with algal blooms in the last 15 years. The M. aeruginosa blooms appeared to be associated with pH ≥8, temperatures >20°C, freshwater, and a balance of nutrients with an N:P ratio of ~13:1. However, there was no apparent correlation between the intensity and toxicity of the blooms. Three distinct blooms occurred during the study period: March to May 1994 with a maximum of >9,000 μg chl a/l from Rio Grande to Feitoria (~45 miles); late September 1994 with increased levels of chl-a above the winter normal value of 10 μg/l due to strong
NE winds causing resuspension of deposited cyanobacteria; and December 1994 to March 1995 with raised chl-a above the winter normal values. The levels of toxicity (LD$_{50}$) of toxic boom samples tested in mice varied from 22 to 250 mg/kg body weight, and in the brine shrimp varied from 0.47 to 2.44 mg/ml.

Matthiensen et al. (1999) identified and quantified the main phytoplankton groups distributed in the estuary during a twelve month survey. The concentrations of *M. aeruginosa*, which were found to originate from the north of the estuary and coincident with high chlorophyll-a levels, ranged from $1.5 \times 10^5$ cells in August 1995 to $1.3 \times 10^6$ cells in December 1994. *M. aeruginosa* blooms were considered highly toxic, presenting a 24 hour LD$_{50}$ <100 mg/kg, and a toxin content higher than 1 µg/mg dry weight. Matthiensen et al. (2000) conducted further research on hepatotoxic Microcystis blooms in the estuary, and found that [D-Leu(1)]Microcystin-LR was the most abundant microcystin.

### 2.4.3 Metals and Trace Elements

Most of the present understanding of processes affecting trace element transport through estuaries is based on studies of systems where mixing is relatively fast so biological processes do not proceed to completion, and resolution is poor at low salinity ranges (Windom et al., 1999). The Patos lagoon lends itself well to this type of study because of its long residence time and slow mixing rate during low freshwater discharge. Heavy metals entering riverine or estuarine waters are quickly absorbed onto suspended material and ultimately removed to coastal bed sediments (Niencheski et al., 1994).
In addition to the high nutrient concentrations associated with freshwater inputs, there are also inputs of trace metals from industry and nutrients from domestic sewage, which increases phytoplankton production. The transport and fate of trace metals is inter-related with nutrient concentrations and biological processes such as uptake and remineralisation (Sánchez-Arcilla, 2000).

Some typical concentrations of metals and trace elements in the Patos lagoon estuary are presented below in Table 2.6.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value/Range</th>
<th>Source</th>
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<tbody>
<tr>
<td>Cadmium (Cd)</td>
<td>0.1 - 20 (μg/g dry weight)</td>
<td>Baisch et al. 1988</td>
</tr>
<tr>
<td>Lead (Pb)</td>
<td>8 - 267 (μg/g dry weight)</td>
<td>Baisch et al. 1988</td>
</tr>
<tr>
<td>Zinc (Zn)</td>
<td>20 - 214 (μg/g dry weight)</td>
<td>Baisch et al. 1988</td>
</tr>
<tr>
<td>Chromium (Cr)</td>
<td>8 - 337 (μg/g dry weight)</td>
<td>Baisch et al. 1988</td>
</tr>
<tr>
<td>Copper (Cu)</td>
<td>0.8 - 20 (μg/g dry weight)</td>
<td>Baisch et al. 1988</td>
</tr>
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</table>

Table 2.6 Typical Values for Metals and Trace Elements in the Patos Lagoon Estuary

The green alga *Enteromorpha sp.* was tested under controlled culture conditions for uptake of copper (Cu) and mercury (Hg) over metal, salinity and chelator gradients and for retention of both metals after accumulation (Seeliger & Cordazzo, 1982). Results showed that the species could be used as a monitoring organism in highly variable estuarine conditions.

In a concurrent field study by Seeliger and Braga Knak (1982), monthly water samples were collected from four sites in the lower Patos estuary and one control site 16 km up-estuary, and analysed for dissolved and particulate Cu for samples collected between April 1980 and June 1981, and for total Hg for samples collected between November 1979 and October 1980. *Enteromorpha sp.* samples were also analysed for tissue levels of both metals. Hg concentrations were found to be close to natural background levels and
Chapter 2 - Reviewing the Literature

originated from freshwater run-off, and Cu concentrations were found in elevated background or low pollution levels, with a significant contribution from resuspended estuarine sediments. Inputs from industrial and port activities also seemed to contribute to the budget of both metals in the lower estuary.

At the control station located at the head of the estuary, no seasonal distribution of salinity and suspended matter or of Cu and Hg was apparent in water and algae samples, but this may have been due to low sampling frequency. There was no significant difference in total Hg concentrations in water samples between stations 2 and 5 (only 2 km apart), however, concentrations decreased substantially between the control station and station 2 (Rio Grande) which were located 16 km apart, and so subjected to high seawater dilution. Dissolved particulate Cu was homogeneous in the lower estuary. Results of the algal tissue analyses showed highest Hg values at station 2 with a concentration gradient to mouth, which indicated a possible contribution from Rio Grande. Results of this study showed negligible contribution to the estuary from offshore waters, where total Cu and Hg were below the limit of detection (~1 μg/l).

Windom (1975) reported concentrations of Cu and Hg in estuarine waters to be a function of salinity, with concentrations generally inversely proportional to salinity in an undisturbed system, which concurs with the results of Seeliger & Braga Knak (1982) who reported low suspended matter at salinities >7 g/kg, and high suspended matter at salinities <5 g/kg, however, in calm weather particles settled out giving low suspended matter with low salinity.
Baisch et al. (1988) measured levels of Cu, Chromium (Cr), Zinc (Zn), Cadmium (Cd), and Lead (Pb) in surface sediment samples from 61 sites in the estuary, which were grouped in two areas impacted by industrial and urban discharges, and one area outside anthropogenic influence. Total metal concentrations (μg/g dry weight) ranged from 0.1 to 20 Cd (0.23), 8 to 267 Pb (28.5), 20 to 214 Zn (83), 8 to 337 Cr (31), and 0.8 to 20 Cu (7.7). The values in brackets, presented for comparison, were found in uncontaminated sediments sampled further north along the Brazilian coast at Riberia Bay (Pfeiffer et al., 1988). Results of the study showed that extremely high values of Cd and Cr (comparable levels to Australian mining effluent) were found in the industrial and harbour areas, but have low availability and mobility due to the oxidising conditions in the shallow estuary. Patterns of Zn, Cu, and Pb indicated both industrial and urban sources.

Baumgarten & Niencheski (1990) used measurements of temperature, salinity, pH, Balanus improvisus and suspended matter from estuarine waters to study levels of Cu, Pb and Manganese (Mn). Results showed that variations in salinity and basal diameters of B. improvisus influenced the concentrations of bioaccumulated metals, and it was concluded that this species would be a suitable indicator of heavy metals pollution in the estuary.

An assessment of the natural and unnatural contributions of particulate metal concentrations was made by Niencheski et al. (1994), using data collected from vertical profiles of temperature, salinity, and conductivity at 1m intervals, and surface and bottom water samples of total suspended matter, particulate organic carbon, and dissolved and particulate metals (Aluminium (Al), Iron (Fe), Nickel (Ni), Cu, Zn, Cd, Pb, Lithium (Li), Phosphorus (P), Vanadium (V), Cr, Arsenic (As), Ag, Barium (Ba), and Mn). Samples were collected from 12 sites in the estuary during high fluvial discharge conditions (5,288...
m$^3$/s) on 1st August 1990, when the waters were fresh, and during low fluvial discharge conditions (1,400 m$^3$/s) on 30th August 1990, when salinities varied from 0 g/kg up estuary to 30.5 g/kg at the mouth. An enrichment factor, EF, was used to assess the proportion of natural to anthropogenic metal concentrations, and it was found that the main contribution to the estuary came from the Patos lagoon. Natural metal concentrations in suspended material derived mainly from the bed sediments and were not altered by anthropogenic inputs from Rio Grande, however, the high excess metal fluxes observed for copper reflected inputs from industrial activity.

Research conducted by Windom et al. (1999) discussed the processes involved in the transport and fate of trace metals throughout the Patos lagoon estuary. Water samples were collected from 2 to 4 m below the surface at 22 sites on the 14th and 15th December 1995, and determined for sodium, potassium, magnesium, calcium, silicate, phosphate, ammonia, nitrate, nitrite, pH, dissolved oxygen, Al, Cd, Cobalt (Co), Cu, Fe, Mn, Ni, Pb, Zn, temperature, and salinity. Results enabled the authors to divide the study area into three zones of dominant processes. In the northern zone (sites 1 to 12) where salinities ranged from zero to ~5-7 g/kg, nutrient and particle removal were the dominant processes as fresh water mixed with seawater, which reflected high primary production, flocculation and particle scavenging. The middle zone (sites 13 to 18) was characterised by rapidly increasing salinity up to ~25-27 g/kg, downstream, and was dominated by organic matter remineralisation, resulting in metal release and nutrient regeneration, although mobilisation from bed sediment was also considered important. The southern zone, where salinities were greater than ~27 g/kg, was dominated by conservative mixing. Figure 2.4 below depicts the features described.
Neincheski and Baumgarten (2000) applied the analysis of suspended matter from monthly surface water samples collected between May 1990 and July 1991 from 7 sites in the Rio Grande Channel, Saco da Mangueira, and Saco do Rio Grande to find out whether the anthropogenic inputs of heavy metals (Cu, Zn, Pb, Fe) from Rio Grande significantly affected concentrations in the southern part of the Patos lagoon estuary. The results and subsequent data analysis showed that the suspended sediments of Saco da Mangueira, and Saco do Rio Grande were enriched with Cu, Pb, and Zn above natural levels due to anthropogenic inputs originating from urban, industrial and harbour activities. High levels of metals of natural origin from resuspended sediments, however, masked the local inputs to the Rio Grande Channel. The report concluded firstly, that spatial variations were mainly due to hydrodynamic conditions and distance from the harbour activities, and
secondly that anthropogenic inputs were masked by high concentrations of resuspended sediment due to meteorological conditions.

2.5 Hydrodynamics and Water Quality of the Saco da Mangueira

The shallow semi-enclosed bay of Saco da Mangueira is oval in shape and orientated southwest to northeast between the city of Rio Grande to the north and the Industrial District of Rio Grande to the south (Figure 2.5). It has an area of 27.2 km$^2$, with sediments composed mainly of fine sand, and a maximum depth of just 1.5m (Persich, 1996). The bay has a weak hydrodynamic circulation, and is connected to the Patos Lagoon Estuary to the west via a narrow entrance channel currently 11m deep, which has been reduced to approximately 200m wide by the construction of a bridge. The Saco da Mangueira was a sediment trap before the entrance was narrowed, but now it appears to be stable, though more information is needed to confirm this (Tagliani, P. pers. comm.). This narrowed entrance appears to act as a barrier to the domestic pollution from the northern area of Rio Grande, however, studies conducted to date have shown high concentrations of nutrients, faecal coliforms, detergent and oxygen demands in the areas adjacent to the main the domestic effluent discharges, which have resulted in eutrophication of the embayment.
Figure 2.5 Sources of Pollution in the Vicinity of Rio Grande and the Saco da Mangueira

The waters of the Saco da Mangueira are polluted by various sources including untreated domestic sewage (Rio Grande population approx. 200,000); industrial effluent; two fertiliser plants to the south (average production around 900,000 ton/yr); landfill; and an increasing number of slums to the north. However, there is a pristine watercourse of 10-20 m³/s (cumecs) at the head of the embayment, which, together with beds of seagrass, help to maintain the water quality. There are plans for a number of shrimp hatchery farms in the southern part of the embayment, which will become another source of pollution for which the impact needs to be assessed.
No direct measurements of the hydrodynamic regime within the Saco da Mangueira had been made prior to this research project, and water quality data are sparse, because most of the studies have concentrated on the Patos lagoon estuary as described in the previous sections. Of the water quality studies that have been conducted in the southern part of the estuary, many have focussed on the shallow areas to the north of Rio Grande (Saco do Arraial, Saco do Rio Grande, and Canal do Norte). These studies have been reported by Baptista (1984), Baumgarten et al. (1982), Cruz et al. (1982), Kantin (1982), Kantin et al. (1982), Almeida et al. (1984), Bergesch (1990), Proença (1990), Aznar et al. (1993), Proença et al. (1994), Bergesch et al. (1995), De Lorenzo (1995), and Santos et al. (1997).

A number of studies have also been completed in the area to the southeast of the city in the Canal do Rio Grande and the Coroa do Boi, which is situated just outside the mouth of the Saco da Mangueira and is the receiving water for the main untreated sewage discharge for Rio Grande. These studies have been reported by Kantin et al. (1981 and 1984), Costa et al. (1982), Kantin and Baumgarten (1982), Kantin (1983), Almeida et al. (1993), Bonilha (1996), and Baumgarten et al. (1998).

Water quality studies in the Saco da Mangueira have been conducted by Kantin et al. (1981), Marchiori et al. (1982), Baumgarten et al. (1982), Persich (1993), Baumgarten et al. (1995), and Persich et al. (1996). The locations of the parameters that have been studied in the vicinity of Saco da Mangueira are presented in Figure 2.3, and a summary of the data is provided in Table 2.7, and will be discussed in further detail in Chapter 3.
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<th>Location</th>
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<th>total nitrogen</th>
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Table 2.7 Summary of Water Quality Data for Saco da Mangueira
Kantin et al. (1981) made monthly determinations of phenolic compounds and oil in Saco da Mangueira and the Access Channel of the estuary for the period of March 1978 to March 1979. Results showed chronic pollution of these waters with mean values of 20.8 ± 4.6 ppb and 4.2 ± 0.6 ppm for phenolic compounds and oils respectively from Saco da Mangueira, and 37.2 ± 11.5 ppb and 4.8 ± 1.5 ppm from the Access Channel.

The concentration of nutrients in Saco de Mangueira and Saco do Arraial were reported by Baumgarten et al. (1982). For both embayments, salinity values ranged from 1.5 to 25 g/kg, and suspended matter ranged from 11 to 50 mg/l. The high concentrations of nutrients showed that both areas were eutrophic, with values of 12.1 ± 8.8 μM (0.169 ± 0.123 mg/l) ammonical nitrogen (N-NH₄); 18.7 ± 9.6 μM (0.262 ± 0.134 mg/l) nitrate (N-NO₃); and 8.9 ± 4.1 μM (0.276 ± 0.127 mg/l) phosphate (P-PO₄) for the Saco de Mangueira, and nitrate concentrations of 60 μM (0.840 mg/l) for the Saco do Arraial. In the summer, the phosphate concentration was greater than 5 μM (0.155 mg/l) for the Saco da Mangueira and 2 - 5 μM (0.062 – 0.155 mg/l) for the Saco do Arraial.

Cruz et al. (1982) described the results from hourly measurements in 24-hour periods, of current speed and direction, water elevation, salinity, temperature, suspended matter, phosphate and nitrate at surface, 8 m and 16 m depths in the narrower point of the Canal do Norte. Results for salinity in winter and summer/autumn were 3 g/kg and 25 g/kg respectively with a homogeneous distribution through depth, whereas those in spring varied by more than 20 g/kg with the water column varying from well mixed to stratified. Current velocity ranged from 10 to 130 cm/s. Variations in suspended and dissolved nutrients were significant, and did not follow the salinity variations. The maximum values
were > 2 μM (>0.062 mg/l) for phosphate; >30 μM (>0.420 mg/l) for nitrates, and 100 mg/l for suspended particulate matter.

Baumgarten et al., (1995), reported on surface water samples collected from 7 sites in the semi-enclosed bays surrounding Rio Grande during 15 monthly cruises from May 1990 to July 1991. It was found that mean levels of phosphate within Saco da Mangueira (0.094 mg/l) were about three times the averages registered for waters to the north and the east of the city (0.033 mg/l). Levels of dissolved available inorganic nitrogen (DAIN), which is the total of ammonium, nitrite, and nitrate for these surveys ranged from 0.178 mg/l to 1.276 mg/l, with a mean concentration of 0.298 mg/l, and the highest values occurred in winter. The main conclusions from the studies were:

- Temporal (seasonal, annual, and inter-annual) and spatial variations in concentrations of the measured parameters were influenced by variations in wind, rainfall, estuarine circulation, and pollutant sources.
- Variations in salinity affected the interactions of nutrients between water column, sediment and atmosphere;
- Spring conditions were marked by the addition of ammonium, nitrate and silicate and the removal of phosphate, whereas the addition of nitrite and phosphate occurred in summer;
- Nitrogenous nutrients and phosphate behaved non-conservatively, whereas silicate showed a conservative trend;
- Having the largest concentrations of phosphate, the Saco da Mangueira acted as a phosphate reservoir for the rest of the estuary, and primary production here was therefore limited by nitrogenous nutrients;
The impact of effluent was more evident in the peripheral areas of the embayments due to weak currents and stagnation of water.

Studies by Persich et al., (1996) were conducted at two sites in the Saco do Arraial, and Saco da Mangueira, for a comparison of chlorophyll-a and physico-chemical parameters in terms of trophic state using ratios of N:P, N:Si, P:Si. Results were as follows:

- Saco da Mangueira had statistically higher chlorophyll-a, nitrogen and phosphorus;
- Saco da Mangueira was predominantly mesotrophic to eutrophic, due to anthropogenic sewage inputs, and discharges from the fertiliser industry;
- Saco da Mangueira had a higher phytoplankton biomass probably due to the longer residence time because of lower exchange of water with the estuary;
- Levels of silicate were generally high in both areas.

Santos et al., (1997) reported on surface water samples collected weekly, between 15\textsuperscript{th} January and 26\textsuperscript{th} February 1996, from three stations close to the Rio Grande City (Station A, Rio Graride North; Station B, close to Saco da Mangueira mouth; Station C, close to the West jetty near the mouth of the Patos estuary). Water temperature, salinity, Secchi disk depth, inorganic nutrients (ammonium, phosphate, nitrate, and nitrite), pH, seston weight, chlorophyll a, dissolved oxygen, BOD, and total and faecal coliforms were measured at all stations. The conclusions were as follows:

- The worst sanitary conditions (up to 160,000 faecal coliforms/100ml) were found at Station A, with mean values higher than for previous studies by Almeida et al. (1984) which substantially exceeded the water quality standards established by
CONAMA and FEPAM (see section 2.7). Pronounced eutrophication conditions (high nutrients and chlorophyll-a concentrations) were evident;

- Stations B and C showed mean values comparable to previous studies by Costa et al. (1982) and Almeida et al. (1984), and within the established water quality standards;
- Hydrodynamics were the main controlling factor for eutrophication conditions in the Patos lagoon estuary.

Baumgarten et al. (1998) reported on the findings of a one year survey to assess the impact of the domestic sewage system of Rio Grande, which discharges into the shallow semi-enclosed embayment of Coro do Boi adjacent to the entrance of Saco da Mangueira. In 1992 and 1993, 15 expeditions were undertaken during ebb and flood stream conditions, and surface water samples were collected in 5 areas from the effluent discharge up to a distance of 800m. At the effluent discharge location, the mean ± standard deviation for the concentrations of water quality variables for ebb and flood stream respectively were: ammonium 398.1 ± 216 µM (5.573 ± 3.024 mg/l) and 288.7 ± 168 µM (4.042 ± 2.352 mg/l); phosphate 27.8 ± 11 µM (0.862 ± 0.341 mg/l) and 13.2 ± 6 µM (0.409 ± 0.186 mg/l); BOD 123.8 ± 150 mg/l and 76.0 ± 49 mg/l; chemical oxygen demand (COD) 26.7 ± 34 mg/l and 74.4 ± 101 mg/l; total suspended material 99.2 ± 34 mg/l and 52.8 ± 22 mg/l. In this area low average concentrations were found for oxygen 3.5 ± 3 mg/l and 4.4 ± 3 mg/l and for nitrate 4.6 ± 3 µM (0.064 ± 0.042 mg/l) and 1.9 ± 2 µM (0.027 ± 0.028 mg/l).

These results showed heavy contamination in the region with poor dispersion of the effluent contributing to levels of ammonium and phosphate being at least twice as high as those considered acceptable for non-polluted estuaries (see Appendix 1). About 800m
away from the discharge point, the hydrodynamics were more efficient in the dispersion and dilution of the effluent, and this was shown by the significant decrease in the values of ammonium, phosphate, BOD, COD, and suspended material, together with an increase in oxygen and nitrate, indicating a complete oxidation of the anthropogenic ammonium (nitrification) suggesting a better recovery of the water system. Although the average ammonium and phosphate concentrations decreased significantly at a certain distance from the discharge location, these values were still at least about twice as high as those considered acceptable for non-polluted estuaries.

2.6 Artisanal Fisheries

The pink shrimp *Penaeus paulensis* is commercially the most important decapod crustacean in the Patos estuary. Shrimps spend most of their lives in freshwater but must complete their early development in seawater (Landau, 1992). Larvae hatch on the continental shelf in spring (September/October to December), and swim into the shallow vegetated areas of the estuary which are dominated by *Ruppia maritime* and offer a protected leafy substrate for the juveniles. During autumn most of the adult females migrate back out to sea to reproduce, completing the life cycle (Bemvenuti, 1997). According to Santos and Bianchini (1997), *Penaeus paulensis* are adapted to cope with highly unpredictable and fluctuating temperature, salinity and pH conditions in order for successful settlement in the Patos Lagoon estuary. Larvae are able tolerate temperatures between 8 and 38°C, however, larval development is inhibited above ammonia concentrations of 2.8 mg/l, and the LC$_{50}$ for post-larvae is 1.33 ppm Cu.

The studies reviewed in the previous sections have described the environmental degradation of some of the aquatic environments of the Patos Lagoon and estuary, in
particular the shallow bays which supply vital shelter and harvesting areas for fish and benthic organisms. The fish species have suffered serious decline, and consequently, the traditional artisan fisheries have started to depend exclusively on shrimp harvesting. The number of artisanal shrimp fisheries has reduced over recent years from 25 to 2 (P. Tagliani *pers com.*), and a possible explanation for this decline has been attributed to the inverse relationship between rainfall and shrimp catch, which was reported by Castello and Möller (1978). When heavy rains coincide with the period when shrimp spawn enter the estuary, increased current speeds in the narrow access channel will restrict the recruitment of shrimp larvae to the estuarine nursery areas. This behaviour is contrary to that of other areas of the world where rainfall has a positive effect on fisheries. It has also been shown that the El Niño Southern Oscillation (ENSO) phenomenon, which causes increased rainfall giving rise to an outflow through that estuary channel of up to 10,000m$^3$/s, also has a negative effect on fisheries, whereas for example in the Pacific and Mississippi the effects of ENSO are positive.

In order to try to halt the decline in the artisanal fisheries, and to protect the economy of the area, there are plans for a number of shrimp hatchery farms in the southern part of Saco da Mangueira, and, according to Midlen & Redding (1998), the limiting factor for farming marine shrimps in ponds is the provision of sufficient oxygen for cultivation and waste assimilation. Aeration is increased by the presence of plant and microbial communities, and also by frequent water exchange. More intensive aquaculture systems are ecologically unbalanced, and consequently can contribute to environmental degradation. This could be the case for the Saco da Mangueira if the impacts of the proposed shrimp farms are not fully assessed. The modelling studies conducted in this research may assist with this aspect.
2.7 Water Quality Legislation

The waters of the southern region of the Patos lagoon estuary are protected by environmental criteria prescribed by a water framework established for Rio Grande do Sul by the State Foundation of Environment Protection (FEPAM, 1995), which was derived from the water quality classification system established by the National Council for the Environment (CONAMA, 1986). The FEPAM classification is sub-divided for the protection, conservation, and use of freshwater (Special Classes, 1 and 2) and brackish water (Classes A, B, and C). Specifically, the waters of Saco da Mangueira are Class B, which means that the quality of the water must be maintained for primary water contact sports (swimming, water skiing, scuba diving); the protection of aquatic communities; and the cultivation of species for human consumption (Baumgarten et al., 1995; Santos et al., 1997; Baumgarten & Pozza, 2001). The waters in the estuary adjacent to Saco da Mangueira are Class C, and must be maintained for the protection of aquatic communities; primary and secondary water contact sports; and navigation. The water quality standards associated with these classifications together with other international water quality standards for general water quality parameters including bacteria and nutrients are summarised in Appendix 1 and will be used later in this study to give context to the water quality modelling results.

Currently there are no statutory water quality standards for nutrients in the UK and the determination of the nutrient status of estuaries, and ecological consequences, remains a notoriously contentious issue (Langston et al., 2003) because nutrient concentrations vary with salinity, season, and river flow, so measurements may show considerable temporal and spatial variability and not be truly representative of water quality. Therefore, it is essential to monitor nitrogen, phosphorus, chlorophyll-a, dissolved oxygen, and turbidity...
for input to models for the development of criteria for the selection of numerical water quality objectives. Langston *et al.* (2003) summarised existing nutrient quality guidelines:

- The EU nitrates directive 91/675/EEC (nitrates from agricultural sources) calls for the identification of all waters that contain 50 mg/l nitrate.
- The USEPA proposed a limit of 10 mg/l nitrate for the protection of domestic water supplies, and a phosphorous criteria of 0.1 μg/l (as P) to protect estuarine and marine organisms against the consequences of bioaccumulation. However, this was not established as a threshold for eutrophication and is currently under review.
- The North Sea Status report stated that hypenutrification in sea water exists when winter maximum TIN values exceed 0.144 mg/l (provided P>0.006mg/l). In estuaries however it seems likely that thresholds will be higher.
- Based on work in 2 eastern USA estuaries, Deegan *et al.*, (1997) have suggested that a value of at least ~ 1mg/l DIN might lead to poor habitat quality for fish populations, which may be due in part to cloaking effects of macroalgal mats on *Zostera* (sea grass) beds.
- There are proposed UK Environmental Quality Standards (EQS) of 0.021 mg/l un-ionised ammonia (NH$_3$-N) and 0.78 mg/l total ammonia for the protection of saltwater fish, shellfish, and EC designated salmonid and cyprinid freshwaters.

In summary, it is evident from this review that the physical and chemical conditions prevailing in the Patos Lagoon and Estuary System have been studied in some detail by the researchers of FURG over the past 2 decades. Much of this information together with new data collected specifically for this project will be used for calibration and validation of a numerical model which is the focus of this study.
Chapter 3

Data Collation and Field Studies

3.1 Introduction

This Chapter builds upon the literature review by presenting a detailed description and analysis of the data used for this research. The quality and quantity of the field data are also considered in order to provide a basis for the level of confidence and detail possible for the models. Most of the data were collected by others in previous surveys, however, new measurements were personally made during two site visits in 2002 and 2003, designed to provide additional site specific information for the hydrodynamic and water quality models. The data-sets are summarised below in Table 3.1 and Figure 3.1.

<table>
<thead>
<tr>
<th>Survey Period</th>
<th>Sampling Frequency and Location</th>
<th>Parameters in addition to a typical water quality suite*</th>
<th>Source Publication</th>
<th>Data provided by</th>
</tr>
</thead>
<tbody>
<tr>
<td>1983</td>
<td>11 x monthly survey @ 3 sites mid &amp; lower estuary</td>
<td>Secchi depth</td>
<td>Niencheski et al. (1986)</td>
<td>Felipe Niencheski, Graça Baumgartcn (FURG)</td>
</tr>
<tr>
<td>1989</td>
<td>5 x 1 day survey (Winter, Spring, Summer) @ 23 sites in estuary</td>
<td>Secchi depth; chlorophyll-a</td>
<td>Abreu et al. (1995)</td>
<td>Data extracted from publication</td>
</tr>
<tr>
<td>1989-1991</td>
<td>8 x 1 day survey (Winter, Spring, Summer, Autumn) @ 21 sites in estuary</td>
<td>Secchi depth; chlorophyll-a, light intensity</td>
<td>Niencheski &amp; Wisdom (1994)</td>
<td>Felipe Niencheski (FURG)</td>
</tr>
<tr>
<td>1990-1991</td>
<td>9 x monthly survey @ 2 central sites &amp; weekly @ 2 outer sites in Saco da Mangueira</td>
<td>Secchi depth; chlorophyll-a; dissolved oxygen; biochemical oxygen demand</td>
<td>Persich et al. (1993 &amp; 1996); Niencheski &amp; Baumgartcn (2000)</td>
<td>Giazaio Persich via Clarisse Odebrecht (FURG)</td>
</tr>
<tr>
<td>1992-1993</td>
<td>15 x 1 day survey (Winter, Spring, Summer, Autumn) @ 8 sites close to main Rio Grande sewage outfall</td>
<td>Dissolved oxygen; biochemical oxygen demand</td>
<td>Baumgartcn et al. (1998)</td>
<td>Data extracted from publication</td>
</tr>
<tr>
<td>1994-1995</td>
<td>16 x monthly survey (Winter, Spring, Summer, Autumn) @ 3 sites in Saco da Mangueira</td>
<td>Dissolved oxygen; biochemical oxygen demand; coliforms</td>
<td>Santos et al. (1997)</td>
<td>JICA (2000)</td>
</tr>
<tr>
<td>1996</td>
<td>3 x weekly survey for 2 Summer months @ 3 sites in the lower estuary</td>
<td>Secchi depth; chlorophyll-a; dissolved oxygen; biochemical oxygen demand</td>
<td>JICA (2000)</td>
<td>Felipe Niencheski (FURG)</td>
</tr>
<tr>
<td>1999</td>
<td>12 x monthly survey (Winter, Spring, Summer, Autumn) @ 32 sites in the lagoon, estuary, rivers, ocean</td>
<td>Secchi depth; dissolved oxygen</td>
<td>JICA (2000)</td>
<td>Felipe Niencheski (FURG)</td>
</tr>
<tr>
<td>1999</td>
<td>Hourly @ lagoon sites: Farol de Itapua; Santa Rita; Rincão do Cristóvão Pereira; Bojáu; São Lourenço do Sul, Half-hourly @ Pratinagam</td>
<td>Winds, Water Levels and Daily Rainfall</td>
<td>JICA (2000)</td>
<td>Osmar Müller (FURG)</td>
</tr>
<tr>
<td>1999-2003</td>
<td>Hourly @ Pratinagam</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2000</td>
<td>6 x 1 day survey fortnightly Jul, Aug, Sep @ 8 sites in mid &amp; lower estuary</td>
<td>Secchi depth; dissolved oxygen; biochemical oxygen demand</td>
<td>Niencheski et al. (2002)</td>
<td>Felipe Niencheski (FURG)</td>
</tr>
<tr>
<td>2002</td>
<td>1 day survey (09/10/02) @ 10 sites in Saco da Mangueira and lower estuary</td>
<td>Secchi depth; dissolved oxygen; biochemical oxygen demand; chlorophyll-a</td>
<td></td>
<td>ECOSUD team lead by Felipe Niencheski (FURG)</td>
</tr>
<tr>
<td>2002</td>
<td>4 x 1 day survey (10-11/10/02, 17-18/10/02) @ entrance to Saco da Mangueira and lower estuary</td>
<td>Current velocity, temperature, &amp; salinity profiles</td>
<td></td>
<td>ECOSUD team lead by Osmar Müller (FURG)</td>
</tr>
<tr>
<td>2003</td>
<td>1 day survey (04/06/03) @ 6 sites in Saco da Mangueira and lower estuary</td>
<td>Secchi depth; dissolved oxygen; biochemical oxygen demand</td>
<td></td>
<td>ECOSUD team lead by Felipe Niencheski (FURG)</td>
</tr>
<tr>
<td>2003</td>
<td>3 x 1 day survey (21-23/05/03) @ entrance to Saco da Mangueira</td>
<td>Current velocity, temperature, &amp; salinity profiles</td>
<td></td>
<td>ECOSUD team lead by Osmar Müller (FURG)</td>
</tr>
</tbody>
</table>

Table 3.1 Summary of Data-sets (* parameters in addition to: temperature; salinity; suspended solids; ammonium; nitrite; nitrate; phosphate; silicate)
Figure 3.1  Map Showing Locations of Water Samples and Oceanographic Measurements used for the Model
3.2  Meteorological and Oceanographic Data

The physical quantities described in this section are those of water level; wind velocity; fluvial discharge; and current velocity, all of which are required to build the hydrodynamic model. Most of the data were collected in 1999 (Figure 3.2) as part of an extensive study conducted by the Japan International Cooperation Agency (JICA, 2000), with additional site specific studies undertaken in 2002 and 2003 (Figure 3.3).

3.2.1 Water Level Data

Hourly water level records were obtained for 1999, 2002, and 2003 from a permanent tide-pole installation (Plate 3.1) operated by the Rio Grande Pilots at Praticagem da Barra close to mouth of the estuary. The only processing necessary for these data was to reduce the levels provided for 1999 by a value of 0.679m to Chart Datum.

Plate 3.1  Tide Pole at the Rio Grande Pilot Station, Praticagem
Hourly water levels were also measured at five locations in the lagoon during 1999 (Table 3.2, and Figure 3.1), which were used during the calibration and validation of the hydrodynamic model to assess whether the model could reproduce the correct water levels within the lagoon.

<table>
<thead>
<tr>
<th>Location</th>
<th>Easting (UTM)</th>
<th>Northing (UTM)</th>
<th>Start Date of Record</th>
<th>End Date of Record</th>
</tr>
</thead>
<tbody>
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<td>Praticagem</td>
<td>396540</td>
<td>6443330</td>
<td>17/04/99 06:00</td>
<td>01/10/99 00:00</td>
</tr>
<tr>
<td>Praticagem</td>
<td>396540</td>
<td>6443330</td>
<td>01/05/02 00:00</td>
<td>01/08/03 00:00</td>
</tr>
<tr>
<td>Farol de Itapuã</td>
<td>494022</td>
<td>6640650</td>
<td>14/02/99 14:00</td>
<td>11/01/00 23:00</td>
</tr>
<tr>
<td>Santa Rita</td>
<td>457801</td>
<td>6560430</td>
<td>14/02/99 00:00</td>
<td>11/01/00 23:00</td>
</tr>
<tr>
<td>São Lourenço do Sul</td>
<td>406175</td>
<td>6516500</td>
<td>14/02/99 00:00</td>
<td>11/01/00 23:00</td>
</tr>
<tr>
<td>Bojuru</td>
<td>459200</td>
<td>6515900</td>
<td>26/02/99 00:00</td>
<td>11/01/00 23:00</td>
</tr>
<tr>
<td>Rincão do Cristóvão Pereira</td>
<td>488900</td>
<td>6561400</td>
<td>14/02/99 00:00</td>
<td>11/01/00 23:00</td>
</tr>
</tbody>
</table>

Table 3.2  Details of Wind and Water Level Data-sets

In macrotidal regions such as parts of the United Kingdom, water circulation patterns are dominated by tidal forces, and the astronomical component of the tidal signal is readily extracted by harmonic analysis and used to forecast or hindcast tidal amplitude and phase to a high degree of accuracy. Tidal forcing is therefore a vital component of any oceanographic study conducted in such areas, and necessitates a thorough tidal analysis prior to numerical modelling. In contrast to this, but in common with most choked coastal lagoons, the Patos System is wind forced rather than tidally driven, with the microtidal signal from the Southern Atlantic Ocean effectively attenuated by the entrance to the system, which causes a reduction in water level fluctuations inside the lagoon. These aspects have been studied extensively by Möller et al. 1996, and Fernandes, 2001 (see Chapter 2), therefore, no further analysis of tidal data has been undertaken for this research.
Figure 3.2  Hydrodynamic Time Series for 1999 with Water Quality Surveys Indicated
3.2.2 Meteorological Data

In addition to the tide-pole, the Rio Grande Pilots at Praticagem also operate a meteorological station that records wind speed and direction, rainfall, air temperature, pressure, and humidity. Hourly records of these parameters were obtained for 1999 to 2003 (with some gaps). Wind measurements were also recorded as part of the 1999 study (JICA, 2000) for the period 01/01/99 to 04/07/99, at a temporary meteorological station at Santa Rita which is situated towards the central latitude of the lagoon (Figure 3.1).

Two analyses of these wind data were completed, firstly, a spatial comparison to establish whether the data for Praticagem could be considered representative of the study area, or if a spatially variable wind parameter would be required for the model. Concurrent records at Praticagem and Santa Rita were resolved parallel to the principal axis of the lagoon (037°), and the longitudinal wind components (labelled WY) were compared. The data are presented in Figure 3.4 as a time series, with positive values indicating winds blowing into the lagoon.

![Figure 3.4](image-url)  
**Figure 3.4** Comparison of Wind at Praticagem and Santa Rita 1st January to 4th July 1999
From Figure 3.4, the two locations clearly share a very similar wind regime ($R^2 = 0.83$), despite being separated by at least 130 km. However, this correlation seems reasonable since the region is a flat coastal plain with few significant topographical features to modify wind patterns. Therefore, the wind data at Praticagem were considered representative of the macroscale wind regime of Patos System, and subsequently used to force the model rather than specifying a spatially variable wind field.

A second analysis of the wind data at Praticagem was undertaken to assess whether the 1999 data showed typical temporal variations compared with other years, since the model would be calibrated using the 1999 data, but would be used for simulations in other years. An indication of the annual and inter-annual variability would also help quantify the level of confidence placed upon selection of the surface friction coefficient of the model during calibration. Ideally, a time series spanning at least ten years would be recommended for a comprehensive investigation of wind climate, however, since the wind regime of the study area is relatively well-known (see Chapter 2), the data available for 1999 to 2003 were considered sufficient within the scope of this study.

In order to compare annual and inter-annual variations, the monthly frequency distributions of wind speed and direction were extracted from the data (Table 3.3), and combined to give seasonal distributions which are presented as histograms in Figures 3.5 and 3.6, and as wind roses in Figure 3.7.
### Table 3.3 Percentage Frequencies for Wind Speed and Direction

<table>
<thead>
<tr>
<th>Wind Speed (m/s)</th>
<th>Monthly Percentage Frequencies for 1999</th>
<th>Mean Monthly Percentage Frequencies for 1999 to 2003</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>J</td>
<td>F</td>
</tr>
<tr>
<td>M</td>
<td>A</td>
<td>M</td>
</tr>
<tr>
<td>J</td>
<td>A</td>
<td>S</td>
</tr>
<tr>
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<td>O</td>
<td>N</td>
</tr>
<tr>
<td>Speed (m/s)</td>
<td>0-1</td>
<td>1</td>
</tr>
<tr>
<td>Speed (m/s)</td>
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<td>2</td>
</tr>
<tr>
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<td>Speed (m/s)</td>
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<td>10</td>
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<td>Speed (m/s)</td>
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<td>15</td>
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<tr>
<td>Wind Direction</td>
<td>N</td>
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<tr>
<td>Wind Direction</td>
<td>NNE</td>
<td>5</td>
</tr>
<tr>
<td>Wind Direction</td>
<td>NE</td>
<td>7</td>
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<tr>
<td>Wind Direction</td>
<td>ENE</td>
<td>9</td>
</tr>
<tr>
<td>Wind Direction</td>
<td>E</td>
<td>11</td>
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<tr>
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</table>

![Figure 3.5](image1.png)  

title: Seasonal Variations in Wind Speed for 1999 and 1999 to 2003  

![Figure 3.6](image2.png)  

title: Seasonal Variations in Wind Direction for 1999 and 1999 to 2003  

Chapter 3 - Data Collation and Field Studies
Figure 3.5 indicates that approximately 55% of the wind speeds are in the range 3-7 m/s with the most frequent speed being 4-5m/s. Stronger winds appear to be more prevalent during the Spring months, however, the seasonal variation for any given wind speed is low at less than 5%. Wind directions, on the other hand, show greater seasonal variation with winds during Spring and Summer months occurring for ~50% of the time from the north by northeast to east, and ~21% from westerly sectors, whereas during Autumn and Winter, winds from the northerly sectors occur for ~35%, whereas winds from the westerly sectors occur more frequently at ~37%. This pattern is clearly evident in Figure 3.7, and agrees with the descriptions of the wind climate given in Chapter 2.

![Wind Roses for 1999 and 1999 to 2003](image)

**Figure 3.7** Wind Roses for 1999 and 1999 to 2003

With respect to the inter-annual frequency distribution, the wind velocity for 1999 is extremely well correlated with that for the period 1999 to 2003, with $R^2$ values of greater than 0.85 and 0.78 for each season for speed and direction respectively, which would strongly suggest that the 1999 data are representative of the typical annual wind regime for the Patos system, and that a high level of confidence can be assigned to selection of the surface friction coefficient for the model in terms of inter-annual simulations.
3.2.3 River Flow Data

Fluvial discharges and rainfall are measured throughout Brazil via a network of hydro-meteorological stations operated by the Hydrological Information Department (HID), which is a part of the Brazilian National Water Agency (Agência Nacional de Águas, www.ana.gov.br). River flow data for the principal freshwater sources to the Patos System between 1940 and 1999 (with some gaps) were obtained from HID by FURG and provided for this research. The data consisted of mean monthly flows for the rivers Jacui and Taquari which account for 85% of the flow input at Guaíba at the northern extremity of the system, and the Camaquã River which is situated close to central region of the lagoon (Figure 3.1). Thus, flows for the Jacui and Taquari were combined and increased by a factor of 100/85 to give an estimate of the total flow for the Guaíba River. Ideally, mean daily flows would give greater detail for model predictions; however, this study is concerned with longer timescales for water quality simulations, and given the immense volume of the system, mean monthly flows were considered acceptable for this study.

Another fluvial discharge of significant magnitude is the São Gonçalo Channel, which connects the Patos with the Mirim Lagoon and enters the upper part of the Patos Estuary from the west. There were no measured flows for this discharge, however, they have been estimated to be ~50% of the total flow for the Jacui and Taquari rivers combined (Osmar Möller pers com.). Therefore, flows for the São Gonçalo Channel were calculated on this basis, and total fluvial flows for the study area were determined for each month and each season, and are presented in Figure 3.8 below.
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Figure 3.8  Seasonal Variations in Total River Flow for 1940 to 1999

The data show a general trend for greater flows during Spring and Winter, with long-term averages for each season of 2671, 1316, 1756, and 3655 cumecs for Spring (September to November), Summer (December to February), Autumn (March to May), and Winter (June to August) respectively. It is relevant to this study to note that the river flows for 1999 are below average for all four seasons. The river flow data will be discussed further in Section 3.4 which presents an investigation of the relationship between fluvial discharge and the El Niño Southern Oscillation (ENSO).

3.2.4 Current Velocity Data

Current velocity data for the Patos Lagoon and estuary are sparse (see Chapter 2), however, during the 1999 study (JICA, 2000), a pair of Aanderaa RCM-7 recording current meters were deployed near-surface (3m) and near-bed (10m) at Praticagem for the period 02/08/99 to 20/08/99. Current velocities were measured at other locations in the estuary and lagoon during the 1999 study, but unfortunately these data were not available.

The velocities have been resolved relative to the main axis of the lower estuary (011°T), and the landward component plotted in Figure 3.9 together with salinity, water surface
elevation, and the up-estuary component of wind, in order to further illustrate the mechanisms controlling the estuarine circulation, which have been described in Chapter 2.

![Figure 3.9 Current Meter and Associated Oceanographic Data for August 1999](image)

Figure 3.9 Current Meter and Associated Oceanographic Data for August 1999

The data presented in Figure 3.9 give an overall summary of the circulation patterns close to the mouth of the estuary during a Winter month. It is clear that the majority of flow is seaward due to the freshwater discharge and wind forcing from the northerly sectors, however, two periods of landward flow are evident during 7th to 9th and 11th to 16th August 1999, which correspond to winds blowing up-estuary associated with the passage of frontal systems from the SW that are a common feature of the Winter weather pattern for this region. Salt water intrusion is also apparent during these periods, with the leading edge of the salt wedge advancing in the lower part of the water column (dashed lines) and the freshwater above flowing in the opposite direction.
3.3 Oceanographic Field Studies in 2002 and 2003

Two field campaigns were conducted as part of this research, the first during October 2002, and the second in May 2003, representing Spring and Autumn respectively (see Table 3.1 and Figure 3.1 for details and locations). The oceanographic studies were designed to fill gaps in the existing knowledge with respect to current velocities in the lower estuary and the entrance to Saco da Mangueira (Plate 3.2), where no data had previously been collected. Profiles of currents, temperature and salinity were also conducted along the lower part of the estuary and at the mouth in the 2002 survey to assess the structure of the water column, since the system had been flooded during the months leading up to the survey due to an excess of rainfall intensified by an El Niño event. Unfortunately, surveys in the lower estuary during the second field trip were cancelled due to mechanical problems with the survey vessel *Larus*. Local winds were recorded at hourly intervals during all surveys using a hand-held anemometer.

Plate 3.2  French Bridge (the entrance to Saco da Mangueira)

The equipment is presented in Plate 3.3 and consisted of a Broadband 614.4 kHz RDI...
Workhorse ADCP (Acoustic Doppler Current Profiler) (www.rdinstruments.com), which I calibrated prior to the survey, and a Sea-Bird Electronics SBE 19plus SEACAT Profiler (www.seabird.com), which was set-up and operated by FURG;

Plate 3.3 Instrumentation (ADCP, CTD Profiler, Water Level Recorder)

Current velocity profiles were collected using the ADCP at four locations on the French Bridge on 17th to 18th October 2002, and 21st to 22nd May 2003 (Figure 3.10). The ADCP was set up to average data over depth intervals (bins) of 1m, and I deployed it at each location to acquire a transect of current velocities each hour during daylight hours (Plate 3.4). A short time series of current velocities averaged every 10 minutes was also completed at Station 2 on 23rd May 2003.

Figure 3.10 Current Velocity Profiling Locations and Soundings at French Bridge
Since the bathymetry across the entrance to Saco da Mangueira had not been surveyed, the ADCP was also used to measure soundings to the nearest metre at intervals of 3.5m across the length of the bridge. These data are presented in Figure 3.10, and although they could not be reduced to chart datum, the tidal range is small enough that they were considered as a first order estimate for use in the model and subsequent volumetric calculations.

The current velocity profile data were processed using the WinADCP™ software, and the longitudinal components representing flows entering (-ve) and exiting (+ve) the Saco da Mangueira are presented in Figures 3.11 and 3.12, with each row of charts showing one day of data at each station across the entrance as a vertical time series for each water depth, together with wind velocities.

A number of important features describing the water movement at the entrance to the Saco da Mangueira are inferred from the data and summarised as follows:
Figure 3.11  Longitudinal Current Velocity Profiles at the Entrance to Saco da Mangueira
Flows entering and exiting the Saco da Mangueira reached speeds of up to 0.60 m/s and 0.61 m/s respectively, and up to 0.46 m/s and 0.55 m/s respectively for depth averaged longitudinal velocities.

There is a quasi-periodicity to the flow reversals which is of the order of 2 to 3 hours, and appears to be independent of the wind direction, but a longer series of observations under a variety of wind conditions would be required to confirm this feature;

With respect to lateral variation, the current velocities appeared to be relatively consistent across the entrance; however, water in the very shallow margins at the entrance was observed to be flowing in the opposite direction to the main flow and against the wind during a surface float experiment conducted on 23rd May 2003. This would suggest some degree of horizontal shear in the circulation pattern which could give an indication of the suitability of a two-dimensional model, compared with the requirements of a three-dimensional model for deeper water systems exhibiting significant vertical shear;

With respect to the vertical pattern of water movement there was some temporal and spatial variation in current speeds with a maximum depth differential of up to 0.5 m/s. At Station 1, the maximum flows entering the Saco tended to occur at between 5 and 7m depth (Figures 3.11d, h & l) and exited more rapidly closer to the surface, with a similar pattern also evident at Station 3 (Figures 3.11b & j). Conversely, at Station 2 located close to the centre of the entrance, the flows entering the Saco da Mangueira were greatest near to the surface, and between 5 and 6m on exit. Flows at Stations 1 and 3 were consistent with Station 2 only on the 22/05/03 (Figures 3.11n, o, & p).

Vertical shear occurred only at speeds of less than 0.05 m/s e.g. Figures 3.11m to p,
which would indicate that a two-dimensional model may be able to correctly reproduce flows at the entrance to Saco da Mangueira.

![Figure 3.12 Longitudinal Current Velocity Profile at Station 2 on 23rd May 2003](image)

Figure 3.12 Longitudinal Current Velocity Profile at Station 2 on 23rd May 2003

The pattern of flows presented in Figure 3.12 is consistent with the other data previously described for Station 2.

The vertical profiles of salinity and temperature conducted in the lower part of the estuary on 11\textsuperscript{th} October 2002 served only to demonstrate that no salty water was present at locations to the north of Praticagem, and according to the team from FURG this had been the case for several months due to heavy rainfall and flooding of the system. Saline water was measured as a layer extending from 8m below the surface to the bed (19m) at the mouth of the estuary, and an ADCP deployment confirmed the salt wedge entering with freshwater flowing downstream at the surface. During the surveys in 2003, CTD profiles also confirmed the absence of saline water at the entrance to Saco da Mangueira.
3.4 Relationship Between River Flows and the Southern Oscillation Index

In order to conduct model scenarios using the hydrodynamic field data collected in 2002 and 2003, measured river flows for this period were required, but unfortunately these were not available. Therefore, it was necessary to synthesise a representative set of fluvial data which took into account the El Niño Southern Oscillation (ENSO). This is a disturbance of the ocean-atmosphere system in the tropical Pacific which affects global weather systems, with high precipitation rates in southern Brazil causing increased fluvial inputs to the Patos System (see Chapter 2). This relationship was investigated and is presented here.

The most widely used intensity scale for ENSO is the Southern Oscillation Index (SOI), which is given in normalised units of standard deviation, and is based on the anti-correlation of the atmospheric pressure difference between Tahiti and Darwin (oar.pmel.tao group@noaa.gov). High pressure in Tahiti indicates normal trade winds blowing from the southeast, whereas under conditions of low pressure the winds blow from the west signifying El Niño. The index is positive for La Niña events and negative for El Niño events.

The monthly SOI values for the period 1940 to 2003 were downloaded from the website of the Pacific Marine Environmental Laboratory www.pmel.noaa.gov, and are presented as a time series in Figure 3.13, together with the monthly total river discharge to the Patos System. Both data-sets were smoothed using a 1 year running mean; the sign was reversed for the SOI; and the river discharges were scaled to give deviations around the mean value for the total data-set.
Figure 3.13  Comparison of Southern Oscillation Index and Total River Flow

The correlation between SOI and riverine discharge is apparent from the value of \( R^2 = 0.46 \) particularly for the period from 1979 to 1988 (\( R^2 \) is the coefficient of determination i.e. the covariance divided by the standard deviations). It is relevant to this study that 1999 was a La Niña year, whereas during 2002-03 there was a moderate El Niño event. The third time series on Figure 3.13 shows the results obtained from the following analysis, for which I am indebted to my supervisor Dr. Ken George. Firstly, the monthly mean discharges for each year of complete dataset were subjected to Fourier analysis. It was assumed that in any given year the discharge varied sinusoidally; viz.

\[
y = y_0 + A \cos (\sigma t - \epsilon)
\]

where \( y = \log \) (discharge in cumecs),
\( t = \) time measured from the start of the year;
\( \sigma = 2\pi/(\text{length of year}) = \) fundamental frequency

The results of the analyses were, for each year:

- \( y_0 \)  the annual mean of the quantity \( \log(\text{discharge}) \);
- \( A \)  the amplitude of the annual variation;
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- $\varepsilon$ the phase of the annual variation

These quantities were plotted against the SOI (Figures 3.14a–c), with the following results:

![Graphs showing relationships between SOI and riverine discharge characteristics](image)

**Figure 3.14** a. Mean Annual Discharge; b. Mean Annual Amplitude; c. Mean Annual Phase

- the mean annual discharge decreases as the SOI increases, i.e. the rivers discharge more water during El Niño events;
- there was no clear relationship between the amplitude of the annual variation and the SOI;
- the phase increases with increasing SOI, i.e. in years of El Niño, the peak of the annual variation in riverine discharge occurs later in the year than in years of La Niña.
The results were then fitted to the formula:

\[ y = <y_0> + (\alpha_0 + \alpha_1 x) \cos \sigma t + (a_0 + a_1 x) \sin \sigma t \]  

(3.2)

where \( x = \text{SOI} \);

\( <y_0> \) is the long-term average of the annual mean of \( \log(\text{discharge}) \); 

\( \alpha_0 \) and \( a_0 \) express the long-term mean of the complex amplitude of the annual variation of \( \log(\text{discharge}) \); and

\( \alpha_1 \) and \( a_1 \) express how the complex amplitude varies with the SOI.

The values of the coefficients \( <y_0> \), \( \alpha_0 \), \( \alpha_1 \), \( a_0 \) and \( a_1 \) were determined by least squares, and subsequently used to generate values of riverine discharge for a given value of SOI, which are presented in Figure 3.15.

![Figure 3.15: Annual Variation Including El Niño](image)

**Figure 3.15** Annual Variation Including El Niño

The total river flows calculated using this method for 2002 and 2003 are shown by the light blue lines in Figure 3.13, and were subsequently converted into flows for the individual rivers and used to drive the model during the validation of the hydrodynamic model and for water quality simulations.
3.5 Data Used for the Water Quality Modelling

Our existing knowledge of the water quality of the Patos System has been described in Chapter 2. This section provides details of the subset of hydro-chemical data collated for this modelling study, together with details of the fieldwork conducted in 2002 and 2003. Survey details and sampling locations are summarised in Table 3.1 and Figure 3.1.

The data are described in terms of quality, quantity, and spatial coverage, in order to assess the level of detail possible for the water quality model. Ideally, a data-set with high spatial and temporal resolution, combined with accurate and consistent laboratory analysis will give optimum confidence in the model calibration and predictive capability, within the chosen scope of study. This situation is rarely achieved mainly due to the expense of fieldwork campaigns, or poor survey planning and design, so it is more often the case that the data available will dictate the resolution of the model.

3.5.1 Water Quality Data Pre 2002

A total of ten sets of data were compiled, three of which were extracted from published literature, and the rest supplied by academic staff at FURG. Water samples were collected in most years from 1983 to 2000, from a total of 75 locations varying with each survey throughout the lagoon, estuary, and shallow embayments including the Saco da Mangueira. The determinands common to almost all of the surveys were temperature; salinity; suspended solids; ammonium; nitrite; nitrate; phosphate; and silicate, with additional measurements of water transparency (Secchi depth); chlorophyll-a; dissolved oxygen (DO); and biochemical oxygen demand (BOD), made during some of the surveys. In this analysis, nitrogen is reported as dissolved available inorganic nitrogen (DAIN), which is the sum of ammonium; nitrite; nitrate, and accordingly, phosphorus is as dissolved
available inorganic phosphorus (DAIP). Temporal and spatial variations for each parameter are presented in Figures 3.16 and 3.17 as box and whisker plots which were designed to show the variation in a sample population by summary statistics as follows:

The dotted lines in plots d. to h. in each figure indicate the concentration of the parameter expected in uncontaminated estuarine waters. There are a variety of values in the literature quoted as indicators of pollution, which aid government departments and regulatory bodies when assessing water quality standards and criteria. These have been summarised and are presented in Appendix 1. For this study the following levels have been adopted:

- A median concentration of at least 7mg/l dissolved oxygen will allow the passage of migratory fish, support a resident fish population, and sustain breeding populations appropriate to the physical and hydrographical conditions of the water body (MPMMG, 1997).

- Values of 150μM (4.214mg/l) for silicate (Aminot & Chaussepied, 1983), and 1μM (0.031mg/l) for phosphate (Aminot & Chaussepied, 1983; Day et al., 1989; Pomeroy et al., 1965), are considered typical of non-polluted estuaries.

- If the concentration of DAIN significantly exceeds 12μmol (0.168mg/l) in the presence of >0.2μmol (0.006mg/l) DAIP, the water is considered to be hypernutrified (MPMMG, 1997).

- Regular exceedence of 10μg/l chlorophyll-a implies eutrophic conditions (MPMMG, 1997; OSPAR Commission, 2002; DoE, MAFF, Welsh Office, 1993).
Figure 3.16  Seasonal and Spatial Variability of Selected Water Quality Parameters
Figure 3.17  Box and Whisker Plots Showing Seasonal Variability of Parameters from Locations in the Lower Estuary and Saco da Mangueira
Figure 3.16 presents the seasonal and spatial variation of water quality data compiled for this study, which have been sub-divided into eight geographical areas (see Figure 3.1a-c) as follows: the fluvial inputs of Guaíba, Camaquã, and the São Gonçalo Channel; the Patos Lagoon; Upper and Lower Patos Estuary; Saco da Mangueira; and an ocean site adjacent to the entrance of the estuary. Seasonal statistics for the entire data-set are also presented.

The water quality modelling study will focus on the Saco da Mangueira, therefore, the data for this embayment are presented in more detail in Figure 3.17, together with the lower part of the Patos Estuary for comparison. The data for Saco da Mangueira have been subdivided into five sampling locations (see Figure 3.18, p.81) as follows:

1. French Bridge, which spans the entrance to Saco da Mangueira, where the water quality is heavily influenced by contaminants from the main sewage outfall of Rio Grande located ~800m outside the entrance in a shallow cove named Coroa do Boi;

2. An area adjacent to Rio Grande which is influenced by urban wastewater from both domestic and industrial discharges described in Chapter 2 (see Figure 2.5, p.39);

3. An area affected by discharges from three fertiliser factories situated in the industrial district on the southern shore of Saco da Mangueira;

4. The central region of Saco da Mangueira;

5. An area adjacent to Simão Creek which is a small stream discharging ~20 cusecs of freshwater into the Saco da Mangueira at the southern end remote from the influence of discharges from the city and industrial district.

Before proceeding with a description of the data, it is clear that there is a very wide range
of sampling frequencies for each parameter on both spatial and temporal scales. As a rule of thumb, a sample size of less than 20 is considered small when assessing water quality data on annual time scales, and therefore, average values taken from such data-sets are likely to be attributed with a low level of confidence as to whether the data are truly representative of the population. This is the case for the fluvial data, where the maximum number of samples for any given parameter is 20 on an annual scale. A much higher level of confidence can be placed upon data elsewhere in the study area, where in general the number of samples ranges from 30 to 60 on a seasonal scale and >100 annually, apart from chlorophyll-a and DO which also have low sample frequencies on a seasonal scale. This aspect will be revisited in Chapter 7 where the maximum resolution that can be reasonably obtained from the water quality model in terms of boundary and initial conditions will be evaluated.

Returning our attention to the data presented in Figures 3.16 and 3.17, the most notable features of the water quality of the Patos System are as follows:

a. **Water temperatures** show a consistent pattern throughout the study area, ranging from $<15^\circ C$ during Winter months followed by a gradual rise during Spring to peak at $\sim 25^\circ C$ in the Summer, then a gradual fall in Autumn. The highest and lowest temperatures are found in Saco da Mangueira, where water depths are extremely shallow, averaging just 0.8 m;

b. **Salinities** range from 0 to 35ppt, and are lower in the Spring due to the elevated river flows and strong northeasterly winds characteristic of this season, which generally enhance the flushing of the system. Values increase during Summer and Autumn as a result of reduced fluvial inputs allowing the intrusion of oceanic water which is generally confined to the estuary and Saco da Mangueira. During
this period, salinities appear to be higher inside the embayment which would suggest a longer residence time than in the estuary, which is investigated in Chapter 6. On average, values marginally decrease during Winter months through the action of increased river flows, but do not reduce to levels found in Spring because of the predominance of weather systems from westerly sectors which facilitate the transport of some salty water into the estuary.

c. Levels of suspended solids are generally high throughout the study area, with an overall proportion of ~50% in excess of 30mg/l, and 20% greater than 80mg/l. Highest concentrations in all areas are evident during Spring, when the action of strong seasonal winds enhance the resuspension of bottom sediments in shallow waters, and favour an increase in inputs from the north of the system and continental shelf (Proença, 1990);

d. The water in all areas appears well oxygenated throughout the year, with DO levels rarely falling below 7mg/l, apart from on occasion during Summer months. Indeed, DO saturation would seem reasonable in the Patos System due to continual aeration from wind action on the shallow water and high levels of primary production, however, the sampling frequency is sparse, so we cannot be certain whether the true variability of DO is reflected by these data. It should also be noted that the data are not in-situ measurements, and where both in-situ and laboratory values exist for the same sample, the in-situ data are on average ~2.5mg/l less than the laboratory results;

e. Levels of silicate are moderate throughout the year with peaks occurring in the fluvial inputs during Winter and Spring months, due to the climatological processes common in these seasons which favour the redissolution of silicon from
sediments. The processes affecting nutrient cycling have been described in the previous Chapter.

f. Concentrations of dissolved available inorganic nitrogen (DAIN) concentrations are high throughout the study area, particularly during Spring and Summer, with an overall proportion of ~55% in excess of 0.168mg/l. This would suggest that the whole of the Patos System is hypernutrified and likely to have a trophic status ranging from mesotrophic to eutrophic, which has been evidenced by the occurrence of persistent algal blooms (see Chapter 2);

g. Concentrations of dissolved available inorganic phosphorus (DAIP) are generally unremarkable on both seasonal and temporal scales apart from in the Saco da Mangueira, where mean concentrations are ~0.15mg/l, which is around five times higher than elsewhere. Levels have also been recorded of at least an order of magnitude higher than those expected in uncontaminated waters, and this is without doubt due to the wastewater discharges from the fertiliser factories which border the embayment;

h. The highest mean concentrations of chlorophyll-a are present in the Saco da Mangueira and the Guaíba river, with values regularly exceeding 10 μg/l, adding further evidence to the high degree of primary productivity in these areas resulting from nutrient enrichment.

In summary, the data confirm the conclusions made previously in published literature (Chapter 2), that the Patos System sustains high levels of primary productivity, with a tendency for eutrophic conditions in freshwater inputs and particularly in the Saco da Mangueira, which has unique hydrochemical characteristics with levels indicative of the
wide range of pollutants which discharge directly to its waters.

3.5.2 Water Quality Field Studies in 2002 and 2003

Water samples and measurements were taken from 5 cm below the water surface on the 9th October 2002 (Winter), and the 4th June 2003 (Spring) from locations in the lower estuary and the Saco da Mangueira shown in Figure 3.18. The survey vessel Larus (Plate 3.5) operated by FURG was used for locations in the lower estuary, whereas those in Saco da Mangueira were collected from a launch owing to the shallow water. Sampling locations 1, 2, and 3 in the estuary were not visited during the second field trip due to mechanical problems with Larus. The sampling locations in Saco da Mangueira were chosen to represent the water quality in areas affected by human activities (French Bridge (domestic effluent); Inca (domestic and industrial wastewater); Fertiliser; Incobrasa (soy oil manufacturing)), as well as areas not directly impacted (Centre and Simão Creek).

![Figure 3.18 Location of Water Sampling Sites in 2002/2003](image_url)

Measurements of salinity, conductivity, temperature, and pH were taken using a Yellow
Springs (model 33 SCT) thermo-salinity meter and a portable potentiometer. All instruments were calibrated and operated by staff of the hydrochemistry laboratory of FURG. Water transparency was measured using a Secchi disc, and wind readings were taken using a hand-held anemometer. Water samples were collected for the analysis of total suspended material; biochemical oxygen demand; dissolved oxygen; chlorophyll-a; ammoniacal nitrogen; nitrate; nitrite; phosphate; total phosphorus; and silicate.

Plate 3.5 Survey Vessel Larus

Water samples underwent the necessary pre-treatment on-board and were subsequently transported to the FURG laboratory where they were analysed by the methods described in Baumgarten et al. (1996), based on Strickland and Parsons (1972), and Aminot & Chaussepied (1983). Total Coliforms and Escherichia Coli were enumerated using the methodology recommended by the American Public Health of Water and Wastewater, (APHA, 1992). The results are presented in Table 3.4 below.
### Table 3.4  Water Quality Results for Surveys in 2002 and 2003

<table>
<thead>
<tr>
<th>Date</th>
<th>Location</th>
<th>East</th>
<th>North</th>
<th>Season</th>
<th>Time</th>
<th>Water Temp (°C)</th>
<th>pH in situ</th>
<th>Total Suspended Material (TS) (mg/l)</th>
<th>Water Temp (°C)</th>
<th>Turbidity (NTU)</th>
<th>Secchi Depth (m)</th>
<th>Dissolved Oxygen (DO) (mg/l)</th>
<th>% Dissolved Oxygen (DO) %</th>
<th>Chlorophyll-a (μg/l)</th>
<th>Ammonia Nitrogen (mg/l)</th>
<th>Nitrate (mg/l)</th>
<th>Nitrite (mg/l)</th>
<th>Phosphate (PO₄) (mg/l)</th>
<th>Total Phosphorus (mg/l)</th>
<th>Silicate (mg/l)</th>
<th>Total Coliforms (cfu/100 ml)</th>
<th>Escherichia Coli (cfu/100 ml)</th>
</tr>
</thead>
<tbody>
<tr>
<td>09/10/2002</td>
<td>3 Bocas (3 Mouths)</td>
<td>396678</td>
<td>6461449</td>
<td>Spring</td>
<td>11:00</td>
<td>NE / 15.2</td>
<td>14.0</td>
<td>59.2</td>
<td>21</td>
<td>0.1</td>
<td>1.3</td>
<td>8.8</td>
<td>97</td>
<td>2.6</td>
<td>0.233</td>
<td>0.194</td>
<td>0.055</td>
<td>0.052</td>
<td>0.432</td>
<td>2.430</td>
<td></td>
<td></td>
</tr>
<tr>
<td>09/10/2002</td>
<td>Diamante</td>
<td>397429</td>
<td>6465547</td>
<td>Spring</td>
<td>11:40</td>
<td>NE / 15.2</td>
<td>21.6</td>
<td>100.8</td>
<td>22</td>
<td>0.0</td>
<td>1.1</td>
<td>6.6</td>
<td>94</td>
<td>1.8</td>
<td>0.084</td>
<td>0.293</td>
<td>0.003</td>
<td>0.035</td>
<td>0.380</td>
<td>2.430</td>
<td></td>
<td></td>
</tr>
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<td>6455780</td>
<td>Spring</td>
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<td>ENE / 10.4</td>
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<td>54.0</td>
<td>22</td>
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<td>0.2</td>
<td>6.1</td>
<td>8.6</td>
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<td>0.155</td>
<td>0.213</td>
<td>0.006</td>
<td>0.083</td>
<td>0.374</td>
<td>1.934</td>
<td></td>
<td></td>
</tr>
<tr>
<td>09/10/2002</td>
<td>Buoy 1 (Rio Grande Channel)</td>
<td>398812</td>
<td>6451486</td>
<td>Spring</td>
<td>13:15</td>
<td>ENE / 10</td>
<td>22.9</td>
<td>92.0</td>
<td>22</td>
<td>0.0</td>
<td>1.1</td>
<td>6.6</td>
<td>9.4</td>
<td>104</td>
<td>0.084</td>
<td>0.293</td>
<td>0.003</td>
<td>0.035</td>
<td>0.380</td>
<td>2.430</td>
<td></td>
<td></td>
</tr>
<tr>
<td>09/10/2002</td>
<td>Incoba (human and urban wastes)</td>
<td>396102</td>
<td>6453227</td>
<td>Spring</td>
<td>14:15</td>
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<td>6446906</td>
<td>Spring</td>
<td>15:11</td>
<td>ENE / 10</td>
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<td>137.2</td>
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</table>

**Chapter 3 - Data Collation and Field Studies**
Comparisons of the water quality data collected during 2002 and 2003 with the historical data are summarised as follows:

- The maximum salinity recorded during the Spring survey in 2002 was 1.1 g/kg, reflecting the flood conditions that dominated the system at the time of the survey, due to an excess of rainfall intensified by an El Niño event. In the 2003 survey, some salt water intrusion was recorded in the estuary and Saco da Mangueira (with an accompanying decrease noted in the levels of turbidity), with a maximum value of 8.73 g/kg in the Rio Grande Channel, and a minimum of 1.24 g/kg recorded close to the Simão Creek;

- Levels of total suspended matter were consistent with typical concentrations for the area, ranging from 14 to 232 mg/l with a mean value of 75.3 mg/l. Higher values were experienced during the Spring survey, due to high fluvial discharge throughout the system;

- DO concentrations were within the typical range for the area, with high values at all locations during both surveys ranging from 7.7 to 10.5 mg/l, and percentage saturation levels approaching and exceeding saturation;

- Biochemical oxygen demand values were ≤ 1.6 mg/l in the estuary during the 2002 survey, which is within the normal limit for the estuary of 3 mg/l established by the State Foundation of Environmental Protection (FEPAM, 1995) (see Chapter 2 and Appendix 1), whereas during the 2003 survey, levels were higher between 2.8 and 4.8 mg/l, indicating organic enrichment. Very few samples had been analysed for BOD in previous studies and have not been presented, however, estuarine values were <3 mg/l apart from close to the main sewage outfall of Rio Grande where BOD reached 43.5 mg/l;

- Concentrations of silicate were low and consistent with the historical data for the
2002 survey, but show elevated levels of up to 7.5 mg/l in the estuary during the 2003 survey when more saline water was present, indicating desorption of silicate from particulate matter;

- **Nitrogenous compounds** (nitrate, nitrite, and ammoniacal nitrogen) were within the normal range found in the area, with values of DAIN ranging from 0.076 to 0.877 mg/l, with the highest levels generally found in the estuary during the 2002 survey, and adjacent to the domestic and industrial wastewater discharges and fertiliser factories in Saco da Mangueira during both surveys. Levels of ammonium were highest close to the Simão Creek during the 2002 survey, indicating the input of human waste probably as a result of the flooding in this area;

- **DAIP** levels were also consistent with previous surveys, with a maximum value of 0.435 mg/l measured adjacent to the fertiliser factories during the 2003 survey;

- **Chlorophyll-a** was only analysed during the 2002 survey, with values <5 mg/l recorded in estuarine waters, and high values exceeding 15 mg/l evident throughout the Saco da Mangueira;

- **Total Coliforms and *Escherichia coli*** numbers were exceptionally high adjacent to the human and wastewater discharges during both surveys, and also close to the Simão Creek and fertiliser factories during the 2002 survey. Total coliform concentrations of up to 500,000 no./100ml were measured in these areas which exceed the EC Bathing Waters Directive mandatory standard of 10,000 no./100ml by a factor of 50, and is representative of raw sewage diluted by less than tenfold. The levels experienced during the 2002 survey were undoubtedly enhanced by flood and rainwater carrying bacterial contaminants through surface water drains and other uncontrolled urban sources bordering the Saco da Mangueira.
Chapter 4

The TELEMAC Modelling Suite

4.1 Introduction

The TELEMAC system is a set of finite element programs developed by Electricité de France, Laboratoire National d'Hydraulique (EDF-LNH), (www.telemacsytem.com), which have been designed for open channel flows. The system contains two and three dimensional modules for the study of currents (TELEMAC-2D, TELEMAC-3D); cohesive sediment transport (SUBIEF); sand transport (SISYPHE); and wave dynamics (ARTEMIS, BOUSSINESQ, COWADIS), together with pre-processing software (MATISSE) for the generation of unstructured finite element grids, and post processing software (RUBENS) for viewing and manipulating results. In addition to those modules developed by EDF-LNH, further modules have been developed by HR Wallingford Ltd. (www.hrwallingford.co.uk) for particle tracking (SEDPLUME-3D); pollutant dispersion (PLUME-RW); and water quality (WQFLOW-2D, WQFLOW-3D).

The TELEMAC modules use highly efficient algorithms based on the finite-element method, and space is discretised in the form of an unstructured triangular grid of elements, which means that areas of special interest can be highly resolved, negating the need for the use of nested models, as is the case with the finite-difference method.

The modules of TELEMAC used for this research were TELEMAC-2D and WQFLOW-2D, the formulations of which are described here with general reference to modelling documentation by Hervouet & Van Haren (1999), and HR Wallingford Ltd. (2000).
Chapter 4 - The TELEMAC Modelling Suite

4.2 The TELEMAC-2D Module

TELEMAC-2D is a two dimensional depth-averaged fluid flow model which uses finite element techniques to solve the second order partial differential equations for shallow water, known as the Barré de Saint-Venant (1871) equations, derived from the three dimensional Navier-Stokes equations. The main variables are water depth and current velocity averaged in the vertical, but the transport of a passive tracer and turbulence can also be taken into consideration. The model uses triangular finite element discretisation, but can also work with quadrilateral elements.

4.2.1 The Averaged Navier-Stokes Equations

The Barré de Saint-Venant equations are derived from the Navier-Stokes equations by taking the vertical average, which requires assumptions and approximations regarding the non-linear terms. Before proceeding with formulation, the orthogonal Cartesian frame of reference used in TELEMAC-2D is presented in Figure 4.1, where the x and y axes form the horizontal plane; gravity acts in the negative z direction; Zf and Z are the elevations of the bed and free surface respectively; and the depth of the water h is equal to Z - Zf.

Figure 4.1 Notation for TELEMAC-2D Geometry (from Hervouet & Van Haren, 1999)
For the derivation of the Barré de Saint-Venant equations the following assumptions and approximations apply:

- the fluid is assumed to be Newtonian;
- the density is constant (following the hypothesis of Boussinesq);
- the pressure is hydrostatic (linked to conditions of small vertical movements), which is necessary to convert the pressure in terms of the water head, since the pressure, denoted by \( p(x,y,z) \) at point \((x,y,z)\), is caused only by the water head above that point:

  \[
  \frac{1}{\rho} \frac{\partial p}{\partial z} - g = 0, \quad \text{where} \quad p(x,y,z) = -\rho g z + C
  \]  

  (4.1)

  The constant \( C \) is chosen such that \( p(x,y,Z) = 0 \), and if it is assumed that the atmospheric pressure is 0 (or is a constant \(-0\)), it follows that:

  \[
  p(x,y,z) = \rho g (Z - z)
  \]  

  (4.2)

  and at the bed:

  \[
  p = \rho g (Z - Z_f) = \rho g h
  \]  

  (4.3)

- the vertical velocity is neglected according to the hypothesis of hydrostaticity, which requires the vertical accelerations to be insignificant;
- there is no transfer of water either through the bed or from the surface.

The TELEMAC-2D code solves the equations for mass continuity and momentum simultaneously, over the vertical by integrating from the bed to the surface.
The averaged continuity equation is:

\[
\frac{\partial h}{\partial t} + \frac{\partial (hU)}{\partial x} + \frac{\partial (hV)}{\partial y} = 0 \tag{4.4}
\]

The averaged momentum equations are:

\[
\frac{\partial (hU)}{\partial t} + \frac{\partial (hUU)}{\partial x} + \frac{\partial (hUV)}{\partial y} = -gh \frac{\partial Z}{\partial x} + \frac{\partial}{\partial x} \left( h v_e \frac{dU}{dx} \right) + \frac{\partial}{\partial y} \left( h v_e \frac{dU}{dy} \right) + hF_x \tag{4.5}
\]

\[
\frac{\partial (hV)}{\partial t} + \frac{\partial (hUV)}{\partial x} + \frac{\partial (hVV)}{\partial y} = -gh \frac{\partial Z}{\partial y} + \frac{\partial}{\partial x} \left( h v_e \frac{dV}{dx} \right) + \frac{\partial}{\partial y} \left( h v_e \frac{dV}{dy} \right) + hF_y \tag{4.6}
\]

where:

- \( t \) time (s)
- \( h \) depth of water (m)
- \( U, V \) depth averaged velocity components (m/s)
- \( g \) gravity acceleration (m/s²)
- \( Z \) free surface elevation (m)
- \( v_e \) momentum diffusion coefficient (m²/s)
- \( F_x, F_y \) source terms in the momentum equations including atmospheric pressure, bed friction, surface friction, and rotation

### 4.2.2 Source Terms

The source terms \( F_x \) and \( F_y \) in the momentum equations include friction at the bed and surface (wind influence), the Coriolis parameter, and atmospheric pressure. The formulations used by TELEMAC-2D for these terms are as follows:
Friction at the bed

The form of the equation for bed friction is a quadratic function of velocity:

\[ \tau = \rho C_f U \sqrt{U} \]  \hspace{1cm} (4.7)

where:
- \( \rho \) density of the liquid (kg/m\(^3\))
- \( C_f \) friction coefficient (dimensionless)
- \( U \) velocity of the flow (m/s)

The friction coefficient \( C_f \) is typically replaced by other coefficients such as de Chezy \( (C) \), Strickler \( (K) \), Manning \( (m) \), or the roughness height of Nikuradse \( (k_r) \). The most common of these is the coefficient of de Chezy, which is related to \( C_f \) by the formula:

\[ C = \sqrt{\frac{g}{C_f}} \hspace{1cm} \text{m}^{1/2} \text{s}^{-1} \]  \hspace{1cm} (4.8)

and parameterised into the equations of momentum by:

\[ F_x = -\frac{1}{\cos(\alpha)} \frac{g}{hC^2} u \sqrt{u^2 + v^2} \]  \hspace{1cm} (4.9)

\[ F_y = -\frac{1}{\cos(\alpha)} \frac{g}{hC^2} v \sqrt{u^2 + v^2} \]  \hspace{1cm} (4.10)

where \( u \) and \( v \) are the velocity components, and \( \alpha \) is the slope angle of the bed.
The friction coefficients of, Manning, Nikuradse, and Strickler may be substituted by the following relation with $C_f$:

$$C_f = \frac{g}{C^2} = \frac{gm^2}{h^{1/3}} = \frac{1}{32 \left( \log \left( \frac{14.8h}{k_s} \right) \right)^2} = \frac{g}{S^2 h^{1/3}} \quad (4.11)$$

where:

- $m$: coefficient of Manning ($m^{1/6} \text{s}^{-1}$)
- $h$: water depth (m)
- $k_s$: the grain size at the bed (Nikuradse's coefficient)
- $S$: coefficient of Strickler ($m^{1/3} \text{s}^{-1}$)

An approximation here is that $h = R_H$, the hydraulic radius (the area of cross-section divided by the wetted perimeter), and this is only correct for very wide channels.

**Friction at the surface**

The resistance of the wind at the surface is parameterised into the equations of momentum in TELEMAC-2D by:

$$F_x = \frac{1}{h} \frac{\rho_{\text{air}}}{\rho} a_{\text{wind}} U_{\text{wind}} \sqrt{U_{\text{wind}}^2 + V_{\text{wind}}^2} \quad (4.12)$$

$$F_y = \frac{1}{h} \frac{\rho_{\text{air}}}{\rho} a_{\text{wind}} V_{\text{wind}} \sqrt{U_{\text{wind}}^2 + V_{\text{wind}}^2} \quad (4.13)$$

where,

- $\rho$: density of freshwater ($1000 \text{ kg/m}^3$)
- $\rho_{\text{air}}$: density of air ($1.29 \text{ kg/m}^3$)
- $a_{\text{wind}}$: wind resistance coefficient
- $U_{\text{wind}}, V_{\text{wind}}$: components of the wind velocity with respect to the fluid ($\text{m/s}$)
The wind resistance coefficient is calculated from the formula used by the former Institute of Oceanographic Sciences (United Kingdom):

If $|U_{\text{wind}}| < 5 \text{ m/s}$, then, $a_{\text{wind}} = 0.565 \times 10^{-3}$

If $5 < |U_{\text{wind}}| < 19.22 \text{ m/s}$, then, $a_{\text{wind}} = (-0.12 + 0.137|U_{\text{wind}}|) \times 10^{-3}$

If $|U_{\text{wind}}| > 19.22 \text{ m/s}$, then, $a_{\text{wind}} = 2.513 \times 10^{-3}$

**Coriolis Acceleration**

The Coriolis force at a point of latitude $\phi$ is equal to:

$$F_x = 2\omega v \sin \phi = fv \quad (4.14)$$

$$F_y = -2\omega u \sin \phi = -fu \quad (4.15)$$

where:

$\omega$ angular velocity of the Earth's rotation $= 7.292 \times 10^{-5} \text{ rad/s}$

$f$ Coriolis coefficient (negative in the Southern Hemisphere)

**4.2.3 Boundary Conditions**

For the solid boundaries, conditions of impermeability and friction are imposed in TELEMAC-2D, and for the liquid boundaries the user defines either a prescribed or free value for each point of the mesh, for each of the principal variables ($h$, $U$, $V$). For example, prescribed elevation and free velocity may be defined for a tidal inlet boundary, whereas, conditions of free elevation and a prescribed flow rate may be defined for fluvial input boundaries.
4.2.4 Tracer Equation

In TELEMAC-2D a tracer represents a conservative physical quantity that does not modify the flow, and depends on advection, diffusion, dispersion, source, and sink terms:

\[
\frac{dT}{dt} + u \frac{dT}{dx} + v \frac{dT}{dy} - \frac{1}{h} \text{div} \left( h v \nabla T \right) = \frac{(T_{\text{sce}} - T_{\text{sce}})}{h}
\]  

(4.16)

where,

- \(T\) an index indicating that the diffusion applies to the tracer
- \(\nu_T\) the coefficient of diffusion (laminar or turbulent) of the tracer,
- \(T_{\text{sce}}\) source value of the tracer, in units the tracer is expressed in
- \(Sce\) the source of discharge (m/s)

The right hand side of the equation is 0 if the tracer value of the source is equal to the tracer value where the source arrives, which is not usually the case for an inflow into the domain. The user provides a source flow rate \(Q_{\text{sce}}\) (m\(^3\)/s), \(T_{\text{sce}}\), and the components of the source velocity \(u_{\text{sce}}\) and \(v_{\text{sce}}\) (m/s).

4.2.5 Modelling Turbulence

The averaging of the Navier-Stokes equations over time requires additional terms which form the Reynolds stress tensor, due to the energy transfers between the average movement and the eddies caused by turbulence. The system of equations obtained is not solvable because it is not closed, and this difficulty has given rise to turbulence models called closure models. The closing is achieved by applying the hypothesis of Boussinesq which expresses the Reynolds stress tensor in terms of the local velocity gradient and a turbulent viscosity. This concept is applied in the turbulence model used in TELEMAC-2D, by either
applying a constant viscosity or directly solving the transport equations for the kinetic energy and its rate of dissipation (the k-ε model).

4.2.6 Wetting and Drying

Tidal flats are handled by two different options in TELEMAC-2D, either by treating them integrally in the entire domain and correcting the gradient of the free surface, or by removing all the elements that are not entirely wet from the calculation.

4.2.7 Numerical Methods

The Navier-Stokes equations are solved based on the Operator-Splitting method (Marchuk, 1975; Zienkiewicz & Ortiz, 1995), whose main principle is that the hyperbolic and parabolic parts of the Navier-Stokes equations should be treated separately in order to use well-adapted numerical methods for each part. The solution involves two steps: 1) solution of the advection terms; 2) solution of the propagation, diffusion and source terms.

Advection Step

The Method of Characteristics is applied to solve the advection of u and v (Galland et al., 1991). In TELEMAC-2D the calculation of the characteristics (trajectories) are performed by a first order method of Runge-Kutta, and the interpolation at the foot of the characteristic conforms to the type of finite element chosen for the “propagation-diffusion-source terms” stage.

The Streamline Upwind Petrov-Galerkin method (SUPG) of Brooks & Hughes (1982) has been applied to solve the advection of h. This method was implemented in TELEMAC-2D to ensure mass conservation and an oscillation free solution without excessive mesh refinement, or the addition of artificial diffusivity (Bates et al., 1998). Extended to a Petrov-
Galerkin formulation, the standard Galerkin weighting functions are modified by adding a streamline upwind perturbation. The modified weighting function is applied to all terms in the equation, resulting in a consistent weighted residual formulation.

**Propagation, Diffusion and Source Terms Step**

The propagation, diffusion and source terms are solved by the finite element method, where an implicit time discretisation allows the calculation of the non-linearities in the equations. Variational formulations and space discretisation transform the continuous equations into a linear discrete system where the values of $h$, $u$ and $v$ at the nodes are the unknown variables. This system is solved by an iterative conjugate gradient method (Hervouet & Van Haren, 1999). TELEMAC-2D makes significant savings in both computational time and storage requirements through the use of an element-by-element solution technique, where the matrices in the linear system are stored in their elementary form without recourse to full assembly (Bates et al., 1997).
4.3 The WQFLOW-2D Module

WQFLOW-2D is a two-dimensional depth averaged model which uses water flows and depths from TELEMAC-2D to simulate processes affecting water quality in estuaries, coastal areas and lakes, using a finite element method. These processes are transport and mixing; biochemical interactions; the balance of oxygen and nutrient variables; and algal growth. A schematic representation of the processes simulated is shown in Figure 4.2.

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**Figure 4.2** Schematic of WQFLOW-2D (adapted from HR Wallingford, 2000)

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This eutrophication model actually describes the balance of mass and energy within an ecosystem, and as such, the system is highly coupled since energy and mass balance for individual constituents is invariably linked to several others. The model incorporates interactions between the variables presented in Table 4.1:

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<th>Model Notation</th>
<th>Model Output Units</th>
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<td>T</td>
<td>°C</td>
</tr>
<tr>
<td>Reactions</td>
<td>Salinity</td>
<td>S</td>
<td>g/kg</td>
</tr>
<tr>
<td>Reactions</td>
<td>Dissolved Oxygen</td>
<td>DO</td>
<td>mg/l</td>
</tr>
<tr>
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<td>B</td>
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</tr>
<tr>
<td>Reactions</td>
<td>Fast Dissolved BOD</td>
<td>B</td>
<td>mg/l</td>
</tr>
<tr>
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<td>mg/l</td>
</tr>
<tr>
<td>Reactions</td>
<td>Fast Organic Nitrogen</td>
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<td>mg/l</td>
</tr>
<tr>
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<tr>
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<tr>
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<td>Nitrate</td>
<td>NO3</td>
<td>mg/l</td>
</tr>
<tr>
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<td>Hydrogen Sulphide</td>
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</tr>
<tr>
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<td>Fast Particulate BOD</td>
<td>B</td>
<td>mg/l</td>
</tr>
<tr>
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<td>Slow Particulate BOD</td>
<td>B</td>
<td>mg/l</td>
</tr>
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<tr>
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<td>Orthophosphate</td>
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<tr>
<td>Coliforms</td>
<td>Coliforms</td>
<td>CF</td>
<td>thousands/100ml</td>
</tr>
</tbody>
</table>

Table 4.1 WQFLOW-2D Variables

Temperature is not a simulated variable, but is either specified as a constant value or spatial distribution, which is used to calculate reaction rates and the solubility of oxygen. In addition to the above variables, up to a further ten pollutant variables may be specified by the user.
4.3.1 The Mass Balance Equation

The transport and dispersion of solutes and suspended matter is governed by the mass balance (advection-diffusion) equation, which is solved separately for each variable:

\[
\frac{\partial}{\partial t} (dC) + \frac{\partial}{\partial x} (dC + u dv) + \frac{\partial}{\partial y} (dC + v dw) = \frac{\partial}{\partial s} \left( dD_x \frac{\partial C}{\partial s} \right) + \frac{\partial}{\partial n} \left( dD_n \frac{\partial C}{\partial n} \right) - K C d - F_c - \frac{L_c}{\Delta s^2} + \frac{S}{\Delta s^2} \quad (4.17)
\]

where:

- **C** depth-averaged concentration of a solute (kg/m³)
- **u,v** depth-averaged components of velocity (m/s)
- **D_x** longitudinal (shear flow) dispersion coefficient (m²/s)
- **D_n** lateral (turbulent) diffusion coefficient (m²/s)
- **(x,y)** Cartesian coordinates in the horizontal plane (m)
- **(s,n)** intrinsic coordinates parallel with and normal to the mean flow, respectively (m)
- **t** time (sec)
- **d** water depth (m)
- **Δs** model grid size
- **K** first order decay rate (s⁻¹)
- **F_c** flux of solute between water column and the bed (kg/m²/s)
- **L_c** loading of solute (kg/s)
- **S** source/sink term (kg/s)

The numerical methods for advection and diffusion in WQFLOW-2D are unconditionally stable, and even though the reactions between variables are treated explicitly, a solute should not be advected more than one element per timestep in order to ensure the conservation of mass and momentum. The term for diffusion represents approximately the effects of a number of physical processes such as turbulence and shear dispersion, which
cannot be properly resolved in a depth-averaged model. In WQFLOW-2D, diffusion may be treated in three ways:

- diffusion is neglected entirely;
- diffusion is calculated isotropically;
- diffusion may be resolved into longitudinal and tranverse components relative to the direction of the current flow, in which case the equations are solved using an iterative method (the pre-conditioned conjugate gradient approach).

The source terms for the model are provided by fluvial inflows and point source loadings such as wastewater discharges, and where a solute is discharged into a dry cell (where the depth of water is <0.01m) the loading is relocated to the nearest wet cell on a prescribed bearing. Further gains and losses to the model due to reversible reactions between water quality variables, biological activity and physical processes such as sedimentation are also included in the source/sink term.

4.3.2 Reaction Rates

The decay of organic materials and the nitrification of ammoniacal-nitrogen are expressed by first order kinetics, with the rate of change of a substance due to decay given by:

\[ \frac{dC}{dt} = -KC \quad (4.18) \]

where K is the reaction rate constant, typically expressed as a function of temperature derived from the Arrhenius equation that relates the energy required to initiate a reaction, the temperature and the rate constant:
where $K_0$ is the rate constant at $T^\circ C$; $K_{20}$ is the rate constant at $20^\circ C$; and $\alpha$ is the term controlling the dependence on temperature of the rate constant.

4.3.3 Salinity

Since salt can be treated as a conservative tracer, with temporal and spatial variation being solely due to advection and dispersion, salinity is used to ascertain the constants in the term for longitudinal dispersion in estuarine water quality modelling studies. A longitudinal variation of salinity and hence density can affect gravitational residual circulation, and although this cannot be properly represented by a depth-averaged model, the effects can be approximately mitigated by increasing the coefficients of diffusion. This means that the concentrations in some estuaries may be over-predicted. Salinity variations are also important when predicting the oxygen balance in an estuary, since there is an inverse relationship between the salinity and the amount of oxygen that can be held by the water.

4.3.4 Dissolved Oxygen

Dissolved oxygen is the most essential component of an aquatic ecosystem, since it controls the distribution of plant and animal life, flows of energy and nutrients, and is a surrogate variable indicating the health of a water body. The balance of oxygen in the model is governed by transport, dispersion, and interactions between variables by processes that provide a source of oxygen such as photosynthesis and atmospheric reaeration; and also those which consume oxygen such as the decay of organic material (biochemical oxygen demand); nitrification of ammonia and nitrite; respiration of algae; and sediment oxygen demand.
In WQFLOW-2D, the concentration of dissolved oxygen (DO mg/l) is given by Fox's equation, which expresses dissolved oxygen as a percentage of the maximum amount of oxygen that can be held in the water, known as the saturated concentration (DOS). DOS is a function of temperature (T°C) and salinity (S kg/m³):

$$DOS = 1.43 \left[ \left( 0.291 - 0.28097 + 0.060097T^2 - 0.00006327T^3 \right) + 0.607 \left( 0.1161 - 0.0039227 + 0.00006317T^2 \right)S \right]$$

(4.20)

Reaeration is the process of oxygen exchange from the atmosphere to a water body, and is modelled as the product of a rate constant \(K_{air}\) multiplied by the difference between the saturation concentration (DOS) and the actual dissolved oxygen concentration (DO):

$$\frac{dDO}{dt} = K_{air}(DOS - DO)$$

(4.21)

\(K_{air}\) is a function of the mixing conditions induced by water turbulence and wind, given by:

$$K_{air} = f_{air} \frac{b}{A}$$

(4.22)

where \(b\) is the width of the water surface; \(A\) is the cross-sectional area of flow; and \(f_{air}\) is a constant representing the speed at which a front of oxygen will move through depth, and has typical values between 0.03 - 0.1 m/hour. \(f_{air}\) is also a function of temperature:

$$f_{air}(\theta) = f_{air}(20) \beta^{(\theta-20)}$$

(4.23)

where \(\beta\) is the temperature adjustment factor which has a typical value of 1.024.
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Should modelled levels of dissolved oxygen fall below 5% saturation, anoxic conditions are assumed and oxygen must be obtained from other sources in the following sequence:

• nitrates are denitrified to provide oxygen for the decay of biochemical oxygen demand, and the nitrification of ammonia is halted;
• once the nitrates are depleted, bacteria begin to oxidise organic matter by the reduction of sulphates (anaerobic respiration) which produces hydrogen sulphide.

The concentration of dissolved oxygen is calculated from:

\[
\frac{\partial}{\partial t} (d \text{DO}) + \frac{\partial}{\partial x} (du \text{DO}) + \frac{\partial}{\partial y} (dv \text{DO}) = \frac{\partial}{\partial s} (dD_O \frac{\partial \text{DO}}{\partial s}) + \frac{\partial}{\partial n} (dD_n \frac{\partial \text{DO}}{\partial n}) - H_1(\text{DO})K_B d
\]

\[
-3.43H_1(\text{DO})K_AM d - 1.14H_2(\text{DO})K_NO2 NO2 d + K_A DOD d + F_{DO} - \frac{L_{DO}}{A S^2} + PP
\]

(4.24)

where:

- \(H_2(\text{DO})\) controls the consumption of dissolved oxygen during the oxidation of carbonaceous material, and equals 1 if either \(\text{DO} \geq 5\%\), or if \(\text{DO} <5\%\) and Oxidised Nitrogen (ON) \(\neq 0\). Otherwise the value is 0.
- \(B\) the concentration of BOD (kg/m²) (see Section 4.3.5)
- \(K_B\) is the oxidation rate for BOD (see Section 4.3.5)
- \(H_1(\text{DO})\) controls the consumption of dissolved oxygen during the oxidation of ammonia to nitrate
- \(AM\) is the concentration of ammonia nitrogen (see Section 4.3.7)
- \(K_AM\) is the nitrification rate constant for ammonia (see Section 4.3.7)
- \(NO2\) the concentration of nitrite (see Section 4.3.7)
- \(K_NO2\) is the oxidation rate constant for nitrite (see Section 4.3.7)
- \(K_ADOD\) reaeration through the water surface, where DOD is the deficit of dissolved oxygen
- \(PP\) the net production of oxygen by algae
4.3.5 Biochemical Oxygen Demand

Biochemical oxygen demand (BOD) is a measure of the quantity of dissolved oxygen consumed as aquatic micro-organisms decompose organic matter. It is usually expressed as the amount of oxygen consumed by the decay of the material over 5 days (BOD₅), due to the lengthy measurement period required to obtain the amount of oxygen that would be consumed if the material decays completely, termed the ultimate BOD (BODₜ). The higher the level of BOD the quicker the depletion of oxygen, and this can be caused by elevated levels of organic pollution from, for example, sewage discharges; and by high nitrate levels which trigger accelerated plant growth. In the event of complete depletion of oxygen, BOD will continue to decay by the denitrification of nitrates and the reduction of sulphates.

Different types of organic material are metabolised at different decay rates depending, in the case of wastewater, on the amount of treatment prior to discharge. Empirical experiments have shown that this can be simplified by using either a fast or a slow rate. In WQFLOW-2D, BOD is associated with carbonaceous organic material only, and is divided into dissolved and particulate forms both represented by first order kinetics:

\[
\frac{dB}{dt} = -KB \tag{4.25}
\]

Particulate BOD settles in proportion to the amount of suspended solids settling to the bed, and continues to decay exerting oxygen demand on the overlying water, termed sediment oxygen demand (SOD). Although the input and output of BOD to the model is in terms of BOD₅, the model actually calculates the ultimate oxygen demand (BODₜ), and is related to BOD₅ by:
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\[
BOD_n = \frac{BOD_f}{\left[1 - \left((1 - p)\exp(-k_f) + p \exp(-k_s)\right)\right]} \tag{4.26}
\]

where \( p \) is the proportion of "slow" BOD, and \( k_f, k_s \) are the fast and slow reaction rates respectively. Crude and primary treated sewage effluents are assumed to be all fast (\( p=0 \)) because of readily decomposable organic material and the settling of sewage particles, whilst secondary treated effluent is assumed to be half fast and half slow. The value of \( p \) for industrial effluents is process specific and generally requires determination from a series of laboratory experiments. The equation governing the conservation of BOD is:

\[
\frac{\partial}{\partial t} (d B ) + \frac{\partial}{\partial x} (d u B ) + \frac{\partial}{\partial y} (d v B ) = \frac{\partial}{\partial s} \left( dD_s \frac{\partial B}{\partial s} \right) + \frac{\partial}{\partial n} \left( dD_n \frac{\partial B}{\partial n} \right) - K_b B d - F_i - \frac{L_b}{\Delta s^2} + \frac{S}{\Delta s^2} \tag{4.27}
\]

The output variable TOTAL BOD is the sum of fast and slow, dissolved and suspended particulate BOD.

4.3.6 Suspended Solids

In WQFLOW-2D, suspended solids (also termed 'mud') represent cohesive sediment particles with a mean diameter of less than 60\( \mu \)m, which enter the modelled system via open boundaries or through point source inputs. Transport between model elements is facilitated in the same way as dissolved substances, and particles may also settle to the bottom of an element as a bed load, which can subsequently be eroded and resuspended. The depth-averaged nature of the model excludes vertical variation of sediment concentrations; therefore, mass settling and deposition occur by:

\[
\frac{dm}{dt} = wc \tag{4.28}
\]

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where \( m \) is the mass of solid per unit area; \( w \) is the settling velocity (m/s); and \( c \) is the concentration. The model assumes that near bed sediment concentrations are double the depth-averaged concentrations, and deposition can occur only if the shear stress at the bed \( (\tau_b) \) is less than some critical deposition stress \( (\tau_d) \) usually less than 0.1 N/m\(^2\). The bed shear stress is calculated as a function of velocity:

\[
\tau_b = \frac{f_{\text{bed}} \frac{|u|}{g}}{\rho} \quad (4.29)
\]

where \( f_{\text{bed}} \) is the overall friction factor and \( \rho \) is the density of water. If the bed stress exceeds a critical erosion stress \( (\tau_e) \) typically 0.2 - 0.7 N/m\(^2\) then resuspension occurs at a rate of erosion given by:

\[
\frac{dm}{dt} = M_e (\tau_b - \tau_e) \quad \text{for } \tau_b > \tau_e \quad (4.30)
\]

where \( M_e \) is the erosion rate constant (kg/N/s) \( \sim 0.001 \) kg/N/S, indicating the hardness of the bed. Note that the erosion rate is proportional to excess stress above the critical stress and not to the stress itself, and deposition and erosion processes will vary with time and between elements depending on the local instantaneous velocity.

### 4.3.7 Nitrogenous Compounds

The nitrogen cycle in natural waters consists of the processes of nitrogen fixation, ammonification (hydrolysis), nitrification and denitrification, which control the conversions between organic nitrogen, ammoniacal nitrogen, and oxidised nitrogen (nitrates and nitrites). This section describes how nitrogen is included in WQFLOW-2D.
Organic Nitrogen

Nitrogen from the atmosphere is incorporated, either directly or via ammonia, into protein and other organic nitrogen compounds by the process of nitrogen fixation, which is carried out by micro-organisms such as bacteria and blue-green algae. The organic nitrogen compounds are subsequently converted by bacteria into ammonium compounds by the process of hydrolysis, which is modelled as a first order decay process with both "fast" and "slow" rates in the same way and relative proportions as for BOD. The equation governing the conservation of organic nitrogen is:

\[
\frac{\partial}{\partial t} (dN) + \frac{\partial}{\partial x} (duN) + \frac{\partial}{\partial y} (dvN) = \frac{\partial}{\partial s} (dD_{s} \frac{\partial N}{\partial s}) + \frac{\partial}{\partial n} (dD_{n} \frac{\partial N}{\partial n}) - K_{n} N d - F_{s} \frac{L_{x}}{\Delta s^{3}} + \frac{S}{\Delta s^{2}} \tag{4.31}
\]

where \( N \) is the concentration of organic nitrogen, and \( K_{n} \) is the hydrolysis rate constant.

Ammoniacal Nitrogen

Ammoniacal nitrogen can be formed by the decomposition of organic nitrogen, but mainly enters the aquatic environment through direct loadings from industrial or domestic discharges. It exists in water as either ammonium ions (\( \text{NH}_{4}^{+} \)) or as unionized ammonia (\( \text{NH}_{3} \)) which are related by:

\[
\text{NH}_{3} + \text{H}_{2} \text{O} = \text{NH}_{4}^{+} + \text{OH}^{-} \tag{4.32}
\]

This equilibrium relationship is governed primarily by pH and to a lesser extent by temperature, and although the innocuous ammonium ion is predominant in most natural waters, conditions of high pH and temperature can cause a shift towards the unionized form which is toxic to fish at very low concentrations.
Ammoniacal nitrogen undergoes a series of oxidation reactions to form nitrites and nitrates, which are modelled as a first order decay processes with a rate constant dependent on temperature:

\[ K_\theta = K_{30} (1 + \frac{aN}{100})^{1/20}, \quad (4.33) \]

where aN is a temperature dependence factor for the reduction of nitrogen. The equation governing the conservation of ammonical nitrogen is:

\[
\frac{\partial}{\partial t} (dAM) + \frac{\partial}{\partial x} (duAM) + \frac{\partial}{\partial y} (dvAM) = \frac{\partial}{\partial s} (dD_I \frac{\partial AM}{\partial s}) + \frac{\partial}{\partial n} (dD_n \frac{\partial AM}{\partial n}) - H_1(DO) K_{\text{AM}} AM d + K_s + F_{\text{AM}} + \frac{L_{\text{AM}}}{\Delta s^2} + \frac{S}{\Delta s^2}, \quad (4.34)
\]

where \( H_1(DO) = 1 \) if \( DO > 5\% \) saturation, and \( H_1(DO) = 0 \) if \( DO < 5\% \) saturation.

**Oxidised Nitrogen**

Oxidised nitrogen refers to nitrites (\( \text{NO}_2^- \)) and nitrates (\( \text{NO}_3^- \)), which are formed by the nitrification (oxidation) of ammoniacal nitrogen via a two stage process where the ammonium ion is initially converted to nitrite by \textit{Nitrosomonas} bacteria:

\[ NH_4^+ + 1.5O_2 \rightarrow 2H^+ + H_2O + NO_2^- \quad (4.35) \]

and secondly, nitrite is oxidised to nitrate by \textit{Nitrobacter} bacteria:

\[ NO_2^- + 0.5O_2 \rightarrow NO_3^- \quad (4.36) \]

Combining these two equations gives:
\[ NH_4^+ + 2O_2 \rightarrow 2H^+ + H_2O + NO_3^- \]  

(4.37)

The first stage (ammonium to nitrite) is slower than the second (nitrite to nitrate), and consequently requires more oxygen, and this is shown by the mathematics underlying chemistry (stoichiometry). Of the 4.57 gOgN\(^{-1}\) of oxygen that is consumed per unit mass of nitrogen oxidised in the total process (\(2 \times \frac{32}{14} = 4.57\)), 3.43 gOgN\(^{-1}\) is used to form nitrite, and 1.14 gOgN\(^{-1}\) to form nitrate. The cofactors which are important for nitrification are the presence of sufficient nitrifying bacteria; alkaline pH levels of optimal value 8; and oxygen levels greater than 1 – 2 mg/l.

In WQFLO\(W\)-2D, should the concentration of dissolved oxygen fall below 5% saturation, oxidised nitrogen undergoes denitrification to produce oxygen so that the oxidation of carbonaceous organic matter (BOD) can continue. The nitrogen exits the model as nitrogen gas and the equations are as follows:

\[ 2NO_2^- + 2H^+ \rightarrow N_2 + H_2O + 0.5O_2 \]  

(4.38)

\[ 2NO_3^- + 2H^+ \rightarrow N_2 + H_2O + 2.5O_2 \]  

(4.39)

By stoichiometry, it is shown that 0.35g of nitrate will produce 1g of oxygen (\(2 \times \frac{14}{2.5} \times \frac{32}{2} = 0.35\)), and for nitrite 1g of oxygen is produced for every 0.58g consumed. Should all the oxidised nitrogen be consumed, the reduction of sulphates occurs. The equations used to calculate the concentrations of nitrite and nitrate are:

\[
\frac{\partial}{\partial t}(dNO_2) + \frac{\partial}{\partial x}(duNO_2) + \frac{\partial}{\partial y}(dvNO_2) = \frac{\partial}{\partial s}(dD_s \frac{\partial NO_2}{\partial s}) + \frac{\partial}{\partial n}(dD_n \frac{\partial NO_2}{\partial n}) \\
+ H_1(DO) K_{AM} AMd - 0.58 H_1 K_B Bd - H_1(DO) K_{NO2} NO_2 d + F_{NO2} + \frac{L_{NO2}}{\Delta s^2} + \frac{S}{\Delta s^2} 
\]  

(4.40)

and

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\[ \frac{\partial}{\partial t} (d\text{NO}_3) + \frac{\partial}{\partial x} (d\text{uNO}_3) + \frac{\partial}{\partial y} (d\text{vNO}_3) = \frac{\partial}{\partial s} (d\text{D}_s \frac{\partial \text{NO}_3}{\partial s}) + \frac{\partial}{\partial n} (d\text{D}_n \frac{\partial \text{NO}_3}{\partial n}) \]

\[ + H_1(\text{DO}) K_{\text{NO}_2} \text{NO}_2 d - 0.35 H_3 K_0 B d + F_{\text{NO}_3} + \frac{L_{\text{NO}_3}}{\Delta s^2} + \frac{S}{\Delta s^2} - \text{PP}_{\text{NO}_3} \]  

(4.41)

where NO3 is the concentration of nitrate, PP \text{NO}_3 represents uptake of nitrate by algae, H_3 = 1 if DO <5% and ON >0. Otherwise H_3 = 0.

### 4.3.8 Phosphorus

Phosphorus is present in aquatic systems in several forms; the most important being dissolved available inorganic phosphorous (DAIP) in the form of orthophosphate, which is the most readily available form for uptake by algae and plants during the process of primary productivity.

Importantly, phosphorus can be adsorbed onto the surface of either suspended or deposited sediment particles, and this mechanism is regulated by a number of factors including pH, the binding capacity of the sediment, and the redox potential (a measure, in volts, of the affinity of a substance for electrons compared with hydrogen). However, this form of phosphorus cannot be easily utilised by algae and plants, and in WQFLOW-2D this process is not simulated, so phosphorus is used to influence of primary productivity only. The process controlling the biological uptake and release of phosphate is described below in Section 4.3.10.

### 4.3.9 Silicon

Silicon may be considered a minor nutrient compared with nitrogen and phosphorus, and is most readily available for biological uptake as soluble orthosilic acid, measured in terms of its equivalent silica (SiO_2) concentration. The main sources of silicon to the aquatic
environment are from the breakdown of silicate polymers originating from soil runoff, and the decay of dead diatom phytoplankton which use the dissolved reactive form (mainly as Si(OH)$_4$) to build cell walls. It is only when such species are dominant that silicon becomes a limiting nutrient.

In WQFLOW-2D, silica is modelled as a dissolved substance, the uptake of which is controlled by the silica to carbon ratio which is species dependent (see Section 4.3.10).

4.3.10 Primary Productivity

Primary productivity is defined as the amount of organic material synthesised by plants and phytoplankton (algae) from inorganic salts (primarily phosphate and nitrate) over time via the process of photosynthesis; where plants convert carbon dioxide (CO$_2$) into carbohydrates (C$_6$H$_{12}$O$_6$) using energy from sunlight, with the production of oxygen (O$_2$) as a by-product:

$$\begin{align*}
6\text{CO}_2 + 6\text{H}_2\text{O} &\xrightarrow{\text{photosynthesis}} C_6\text{H}_{12}\text{O}_6 + 6\text{O}_2 \\
\text{respiration} &\xrightarrow{} C_6\text{H}_{12}\text{O}_6 + 6\text{O}_2 
\end{align*}$$ 4.42

The reverse of photosynthesis is termed respiration: a process where algal carbon is depleted, resulting in the release of carbon dioxide and the death of algae which form detritus, the decay of which leads to the return of nutrients to the dissolved phase. The processes of photosynthesis and respiration are important in a water quality model since they affect the balance of oxygen and provide sources and sinks for nitrogenous and phosphate compounds. The quality of a body of water can be greatly reduced by excessive plant growth, and certain types of phytoplankton are toxic.
In WQFLOW-2D, nitrogen and phosphorus are the most likely nutrients to limit algal growth, whereas silicon is important for the growth of diatoms, and inorganic carbon is usually available in excess and not considered in the model. Algae are represented by algal carbon (the proportion of carbon in the algal biomass, dry weight), with inputs and outputs in terms of chlorophyll-a, which is converted to algal carbon by the chlorophyll to carbon ratio. In reality, the amount of carbon in the form of chlorophyll-a depends on the species of phytoplankton, but is denoted in WQFLOW-2D by a single representative species.

The rate of growth of algae depends on the presence of sufficient sunlight and nutrients, and the maximum rate is expressed as an exponential function of temperature:

\[
rate = \exp[2.303(mT + c)]
\]

(4.43)

where \(m\) and \(c\) are constants that depend on the species being modelled, and \(T\) is the temperature (°C). Two sets of rate constants can be input to the model, which determine the shape of the relationship of the rate of above and below the optimal temperature.

There is an optimum light intensity at which maximum primary productivity occurs for a particular species. The model calculates the light induced growth limitation factor from an equation derived from:

\[
\mu_{light} = \frac{I \exp(1 - I/I_{max})}{I_{max}}
\]

(4.44)

where \(\mu_{light}\) is the light limitation factor at depth \(z\) below the surface, \(I_{max}\) is a constant light intensity that will produce maximum productivity (i.e. \(\mu_{light} = 1\)), and \(I\) is the light intensity at depth \(z\), which varies with time and is given by the Beer-Lambert law:
where $I_0$ is the light intensity at the surface, $k$ is the light attenuation factor which is a function of the suspended solids (SS) and algal carbon (AC) concentrations given by:

$$k = k_1 (0.025SS + 0.04) + k_2 AC$$

where $k_1$ is the extinction coefficient relating to the suspended solids, and $k_2$ is the extinction coefficient relating to algal carbon.

The light intensity is input to the model as the ratio $I/I_{\text{max}}$, and the equation for light limitation is integrated over the depth to give an average value for the whole water column. It is clear that primary productivity will be limited by light when $I \neq I_{\text{max}}$.

The effects of nutrients on growth are described by Michaelis-Menten relationships, which were originally referred to as “Monod Kinetics” (Monod, 1949), where growth is dependent upon nutrient availability at low nutrient concentrations but is independent of nutrients at high concentrations. Liebig’s “law of the minimum” (Odum, 1971) indicates that growth is determined by the nutrient in least supply, and the limitation factor for each nutrient is determined by a saturation curve given by a Michaelis-Menten equation:

$$\mu_{\text{nutrient}} = \frac{C_{\text{nutrient}}}{k_{\text{nutrient}} + C_{\text{nutrient}}}$$

where $C_{\text{nutrient}}$ is the concentration of the nutrient source, and $k_{\text{nutrient}}$ is the half saturation constant which corresponds to the concentration of nutrient that would produce half the maximum a 50% growth rate. A low half-saturation constant means that the nutrient is only limiting at very low concentrations, and a high value means that primary production
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will only be unlimited at very high concentrations.

The total growth rate (P) is given by:

\[ P = P_{\text{max}} \cdot \text{light} \cdot \min(\mu_{\text{nitrate}}, \mu_{\text{phosphate}}, \mu_{\text{silicate}}) \] (4.48)

where \( P_{\text{max}} \) is the maximum rate, and it is clear that primary production occurs at the rate determined by the most limiting nutrient. Further, the amount of nutrient assimilated by the algae depends on the proportion of the nutrient in the plant cells, and is expressed as the ratio of the nutrient to carbon in the cell, which varies with species. Thus the total amount of nutrient taken up is equal to the algal carbon produced multiplied by the ratio of nutrient to carbon in the cell, and the increase in algal carbon is given directly by the net production rate. The amount of oxygen released by photosynthesis is also calculated as a proportion of the carbon mass produced, so that 0.67g of oxygen are released for each gram of algal carbon produced.

As stated earlier, algal carbon and oxygen are consumed during algal respiration, the rate of which is a function of temperature:

\[ R_0 = R_{20} \cdot Q_{10}^{(20-0)/10} \] (4.49)

where \( R_0 \) is the respiration rate constant at 0°C, \( R_{20} \) is the respiration rate constant at 20°C, and \( Q_{10} \) is a parameter that controls the temperature dependency of respiration and corresponds to a doubling of the rate for a 10°C rise in temperature.

Algal carbon is also depleted by mortality, which in reality can be due to several processes such as grazing by zooplankton or the natural death of the algae, both of which vary with
time, nutrient supply, and other environmental factors. To avoid the complexities required for the accurate modelling of algae mortality, the loss processes have been simplified in WQFLOW-2D by a single first order decay constant of mortality.

The detrital carbon, which is the product of algal carbon mortality, decays further to return nutrients back into the dissolved phase, and this is also modelled as a first order process: nitrogen converts to slow decaying organic nitrogen; phosphorous converts to orthophosphate; and silicon converts to silica. Detritus also settles at a fixed settling velocity, and once deposited on the bed it continues to decay releasing nutrients to the water column.

4.3.11 Coliforms

Bacteria are represented in WQFLOW-2D as an independent variable that is controlled by a first order decay rate constant (k/day), and does not interact with any other variable. This decay rate, commonly expressed as \( T_{90} \) (hours), is defined as the time taken for a bacterial population to reduce to 10% of its original density, and is calculated by the expression (Chapra, 1997):

\[
T_{90} = \frac{2.3025}{k}
\]  

(4.50)

Coliform concentrations are calculated by:

\[
\frac{\partial}{\partial t} (d \cdot CF) + \frac{\partial}{\partial x} (d \cdot CF) + \frac{\partial}{\partial y} (d \cdot CF) = \frac{\partial}{\partial s} (dD, \frac{\partial CF}{\partial s}) + \frac{\partial}{\partial n} (dD_n, \frac{\partial CF}{\partial n}) - kCFd - \frac{L_e}{\Delta s} + \frac{S}{\Delta s'}
\]

(4.51)

where CF is the concentration of coliforms.
Chapter 5

Calibration and Validation of TELEMAC-2D

5.1 Introduction

This chapter describes the calibration and validation of TELEMAC-2D for the hydrodynamics of the Patos Lagoon and Estuary. The various steps that constitute this process can be divided into four main procedures:

- generating the mesh and defining the boundary conditions;
- sensitivity analysis of the forcing parameters of river flow, wind influence, and free surface elevation;
- calibration of the source terms such as bed and surface friction to obtain an optimal agreement between the model output and an observed set of data;
- validation against further observations to establish the model's robustness.

The locations of the rivers and water level recording sites are presented in Figure 5.1 which is an image of the Patos Lagoon taken by a Multi-angle Imaging SpectroRadiometer aboard the “Terra” Satellite on 27th December, 2001 (NASA/GSFC/LaRC/JPL, MISR Team).
5.2 Generation of the Mesh

The discretisation of space within the domain of the model depends principally on the density of the available soundings. The ideal situation might be uniformly spaced soundings; the corresponding ideal mesh would have nodes coincident with those soundings. In the real world, soundings are not uniformly spaced, but it still appears sensible to design a mesh in which the number of nodes is roughly equal to the number of soundings. A rule of thumb, which ensures neither over- nor under-resolution is that:

\[
\frac{1}{2} < \frac{\text{no. of nodes}}{\text{no. of soundings}} < 2
\]  

(5.1)

The bathymetry and coastline of the Patos lagoon and estuary used for this study originated from the following Brazilian nautical charts:
In addition, the bathymetry for Saco da Mangueira was obtained from an historical chart (Antiga2) of soundings collected between 1882 and 1975. All charts were digitised by the Federal University of Rio Grande (FURG), and supplied in ASCII format. The digitised information was subsequently converted from spherical co-ordinates to the Universal Transverse Mercator (UTM, 1983) co-ordinate system for Zone 22 South, using the co-ordinate calculator within the Trimble HYDROpro™ Navigation software. UTM is a coordinate system where the globe is subdivided into narrow longitude zones, which are projected onto a Transverse Mercator projection, onto which a grid is constructed and used to locate points.

Viewing these data revealed that the lagoon and estuarine area could be roughly divided into five sub-domains based on the density of soundings, which ranged from coarsely aspaced in the main body of the lagoon (0.1 soundings/km²) to densely spaced in the navigation channel (15 soundings/km²). The average spacing between soundings was calculated from the total area of each sub-domain divided by the total number of soundings within each sub-domain. The total area was found from the literature or measured directly from a Geographical Information System (GIS) constructed for this study. The range of inter-node distances for each sub-domain was then calculated and this information is summarised below in Table 5.1.
Chapter 5 - Calibration and Validation of TELEMAC-2D

The target inter-node distances are identified in bold type in Table 5.1. Since the main body of the lagoon was not the focus of the modelling study but would be used to provide inputs to the southern part of the Patos system, a value close to the maximum distance of 6000m between nodes was considered appropriate. For the Guaiba river, estuarine and navigation channel areas, a more refined grid was required; therefore target inter-node distances would need to be closer to the mean value. Finally, the maximum resolution of around 200m was selected for Saco da Mangueira; the area of focus for the water quality studies.

<table>
<thead>
<tr>
<th>Sub-Domain</th>
<th>Brazilian Chart No.</th>
<th>Area (km$^2$)</th>
<th>No. of Soundings</th>
<th>Density of Soundings (per km$^2$)</th>
<th>Mean Spacing (m)</th>
<th>Target Inter-Node Range (m) (Target Distance in bold)</th>
<th>Mesh 12 Typical Inter-Node Distance (m)</th>
<th>Mesh 21 Typical Inter-Node Distance (m)</th>
<th>Source for Sub-Domain Area Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lagoon</td>
<td>2140</td>
<td>9330</td>
<td>1024</td>
<td>0.1</td>
<td>3018</td>
<td>1500, 3000, 6000</td>
<td>5500, 5500</td>
<td>Knoppers &amp; Kjerfve, 1999</td>
<td></td>
</tr>
<tr>
<td>Guaiba River</td>
<td>2140</td>
<td>450</td>
<td>90</td>
<td>0.2</td>
<td>2236</td>
<td>1100, 2200, 4400</td>
<td>2200, 2200</td>
<td>GIS</td>
<td></td>
</tr>
<tr>
<td>Upper Estuary</td>
<td>2101, 2102, 2103, 2106, 2112</td>
<td>1030</td>
<td>5010</td>
<td>4.9</td>
<td>453</td>
<td>250, 500, 1000</td>
<td>750, 1000</td>
<td>GIS</td>
<td></td>
</tr>
<tr>
<td>Navigation Channel</td>
<td>2101, 2102, 2103, 2106, 2112</td>
<td>85</td>
<td>1283</td>
<td>15.1</td>
<td>257</td>
<td>125, 250, 500</td>
<td>500, 350</td>
<td>GIS</td>
<td></td>
</tr>
<tr>
<td>Saco da Mangueira</td>
<td>Antiga2</td>
<td>21.7</td>
<td>156</td>
<td>7.2</td>
<td>373</td>
<td>200, 400, 800</td>
<td>N/A, 250</td>
<td>GIS</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.1  Bathymetric Information Used to Construct the Mesh

These values formed the basis for creating meshes using MATISSE, which is TELEMAC's module for generating an unstructured grid of finite elements. MATISSE automatically produces the mesh from the coastline, but also allows the user to adapt the grid both manually and automatically to enable the required bathymetric representation. Typical inter-node distances for each region were obtained from the resultant mesh and compared with target values.
A secondary requirement, at least of the initial mesh was for the total number of nodes and triangles to be not significantly greater than those of the high resolution TELEMAC mesh of the same domain created by Fernandes (2001), which consisted of 2643 nodes and 4860 triangles.

Initial model sensitivity tests were conducted using a mesh with 3600 nodes 6703 triangles (Mesh 12), which used the bathymetry for the lagoon and estuary, but excluded the shallow embayments in the estuary. This mesh is shown below in Figure 5.2.

Following the first fieldwork campaign in October 2002, and the provision of soundings for the shallow embayments in the estuary, a process of iteration led to a final mesh (Mesh 21) which consisted of 3705 nodes and 6672 triangles. This is presented in Figure 5.3, and
also in Figure 5.4, which shows contours of the average length of each element. From Table 5.1, the typical inter-node distances achieved for Mesh 21 were within the target range and close to the required values, and therefore the mesh was considered suitable to use for the model calibration. The availability of increased computational power justified the greater number of nodes and triangles when compared with Fernandes (2001).

The final stage in creating the mesh was to define the boundary conditions. The flows into and out of the system were described in Chapter 2, and of these, the principal inputs for the model were considered to be represented by four open boundaries: the rivers Jacui and Taquari which account for 85% of the flow input at Guaiba at the northern extremity (average flow 1500m$^3$/s); the Camaquã River which is situated close to central region of the lagoon (300m$^3$/s); the São Gonçalo Channel entering the Patos Estuary from the west (600m$^3$/s); and the ocean boundary at the southern extremity. The three freshwater boundaries (Guaiba River, Camaquã River, and the São Gonçalo Channel) were defined by prescribed velocity ($U$, $V$) and fixed elevation ($\zeta$), whereas the ocean boundary at Praticagem was defined by prescribed elevation and free velocity. The mean monthly river flows for 1999 are presented in Table 5.2.

<table>
<thead>
<tr>
<th>Month</th>
<th>Guaiba River (Jacui + Taquari) (m$^3$/s)</th>
<th>Camaquã River (m$^3$/s)</th>
<th>São Gonçalo Channel (m$^3$/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>April</td>
<td>1074</td>
<td>243</td>
<td>457</td>
</tr>
<tr>
<td>May</td>
<td>611</td>
<td>159</td>
<td>260</td>
</tr>
<tr>
<td>June</td>
<td>2255</td>
<td>458</td>
<td>958</td>
</tr>
<tr>
<td>July</td>
<td>2469</td>
<td>497</td>
<td>1050</td>
</tr>
<tr>
<td>August</td>
<td>1257</td>
<td>277</td>
<td>534</td>
</tr>
<tr>
<td>September</td>
<td>1735</td>
<td>364</td>
<td>737</td>
</tr>
<tr>
<td>October</td>
<td>2148</td>
<td>439</td>
<td>913</td>
</tr>
</tbody>
</table>

Table 5.2 Mean Monthly River Flows in 1999
Figure 5.3  Space Discretisation for the Final Mesh

Figure 5.4  Average Element Length for Final Mesh
5.3 Sensitivity Analysis of the Forcing Parameters

A set of 30 initial simulations was designed to investigate the sensitivity of the system to variations in the forcing parameters of tidal elevation, river flow and wind. For each simulation the model was set-up using Mesh 12 with two liquid boundaries, and run for 72 hours. The parameters used for the set-up are summarised in Table 5.3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Boundaries</td>
<td>10,000 m³/s; 3162 m³/s; 1000 m³/s; 0.3 m; 0.3 m S²</td>
</tr>
<tr>
<td>Time Step (s)</td>
<td>60</td>
</tr>
<tr>
<td>Number of Time Steps</td>
<td>4320</td>
</tr>
<tr>
<td>Coriolis Coefficient (rad/s)</td>
<td>-7.73 x 10⁻³</td>
</tr>
<tr>
<td>Wind Velocity Along X and Y</td>
<td>0; 3.54 (5 m/s SW); 7.07 (10 m/s SW); -3.54 (5 m/s NE); -7.07 (10 m/s NE)</td>
</tr>
<tr>
<td>Coefficient of Wind Influence</td>
<td>7.30 x 10⁻³ (5 m/s); 1.61 x 10⁻⁶ (10 m/s)</td>
</tr>
<tr>
<td>Air Pressure</td>
<td>NO</td>
</tr>
<tr>
<td>Law of Bottom Friction</td>
<td>5 (Nikuradse's Law)</td>
</tr>
<tr>
<td>Friction Coefficient</td>
<td>0.01</td>
</tr>
<tr>
<td>Velocity Diffusivity (m²/s)</td>
<td>10</td>
</tr>
<tr>
<td>Tidal Flats</td>
<td>Option 1 - Submerged/exposed areas are detected and the free surface gradient is corrected</td>
</tr>
<tr>
<td>Type of Advection</td>
<td>Option 1 - U+V - method of characteristics, Option 5 - H - conservative scheme + SUPG</td>
</tr>
</tbody>
</table>

Table 5.3 Set-Up Parameters for the 3 Day Arbitrary Tests

Two tidal elevation scenarios were considered for forcing the model at the ocean boundary: a constant elevation of 0.3m, and an artificial semi-diurnal elevation with a range ζ(t) of 0.3m, which was calculated by:

\[
ζ(t) = 0.25 \times \cos \left( \frac{2\pi t}{43200} \right)
\]  

(5.2)

For each elevation scenario, three constant river flows of 10,000m³/s, 3162m³/s (logarithmically halfway between 0 and 10,000), and 1000m³/s were imposed at the northern boundary to represent conditions of high, medium and low flow respectively.
These six scenarios were modelled with five constant wind velocities of 0 m/s, 5 m/s SW, 10 m/s SW, 5 m/s NE, and 10 m/s NE. With reference to Chapter 4, the resistance of the wind is represented in TELEMAC-2D by the coefficient of wind influence, given by:

\[
\frac{\rho_{\text{air}}}{\rho} a_{\text{wind}}
\]  

(5.3)

where \( \rho_{\text{air}} = 1.29 \text{ kg/m}^3; \rho = 1000 \text{ kg/m}^3 \)

and \( a_{\text{wind}} = (-0.12 + 0.137 \times W) \times 10^{-3} \) (for \( 5 < W < 19.22 \text{ m/s} \))

This is the ratio of air and water densities multiplied by a wind-resistance coefficient \( a_{\text{wind}} \), which is calculated from the formula used by the former Institute of Oceanographic Sciences (United Kingdom). The coefficient of wind influence was calculated for winds \( W \) of 5 and 10 m/s.

The values chosen for the remaining set-up parameters for these tests were based on the work of Fernandes (2001).

### 5.3.1 Response of the Modelled System to Free Surface Elevation

The results for simulations forced by a constant tidal elevation were compared with those for the small semi-diurnal tide, and showed a very similar overall pattern. This demonstrated the diminutive importance of tides on the barotropic circulation, compared to wind and river flow, which concurs with previous studies conducted by, for example, Möller (1994) and Möller & Castaing (1996).
A rough calculation was performed to check whether the model was correctly responding to tidal forcing, by finding the rate of rise $\frac{d\zeta}{dt}$, given the surface area of the lagoon $S$ and the rate of inflow $Q$, with the assumption that no water escapes to the sea:

\[
\text{In a time } \Delta t, \\
\text{inflow} = Q \Delta t \\ = Q \Delta \zeta \\
\text{therefore,} \\
\frac{\Delta \zeta}{\Delta t} = \frac{d\zeta}{dt} = \frac{Q}{S} \\
(5.4)
\]

Let, $Q = 10^4$ m$^3$/s and $S = 10^4$ km$^2$
therefore,
\[
\zeta = 1.0 \times 10^{-6} \text{ m/s} \\
= 8.6 \times 10^{-2} \text{ m/d} \\
= 86.4 \text{ mm/d}
\]
so in 3 days, rise $\Delta \zeta = 0.26 \text{ m}$

Modelled output:
\[
\zeta \text{ at 72 hr at Itapua} = 0.446 \text{ m} \\
\Delta \zeta = 0.15 \text{ m}
\]

Comparison of the expected change in elevation after 3 days against the modelled change in elevation from this calculation shows the results to be in the right order to accept the models treatment of the tide.

### 5.3.2 Response of the Modelled System to Wind and River Flow

Figures 5.5a-c illustrate the model output over the entire domain for free surface elevation at $T = 72$ h for the 15 simulations forced by a constant elevation at the mouth. The
response of the modelled system to forcing by wind and river flow was evaluated in terms of the free surface differential between two locations: Itapua at the northern end of the lagoon; and Feitoria at the tidal limit of the estuary. The differentials were computed at $T = 72\ h$ for each simulation, and are presented in Figure 5.6.

**Figure 5.5a**  Free Surface Elevation at $T = 72\ hrs$ Constant Elevation and $10,000\ m^3/s$ River Flow

**Figure 5.5b**  Free Surface Elevation at $T = 72\ hrs$ Constant Elevation and $3162\ m^3/s$ River Flow

**Figure 5.5c**  Free Surface Elevation at $T = 72\ hrs$ Constant Elevation and $1000\ m^3/s$ River Flow
The results presented in Figures 5.5 and 5.6 show the interaction of wind and river flow on the resultant free surface level of the system in 'quasi' steady state. A positive gradient is evident from Feitoria to Itapua, for all flows influenced by a SW wind, and a negative gradient for strong winds from the NE, i.e. water piling up downwind. Strong winds appear to be the dominant factor over low and medium river flows. These results are in agreement with the explanation given by Moller (1996) for the local wind dominating the circulation through a set-up/set-down mechanism of oscillation for the central and inner lagoon.

The effect of river flow in the absence of wind is also a positive gradient, which is notably higher for the maximum flow condition modelled. This could be explained by a funnel effect caused by water entering the lagoon having to pass through the narrow entrance at the mouth of the Guaiba River.
From the results of these arbitrary simulations, it was concluded that the model was responding reasonably to the forcing parameters, and was ready for further sensitivity tests.

5.4 Calibration of the Source Terms

The next stage in the calibration process was to investigate the sensitivity of the model to the parameters of friction, eddy viscosity, and Coriolis force, which are represented as source terms in TELEMAC. These parameters had previously been evaluated in detail by Fernandes (2001), with the indication that variations of both the eddy viscosity and the Coriolis force had little effect on the circulation of the lagoon. However, since the extents of the domain and the resolution of the mesh used for this study differed significantly from the work of Fernandes (2001), it was necessary to re-evaluate the sensitivity of the model to the principal source terms of bed and surface friction.

5.4.1 Sensitivity of the Model to Bed Friction

The sensitivity and initial calibration of the model to bed friction were investigated using coefficients defined by the laws of Chezy (C), Manning (n), and Nikuradse \((k_s)\). A range of model simulations were completed using the model set-up presented in Table 5.4. Tidal elevation and wind data measured at Praticagem for the period 6\(^{th}\) to 8\(^{th}\) August 1999 were used to force the model (Figure 5.7), and mean monthly river flows of 1257; 277; and 534 \(m^3/s\) for August 1999 (see Table 5.2) were input at the Guaiba; Camaquã; and São Gonçalo Channel boundaries respectively.
### Table 5.4  Model Set-Up for Bed Friction Sensitivity Tests

The mesh used for these simulations (Mesh 21) included the shallow embayments adjacent to the southern part of the estuary, and the narrow entrance to Saco da Mangueira was very finely resolved to 25m to allow flows to enter and exit smoothly. Due to the increased density of triangles in this area, it was necessary to reduce the timestep of the model from 60 to 20 seconds to avoid exceeding the maximum number of iterations for solving the propagation step.

![Figure 5.7 Observed Tidal Elevation and Wind at Praticagem 6th to 8th August 1999](image-url)
The model results of the effect of varying bed friction on the longitudinal velocity at Praticagem are presented as a time series in Figure 5.8. The magnitude of the velocity decreases with increasing magnitude of both Manning and Nikuradse friction coefficients, and conversely, decreases with decreasing Chezy coefficients; as would be expected from the formulation of these laws. These observations are consistent with the work of Fernandes (2001 and 2002).

In order to quantify the variability of the bed friction, the model results were compared with observed longitudinal velocities for the same location and time period. The current velocity observations have been described in Chapter 3, and consisted of a pair of current meters moored at 3m and 10m below surface. The observations presented here are for depth-averaged values that coincide with the depth averaged output of the model. Two measures of data correlation were calculated: $R^2$; and the predictable variance (p.v.), which is the proportion of the observations the model is able to predict, given as a percentage:

$$\frac{\text{Var}_{\text{Obs}} - \text{Var}_{\text{Obs-Mod}}}{\text{Var}_{\text{Obs}}}$$ (5.5)

In later simulations, the model results were also compared with free surface elevation measurements for locations throughout the lagoon. Since these measurements were not corrected to a single datum it was necessary to adjust the measured data. This was achieved by subtracting the mean of the model predictions from the mean of the observations and then subtracting this value from each of the observations. The formula for p.v. thus became:

$$\frac{\text{Var}_{\text{AdjObs}} - \text{Var}_{\text{AdjObs-Mod}}}{\text{Var}_{\text{AdjObs}}}$$ (5.6)

where,
$\text{Var}_{\text{AdjObs}} = \text{Variance of the adjusted observations} = \text{Variance ((Observed minus (Mean Observed minus Mean Modelled))}$

The values of $R^2$ and p.v. for each of the modelled scenarios are presented in Table 5.5, together with the various coefficients in order of increasing friction. The optimal agreements between model output and observations were produced with Manning coefficients of 0.01 and 0.015 (p.v. = 85.55% and 80.90% respectively), and a Nikuradse coefficient of 0.001 (p.v. = 80.53%). The Chezy coefficient of 80 (p.v. = 80.36%) also gave very good agreement. This can be compared to the results of Fernandes (2001) which showed the best correlations obtained using the Manning coefficient between 0.01 – 0.025; Chezy coefficient of 50 and Nikuradse coefficient of 0.008-0.01.

<table>
<thead>
<tr>
<th>Description</th>
<th>Chezy (C)</th>
<th>Manning (n)</th>
<th>Nikuradse (ks)</th>
<th>p.v. (%age)</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>least friction</td>
<td></td>
<td>0.01</td>
<td></td>
<td>85.55</td>
<td>0.83</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.015</td>
<td></td>
<td>80.90</td>
<td>0.83</td>
</tr>
<tr>
<td>clay/mud (deeper channels)</td>
<td>80</td>
<td></td>
<td></td>
<td>80.36</td>
<td>0.83</td>
</tr>
<tr>
<td>fine silt (deeper channels)</td>
<td></td>
<td>0.004</td>
<td></td>
<td>76.94</td>
<td>0.82</td>
</tr>
<tr>
<td>typical value for shelf seas</td>
<td></td>
<td>0.02</td>
<td></td>
<td>73.23</td>
<td>0.80</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60</td>
<td></td>
<td>72.17</td>
<td>0.81</td>
</tr>
<tr>
<td>coarse silt (main lagoon)</td>
<td></td>
<td>0.1</td>
<td></td>
<td>62.94</td>
<td>0.76</td>
</tr>
<tr>
<td>very fine sand (lagoon shallows)</td>
<td></td>
<td>0.13</td>
<td></td>
<td>61.20</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.25</td>
<td></td>
<td>66.14</td>
<td>0.78</td>
</tr>
<tr>
<td>fine/very fine sand (lagoon shallows)</td>
<td>40</td>
<td></td>
<td></td>
<td>57.88</td>
<td>0.76</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.025</td>
<td></td>
<td>57.30</td>
<td>0.73</td>
</tr>
<tr>
<td>medium/fine sand (lagoon shallows)</td>
<td></td>
<td>0.03</td>
<td></td>
<td>59.90</td>
<td>0.75</td>
</tr>
<tr>
<td>most friction</td>
<td></td>
<td>0.035</td>
<td></td>
<td>54.50</td>
<td>0.72</td>
</tr>
</tbody>
</table>

Table 5.5   Bed Friction Coefficients
Figure 5.8  Modelled Bed Friction for the Period 6\textsuperscript{th} to 8\textsuperscript{th} August 1999
The best results from these sensitivity tests provided a range of bed friction values for further 3 day simulations conducted for fine tuning. The coefficients used and results of these tests are summarised in Table 5.6. The best results were obtained using a Manning coefficient of 0.01 (p.v. = 85.55%), and a Nikuradse coefficient of 0.00005 (p.v. = 84.67%).

<table>
<thead>
<tr>
<th>Bed Friction Coefficient</th>
<th>p.v. (%)</th>
<th>R²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chezy = 75</td>
<td>78.77</td>
<td>0.83</td>
</tr>
<tr>
<td>Chezy = 80</td>
<td>80.36</td>
<td>0.83</td>
</tr>
<tr>
<td>Chezy = 85</td>
<td>81.71</td>
<td>0.83</td>
</tr>
<tr>
<td>Manning = 0.005</td>
<td>78.89</td>
<td>0.81</td>
</tr>
<tr>
<td>Manning = 0.01</td>
<td>85.55</td>
<td>0.83</td>
</tr>
<tr>
<td>Manning = 0.012</td>
<td>84.53</td>
<td>0.83</td>
</tr>
<tr>
<td>Manning = 0.014</td>
<td>82.27</td>
<td>0.83</td>
</tr>
<tr>
<td>Manning = 0.015</td>
<td>80.90</td>
<td>0.83</td>
</tr>
<tr>
<td>Nikuradse = 0.00005</td>
<td>84.67</td>
<td>0.83</td>
</tr>
<tr>
<td>Nikuradse = 0.0005</td>
<td>81.87</td>
<td>0.83</td>
</tr>
<tr>
<td>Nikuradse = 0.001</td>
<td>80.53</td>
<td>0.83</td>
</tr>
</tbody>
</table>

Table 5.6 Three Day Simulations Results for the Fine Tuning of Bed Friction

In order to test the model performance for these two coefficients over a longer simulation period, the model was run for 31 days from 21st July 1999 to 21st August 1999, with the set-up shown in Table 5.7. The tidal elevations and wind for this period used to force the model are presented in Figure 5.9. Mean monthly river flows in July and August 1999 are presented in Table 5.2. A third simulation was also completed using a Nikuradse coefficient of 0.001, because the value of 0.0005 was considered unrealistic.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time Step (s)</td>
<td>20</td>
</tr>
<tr>
<td>Number of Time Steps</td>
<td>133920 (31 days)</td>
</tr>
<tr>
<td>Coriolis Coefficient (rad/s)</td>
<td>-7.73 x 10⁻² (at latitude 32° South)</td>
</tr>
<tr>
<td>Coefficient of Wind Influence</td>
<td>1.61 x 10⁻⁴ (wind speed = 10 m/s);</td>
</tr>
<tr>
<td>Air Pressure</td>
<td>No surface pressure field</td>
</tr>
<tr>
<td>Friction Coefficient and Law</td>
<td>Manning = 0.01; Nikuradse = 0.00005; Nikuradse = 0.001</td>
</tr>
<tr>
<td>Velocity Diffusivity (m²/s)</td>
<td>10</td>
</tr>
<tr>
<td>Tidal Flats</td>
<td>Option 1 - Submerged/exposed areas are detected and the free surface gradient is corrected</td>
</tr>
<tr>
<td>Type of Advection</td>
<td>U+V – method of characteristics, H - conservative scheme + SUPG</td>
</tr>
</tbody>
</table>

Table 5.7 Model Set-Up for 31 Day Bed Friction Sensitivity Tests
Results for these tests gave predictable variance values for the longitudinal velocity of 67.77% (Manning 0.01); 77.66% (Nikuradse 0.00005); and 87.82% (Nikuradse 0.001). It was therefore concluded that the most suitable value to use for the coefficient of bed friction was $k_s = 0.001$.

The work of Fernandes (2001) also included an examination of the effect of varying bed friction throughout the domain. Although the results showed an improvement in the reproduction of measurements, it was concluded that varying friction according to the bed sediment was not essential. Therefore, no tests of this nature were completed for this research.

5.4.2 Sensitivity of the Model to Surface Friction

The sensitivity of the model to the effects of wind were evaluated by varying the coefficient of wind influence under conditions of a constant bed friction coefficient of $k_s = 0.001$. The model was run for a period of 31 days from 21st July 1999 to 21st August 1999, with the set-up shown in Table 5.8. A series of six simulations were completed with coefficients of wind influence computed from winds of 2.5, 5, 7.5, 10, 15 and 20 m/s. The mean wind speed for the period was 5.4 m/s.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time Step (s)</td>
<td>20</td>
</tr>
<tr>
<td>Number of Time Steps</td>
<td>133920 (31 days)</td>
</tr>
<tr>
<td>Coriolis Coefficient (rad/s)</td>
<td>$-7.73 \times 10^{-2}$ (at latitude 32° South)</td>
</tr>
<tr>
<td>Coefficient of Wind Influence</td>
<td>$2.87 \times 10^{-7}$ (wind speed = 2.5 m/s); $7.29 \times 10^{-7}$ (wind speed = 5 m/s); $1.17 \times 10^{-6}$ (wind speed = 7.5 m/s); $1.61 \times 10^{-6}$ (wind speed = 10 m/s); $2.50 \times 10^{-6}$ (wind speed = 15 m/s); $3.38 \times 10^{-6}$ (wind speed = 20 m/s)</td>
</tr>
<tr>
<td>Air Pressure</td>
<td>No surface pressure field</td>
</tr>
<tr>
<td>Friction Coefficient and Law</td>
<td>Nikuradse = 0.001</td>
</tr>
<tr>
<td>Velocity Diffusivity (m²/s)</td>
<td>10</td>
</tr>
<tr>
<td>Tidal Flats</td>
<td>Option 1 - Submerged/exposed areas are detected and the free surface gradient is corrected</td>
</tr>
<tr>
<td>Type of Advection</td>
<td>Option 1 - U+V – method of characteristics, Option 5 - H - conservative scheme + SUPG</td>
</tr>
</tbody>
</table>

Table 5.8 Model Set-Up for Surface Friction Sensitivity Tests
The modelled period had an underlying wind direction from the northerly sectors, which was punctuated by several clearly defined frontal systems passing through from the SW, e.g. for the 7th to 9th and 11th to 16th August. These systems have been described in Chapter 2 and are a common feature of the wind pattern of the region during winter months. Therefore this period was considered ideal to test the performance of the model under typical winter conditions.

![Figure 5.9](image)

**Figure 5.9** Observed Elevation and Wind at Praticagem 21st July to 21st August

The model results for longitudinal velocity at Praticagem and free surface elevation at Itapua were extracted for the period 2nd to 21st August and are presented as time series in Figures 5.10 and 5.11, together with the longitudinal wind component (WY), and observations for the scenario that gave the best predictions for each set. The time from the beginning of each simulation to 1st August served as a “run-in” period, to enable the model to reach the correct initial conditions for the lagoon at the start of the calibration period. Table 5.9 presents the correlation statistics for these simulations.
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Figure 5.10  Longitudinal Velocity at Praticagem 2nd to 20th August 1999 for Various Coefficients of Wind Friction

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Figure 5.11  Free Surface Elevation at Itapua 2\textsuperscript{nd} to 20\textsuperscript{th} August 1999 for Various Coefficients of Wind Friction
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Table 5.9  Modelled and Observed Correlations with a Varying Coefficient of Wind Influence for 2nd to 20th August 1999

The top panel of Figure 5.10 shows the model output for the longitudinal current velocity component (V) for the five wind coefficients. As would be expected, the magnitude of the current velocity increases with increasing wind influence, with the differential between the various values of the coefficients being greatest during times of the highest current velocities, particularly in the southern sectors (positive values), which are associated with the passing of frontal systems.

The lower panel of Figure 5.10 shows the model output and observations for the wind coefficient of $1.61 \times 10^6$ (p.v. = 87.82%). In fact the maximum agreement between model output and observations was achieved with a wind coefficient of $7.29 \times 10^7$ (p.v. = 89.62%) however, the highest velocities were best reproduced with the wind coefficient set to $1.61 \times 10^6$. The wind velocity is also included on the lower panel of Figure 5.10 to demonstrate the capability of the model to reproduce the passing of frontal systems.

The top panel of Figure 5.11 shows the model output for free surface elevation at Itapua located at the northern end of the lagoon, for the five wind coefficients. Results show the size of the fluctuations increases with increasing wind influence, which is expected for this wind-dominated system.

<table>
<thead>
<tr>
<th>Coefficient of Wind Influence</th>
<th>Free Surface Elevation</th>
<th>Longitudinal Velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>p.v. (%)</td>
<td>R²</td>
</tr>
<tr>
<td>$2.87 \times 10^{-7}$ (2.5 m/s)</td>
<td>31.89</td>
<td>0.37</td>
</tr>
<tr>
<td>$7.29 \times 10^{-7}$ (5 m/s)</td>
<td>51.72</td>
<td>0.60</td>
</tr>
<tr>
<td>$1.17 \times 10^{-6}$ (7.5 m/s)</td>
<td>64.28</td>
<td>0.69</td>
</tr>
<tr>
<td>$1.61 \times 10^{-6}$ (10 m/s)</td>
<td>70.89</td>
<td>0.72</td>
</tr>
<tr>
<td>$2.50 \times 10^{-6}$ (15 m/s)</td>
<td>69.45</td>
<td>0.73</td>
</tr>
<tr>
<td>$3.38 \times 10^{-6}$ (20 m/s)</td>
<td>51.14</td>
<td>0.72</td>
</tr>
</tbody>
</table>
The lower panel of Figure 5.11 shows the model output and adjusted observations for the wind coefficient of $1.61 \times 10^{-6}$, which had the best agreement with the observations: ($R^2 = 0.72$, p.v. = 70.89%). Therefore, the best overall agreement, when considering the average predictable variance for both elevations and longitudinal velocity was achieved with a wind coefficient of $1.61 \times 10^{-6}$ (p.v. = 79.36%).

In summary, the model has been shown to produce extremely good results under a range of calibration parameters. The optimal bed friction parameter indicated is a Nikuradse coefficient of 0.001, and for the coefficient of wind influence, a value of $1.61 \times 10^{-6}$.

5.5 Model Validation

Following the successful calibration of TELEMAC-2D, the final step was to test the robustness by a process of validation using a further independent data set, modelled with the source terms derived from the calibration. The model was run for a period of 15 days from 19th April to 4th May 1999, with the set-up shown in Table 5.10. The tidal elevations and wind for this period are presented in Figure 5.12, and mean monthly river flows are presented in Table 5.2. Bed friction was set at $k_s = 0.001$, and the coefficient of wind friction value was $1.61 \times 10^{-6}$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time Step (s)</td>
<td>20</td>
</tr>
<tr>
<td>Number of Time Steps</td>
<td>64800 (15 days)</td>
</tr>
<tr>
<td>Coriolis Coefficient (rad/s)</td>
<td>$-7.73 \times 10^{-5}$ (at latitude 32° South)</td>
</tr>
<tr>
<td>Coefficient of Wind Influence</td>
<td>$1.61 \times 10^{-6}$ (wind speed = 10 m/s)</td>
</tr>
<tr>
<td>Air Pressure</td>
<td>No surface pressure field</td>
</tr>
<tr>
<td>Friction Coefficient and Law</td>
<td>$k_s = 0.001$</td>
</tr>
<tr>
<td>Velocity Diffusivity (m²/s)</td>
<td>10</td>
</tr>
<tr>
<td>Tidal Flats</td>
<td>Option 1 - Submerged/exposed areas are detected and the free surface gradient is corrected</td>
</tr>
<tr>
<td>Type of Advection</td>
<td>Option 1 - U+V – method of characteristics, Option 5 - H - conservative scheme + SUPG</td>
</tr>
</tbody>
</table>

Table 5.10 Model Set-Up for Validation Test 19th April to 4th May 1999
Chapter 5 - Calibration and Validation of TELEMAC-2D

Figure 5.12 Observed Tidal Elevation and Wind at Praticagem 19th April to 4th May 1999

Unfortunately there were no current velocity measurements available for this period, so the model results for elevation were compared with measurements at five locations in the lagoon: Farol de Itapuã; Santa Rita; São Lourenço do Sul; Bojuru; and Rincão do Cristóvão Pereira. The results of the correlation between modelled and measured data are presented in Table 5.11, and show an excellent level of correlation. Time series plots of the results are presented in Figure 5.13.

<table>
<thead>
<tr>
<th>Location</th>
<th>Easting (UTM)</th>
<th>Northing (UTM)</th>
<th>Predictable Variance (%age)</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Farol de Itapuã</td>
<td>494022</td>
<td>6640650</td>
<td>89.15</td>
<td>0.91</td>
</tr>
<tr>
<td>Santa Rita</td>
<td>457801</td>
<td>6560430</td>
<td>93.35</td>
<td>0.97</td>
</tr>
<tr>
<td>São Lourenço do Sul</td>
<td>406175</td>
<td>6516500</td>
<td>88.14</td>
<td>0.88</td>
</tr>
<tr>
<td>Bojuru</td>
<td>459200</td>
<td>6515900</td>
<td>89.44</td>
<td>0.90</td>
</tr>
<tr>
<td>Rincão do Cristóvão Pereira</td>
<td>488900</td>
<td>6561400</td>
<td>75.54</td>
<td>0.75</td>
</tr>
</tbody>
</table>

Table 5.11 Correlation Statistics for Model Validation 19th April to 4th May 1999
Figure 5.13  Model Output and Adjusted Observations 19th April to 4th May 1999
As a further validation the model was run for a 165 day period from 18th April to 1st October 1999, using the same set-up as the previous validation simulation. Wind and tidal elevation data measured at Praticagem are presented in Figure 5.14, and mean monthly river flows are presented in Table 5.2.

The results for modelled and measured elevations at the five gauging stations are presented in Figure 5.15. The $R^2$ and predictable variance values for the entire period were calculated: Farol de Itapuã ($R^2 = 0.61$, p.v. = 60.71%); Santa Rita ($R^2 = 0.70$, p.v. = 68.41%); São Lourenço do Sul ($R^2 = 0.59$, p.v. = 58.73%); Bojuru ($R^2 = 0.55$, p.v. = 54.61%); and Rincão do Cristóvão Pereira ($R^2 = 0.64$, p.v. = 63.87%). These correlations were not as high when calculated for the entire data set as those achieved for shorter periods, however, the correlation for the longitudinal velocities at Praticagem for the period 2nd to 21st October was very good ($R^2 = 0.90$, p.v. = 88.46%).
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Figure 5.14  Observed Tidal Elevation and Wind at Praticagem 19th April to 1st October 1999
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Figure 5.15 Model Output and Adjusted Observations 19th April to 1st October 1999
5.6 Hydrodynamic Regime of the Saco da Mangueira

Some insight into the circulation of Saco da Mangueira may be gained from the results of the validated hydrodynamic model. Figure 5.16 presents an animation with a time interval of 3 hours for the period 21st July 1999 to 31st July 1999. The full animation can be seen by readers viewing this as an electronic file, whereas those reading from a printed copy are referred to Appendix 2 and the attached CD for all frames of the simulation.

Figure 5.16 Modelling the Circulation of the Saco da Mangueira

The free surface elevation is shown by coloured contours with superimposed current vectors, and the time series below gives the observed elevations at Praticagem (blue).
together with the longitudinal component of the observed wind (red), where winds from the northerly sectors are negative. Current velocities were extracted from the model results at various locations within the Saco da Mangueira and lower Patos estuary.

Maximum current speeds of up to 1.9 m/s were predicted during the modelled period in the main channel of the lower estuary, which reduced to 1.1 m/s in the estuary adjacent to the entrance to the bay. A localised increase in velocity characterises the narrow entrance to the Saco da Mangueira with model results reaching 1.3 m/s. Average predicted velocities in the estuary and at the entrance were 0.41 m/s and 0.36 m/s respectively. There is a marked decrease in water movement within the Saco da Mangueira compared with the estuary which is shown by the contours of mean current speed presented in Figure 5.17 together with vectors showing the mean current direction.

Figure 5.17 Mean Current Velocities in the Saco da Mangueira
The model indicates a very sluggish circulation within the Saco da Mangueira with mean and maximum velocities ranging from 0.03 m/s and 0.15 m/s respectively in the centre of the bay to 0.06 m/s and 0.23 m/s respectively closer to the shoreline. Circulation patterns can be detected when currents approach their maximum velocities, with movement to the southwest tending to follow the central axis of the bay and return flows towards the mouth occurring in the very shallow margins and reaching slightly higher velocities. These features were observed during a surface float experiment conducted for this research on 23rd May 2003, where water close to the shoreline at the entrance of the bay was observed to be flowing in the opposite direction to the main flow and against the wind.

Another feature of the pattern of water movement recorded at the entrance to Saco da Mangueira during the fieldwork in May 2003 which is also apparent from the model output (see the animation of Figure 5.16 in Appendix 2) is a quasi-periodicity to the flow reversals in and out of the bay of the order of 2 to 3 hours which appears to be independent of the wind direction.
Chapter 6

Transport and Mixing Time Scales in the Patos Lagoon and the Saco da Mangueira

This Chapter describes an assessment of water exchange time scales within the Patos Lagoon System, principally focussing on the semi-enclosed embayment of Saco da Mangueira. The results of volumetric calculations are compared with those derived from simulations using TELEMAC-2D.

6.1 Defining Transport and Mixing Timescales

Temporal quantification of transport and mixing of water and dissolved particles within an aquatic ecosystem is essential when conducting water quality investigations, because the length of time a water parcel is retained within a body of water coupled with the rate of biogeochemical reactions occurring therein, will determine its capacity for assimilation and potential for the build up of contaminants. For a water quality modelling study, an assessment of the factors which affect flushing and an estimation of the residence time will also aid the determination of the most appropriate time scale for simulations, and hence, optimum efficiency of the model.

There are many terms and concepts which describe transport time scales in estuaries, rivers and lakes, for example, residence time (Dronkers & Zimmerman, 1982); estuarine residence time (ERT) and pulse residence time (PRT) (Miller & McPherson, 1991); flushing time (Dyer, 1973); freshwater replacement time; renewal time; age; exchange rate; and freshwater transit time. All of these terms represent physical transport time scales but
tend to be inconsistently defined in the literature (Monsen et al., 2002), with different concepts described by the same name as well as the same concept being described by different names. Methods of calculation are in a state of continual refinement, starting from empirical methods based on the measurement of tracers such as freshwater or dye studies; and progressing to models ranging from the simple and segmented versions of the tidal prism model, to box models, and more commonly in recent times the use of hydrodynamic models in multiple dimensions, which can simulate the physics of a system with a high degree of accuracy, leading to more realistic estimates of transport and mixing timescales.

A range of methods has been reviewed by Kuo & Neilson (1988); Sanford et al. (1992); Jay et al. (1997); Guo & Lordi (2000); Monsen et al. (2002); Sheldon & Alber (2002); and Wang et al. (2004), from which it is concluded that the most commonly used terms are residence time and flushing time, and it is most important to begin an assessment with a correct understanding of the existing terminology and which methods of calculation are appropriate for the system being studied. Some definitions and formulations compiled by Wang et al. 2004 are reproduced here:

**Flushing Time ($T_f$)**

a. The time required to replace the existing freshwater in the whole or a segment of the estuary at a rate equal to river discharge, (Bowden, 1967; Dyer, 1973; Officer, 1976; Fischer et al., 1979):

\[
T_f = \frac{V_f}{R} \tag{6.1}
\]

where:
Chapter 6 - Transport and Mixing Time Scales in the Patos Lagoon and the Saco da Mangueira

\[ V_f \] volume of freshwater accumulated in the whole or a segment of the estuary

\[ R \] river discharge

b. The volume of sea water and river water introduced on the flood stream equals the tidal prism, and the same volume of water is removed on the ebb stream:

\[ T_f = \frac{(V + P)T}{P} \]

(Bowden, 1967; Dyer, 1973) (6.2)

where:

\[ V \] low tide volume of the whole or a segment of the estuary

\[ P \] tidal prism

\[ T \] tidal period

c. The ratio of the mass of a scalar in a reservoir to the rate of renewal of the scalar:

(Geyer et al., 2000)

**Residence Time (T_r)**

d. The average time for all existing water in the whole or a segment of the estuary to remain in the original domain:

\[ T_r = \frac{1}{M(0)} \int_0^t t \left[ -\frac{dM(t)}{dt} \right] dt \]

(Wang et al., 2004): (6.3)

where:

\[ M \] total mass of tracer remaining in the estuary

\[ t \] time
e. The time required for the total mass of a conservative tracer originally within the whole or a segment of the estuary to be reduced to a factor of $e^{-1}$ (i.e. 0.37):

$$T_r = \frac{(V + P/2)T}{(1-b)P + RT} \quad (\text{Sanford et al, 1992}) \quad (6.4)$$

$$T_r = \frac{(V + P)T}{(1-b)P + RT/2} \quad (\text{Luketina, 1998}) \quad (6.5)$$

where:

$b$ return flow factor

f. The time required for a particle to travel from a location to the boundary of the region (Prandle, 1984), which depends on the location where the particle is released. This was further defined by Van de Kreeke (1983) with respect to the phase of tide when the particle is initially released.

Renewal Time

g. The time required to replace a specified fraction of the water in an estuary by the volume flows of freshwater and new ocean salt water, e.g., the 50% renewal time:

$$T_{1/2} = 0.693 \frac{V}{R + Q} \quad (\text{Pritchard, 1960}) \quad (6.6)$$

where:

$Q$ salt water flow rate, or volume of new water entering the estuary on a flood tide

Pritchard equated mean renewal time to mean residence time:

$$T_m = \frac{V}{R + Q} \quad (6.7)$$
Mean Detention Time

h. The mean time that a particle of tracer remains inside an estuary, also confusingly termed flushing time (Fischer et al., 1979).

Turn-over Time

i. Definition similar to the flushing time in a. (Bolin and Rodhe, 1973).

j. Definition the same as that for residence time in e. (Prandle, 1984).

Exchange Time

k. Definition the same as that for residence time in e. (Gillibrand, 2001).

Transit Time

l. The period of time between a particle entering and leaving an estuary (Bolin and Rodhe, 1973).

Age

m. The time that has elapsed since the water parcel enters an estuary (Bolin and Rodhe, 1973).

For this study, the residence time will be determined from the rate of change of the total mass of a conservative tracer, which is commonly referred to as the e-folding time, because the concentrations typically show an exponential decrease with time.
6.2 Volumetric Calculations

A simple analysis of the flushing time for the Saco da Mangueira was completed in order to provide a comparison with results generated from the model simulations. The flushing time ($T_f$) can be calculated as the volume ($V$) of water in a defined system, divided by the volumetric flow rate ($Q$) through the system:

$$T_f = \frac{V}{Q}$$  \hspace{1cm} (6.8)

where,

$V$    the volume of water in the bay ($1.748 \times 10^7$ m$^3$), from the average depth of the bay ($7.6 \times 10^{-1}$ m), and the surface area of the bay ($2.3 \times 10^7$ m$^2$);

$Q$    the discharge through the entrance to the bay ($1.28 \times 10^3$ m$^3$/s), given by the product of:

$A$    the cross-sectional area of the entrance ($7.27 \times 10^2$ m$^2$), obtained from the ADCP soundings made at intervals of 3.5 m across the entrance during the field campaign in 2003 (see Chapter 3, Figure 3.10);

and

$U$    average current speed at the entrance ($1.76 \times 10^{-1}$ m/s), obtained from the ADCP measurements undertaken in 2002 and 2003.

Applying Equation 6.8 to the Saco da Mangueira gave a theoretical time of 1.6 days to replace all the water in the bay; however, this estimate was considered to be a significant under-estimate since the method does not account for return flows and the influence of wind on the hydrodynamics. Since wind is known to be the principal factor controlling water transport in the study area, it was necessary to conduct model simulations to obtain more realistic estimates of the residence time.
6.3 TELEMAC-2D Simulations

The method to evaluate the residence time of the Patos Lagoon and Saco da Mangueira with TELEMAC-2D was to use a conservative tracer \( C \) to calculate the e-folding flushing time \( (T_f) \) given by Thomann and Mueller (1987):

\[
C(t) = C_0 e^{-t/T_f} = C_0 e^{-t/T_f}
\]

where,

\( t \) the time elapsed from the introduction of the tracer

\( C_0 \) the concentration of the tracer at \( t = 0 \)

For each simulation, the model was ‘run-up’ for a period of 1 month and then a unit conservative tracer was instantaneously introduced at each node within the Saco da Mangueira with zero tracer elsewhere, as shown in Figure 6.1.

Figure 6.1 Initial Conditions for Modelling Water Residence Times in the Saco da Mangueira
Each model simulation proceeded for a period of 31 days, and the concentration of the total tracer remaining in the bay was extracted from the results at daily intervals. An example of four model simulations investigating the effects of varying the wind is presented in Figure 6.2. The full animation can be seen by readers viewing this as an electronic file, whereas those reading from a printed copy are referred to Appendix 3 and the attached CD for all frames of the simulation.

Figure 6.2  Comparison of Theoretical and Observed Wind Forcing during May 1999

The concentrations of total tracer extracted at daily intervals were expressed as percentages of the total initial concentration of tracer in the bay, and plotted as a time series. The general trend of tracer decrease was obtained by fitting a curve to the plotted
concentrations, from which the e-folding flushing time (days) was computed for each simulation, i.e. the length of time taken for the concentration of tracer remaining in the Saco da Mangueira to reduce to 1/e (37%) of the initial concentration.

Figure 6.3 presents an example of the graphical output for this method for simulations investigating the effects of varying the wind. The positive phases of the oscillations in the curves are due to the re-entrainment of tracer into the bay during times of net inflow of water from the estuary; and conversely, the negative phases correspond to net outflow. These oscillations are most pronounced for the simulation without wind forcing resulting in very slow overall removal of tracer from the bay, and demonstrating the importance of wind in the transport mechanism for this system.

![Graph showing e-folding flushing times with different wind scenarios](image)

**Figure 6.3** E-Folding Flushing Times in Saco da Mangueira (1st May 1999 to 1st June 1999) - Continuous Low River Flow (1000 cusecs)

Four groups of simulations were designed to investigate the effects of various combinations of wind and river flow using both observed data and constant values to force the model, with observed elevations at the entrance to the estuary. A total of 17
simulations were completed, which are summarised in Table 6.1, together with the calculated e-folding flushing times.

<table>
<thead>
<tr>
<th>Modelled Period</th>
<th>Season</th>
<th>Total River Flow (m³/s)</th>
<th>Wind Conditions</th>
<th>E-Folding Flushing Time (days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group 1: Constant High River Flow with Various Constant Winds</td>
<td>01/05-01/06/99</td>
<td>10,000</td>
<td>No wind</td>
<td>99.4</td>
</tr>
<tr>
<td></td>
<td>01/05-01/06/99</td>
<td>10,000</td>
<td>10 m/s NE</td>
<td>48.8</td>
</tr>
<tr>
<td></td>
<td>01/05-01/06/99</td>
<td>10,000</td>
<td>10 m/s SW</td>
<td>7.2</td>
</tr>
<tr>
<td>Group 2: Constant Low River Flow with Various Constant Winds</td>
<td>01/05-01/06/99</td>
<td>1000</td>
<td>No wind</td>
<td>90.2</td>
</tr>
<tr>
<td></td>
<td>01/05-01/06/99</td>
<td>1000</td>
<td>10 m/s NE</td>
<td>27.7</td>
</tr>
<tr>
<td></td>
<td>01/05-01/06/99</td>
<td>1000</td>
<td>10 m/s SW</td>
<td>6.5</td>
</tr>
<tr>
<td>Group 3: Various Constant River Flows with Observed Winds</td>
<td>01/05-01/06/99</td>
<td>10,000</td>
<td>Observed</td>
<td>26.2</td>
</tr>
<tr>
<td></td>
<td>01/05-01/06/99</td>
<td>5000</td>
<td>Observed</td>
<td>24.4</td>
</tr>
<tr>
<td></td>
<td>01/05-01/06/99</td>
<td>1000</td>
<td>Observed</td>
<td>21.9</td>
</tr>
<tr>
<td></td>
<td>01/05-01/06/99</td>
<td>200</td>
<td>Observed</td>
<td>21.6</td>
</tr>
<tr>
<td>Group 4: Observed River Flows with Observed Winds</td>
<td>01/05-01/06/99</td>
<td>Autumn</td>
<td>1030</td>
<td>Observed</td>
</tr>
<tr>
<td></td>
<td>01/06-02/07/99</td>
<td>Winter</td>
<td>3671</td>
<td>Observed</td>
</tr>
<tr>
<td></td>
<td>01/07-01/08/99</td>
<td>Winter</td>
<td>4016</td>
<td>Observed</td>
</tr>
<tr>
<td></td>
<td>01/08-01/09/99</td>
<td>Winter</td>
<td>2068</td>
<td>Observed</td>
</tr>
<tr>
<td></td>
<td>01/09-01/10/99</td>
<td>Spring</td>
<td>2835</td>
<td>Observed</td>
</tr>
<tr>
<td></td>
<td>01/10-01/11/02</td>
<td>Spring</td>
<td>2466</td>
<td>Observed</td>
</tr>
<tr>
<td></td>
<td>01/05-01/06/03</td>
<td>Autumn</td>
<td>1858</td>
<td>Observed</td>
</tr>
</tbody>
</table>

Table 6.1 E-Folding Flushing Time Results from TELEMAC-2D Simulations of a Conservative Tracer in Saco da Mangueira

The results show a large range of e-folding flushing times for the Saco da Mangueira ranging from 6.5 days (low river flow of 1000 m³/s with a strong SW wind) to 99.4 days (high river flow of 10,000 m³/s with no wind). The main points to note from the results are as follows:

- The condition of no wind was found to significantly extend the flushing time by a factor of between two and three compared with other conditions.
• Constant winds from the SW were found to flush the embayment much quicker than winds from the NE, independent of river flow, which is likely to be due to the orientation of the Saco da Mangueira.

• Simulations with observed wind and various constant values for river flow (Group 3) resulted in a relatively narrow range of e-folding times from 21.6 days for the lowest river flow (200 m³/s) to 26.2 days for the highest river flow (10,000 m³/s).

These observations highlight the dominance of wind compared to river flow with respect to transport and mixing processes within the Saco da Mangueira.

• Flushing times for the simulations using observed wind and river flows (Group 4) ranged from 21.2 to 44.5. This range is considered to be more realistic than the results from simulations using constant winds and river flows since these conditions do not occur naturally.

In contrast to the results obtained for the flushing of Saco da Mangueira, further simulations conducted with a unit tracer imposed throughout the entire Patos system showed river flows to been more important than winds, with e-folding flushing times ranging from 89 days (river flow = 10,000 m³/s, wind = 10 m/s NE) to 428 days (river flow = 1000 m³/s, wind = 10 m/s SW). A value of 303 days was calculated from the results obtained using observed river flows and winds. This is somewhat longer than the value of 82 days given for the flushing half-life by Knoppers and Kjerfve (1999), and the freshwater residence time of ~5 months given by Windom et al. (1999).
In summary, the fastest flushing of the Saco da Mangueira is likely to occur during times of low river flow and long periods of wind from the SW sector, whereas high river flows and winds from the NE will enhance the flushing of the Patos lagoon but restrict that of Saco da Mangueira, due to its orientation relative to the Patos lagoon estuary.

6.4 Processes Controlling Water Transport and Mixing

It is apparent that water transport in and out of the Saco da Mangueira is principally controlled by the wind direction and duration rather than the river flow. The relative relationship between wind, river flow and flushing can be shown by plotting the river flow and the total longitudinal wind component for each monthly period (relative to the principal axis of the Saco da Mangueira) against the modelled flushing results (Figure 6.4). The strongest correlation with flushing ($R^2 = 0.43$) was with winds blowing out of the bay.

![Figure 6.4 Correlating River Flows and Wind Directions with E-Folding Flushing Times in Saco da Mangueira](image)
To investigate when these 'flushing events' are likely to occur and whether they are related to certain months or seasons, it is necessary to consider annual and inter-annual patterns of wind and river flow. The seasonal variations in wind direction for 1999, and 1999 to 2003 were presented in Chapter 3 (Figure 3.7, p.59), and showed the highest percentage of winds from the northeast to east occur during Spring and Summer (~50%), whereas there is a trend for an increase in the occurrence of winds from westerly sectors during Autumn and Winter (~37%). Therefore, the flushing of Saco da Mangueira is likely to be better during Autumn and Winter than during Spring and Summer. This seems to be in agreement with the results of the flushing simulations (Table 6.1, Group 4), since the two slowest e-folding flushing times of 44.5 and 33.3 days were calculated from Spring months, and the fastest times of 21.9 and 21.2 occurred in Autumn and Winter months respectively.

With respect to average seasonal river flows, values for the period 1940 to 1999 are 2671 m$^3$/s (Spring); 1316 m$^3$/s (Summer); 1756 m$^3$/s (Autumn); and 3655 m$^3$/s (Winter). This indicates that given favourable wind directions, the flushing of the Saco da Mangueira may be enhanced during Summer and Autumn.

Further insight into the nature of the circulation patterns within the Saco da Mangueira and exchange at the mouth on a more detailed temporal scale may be gained from tracer simulations. One such simulation showing concentrations of tracer in the bay and lower estuary at intervals of 2 hours for a period of 12.5 days from 19th June 1999 to 30th June 1999 is presented as an animation in Figure 6.5 below. The full animation can be seen by readers viewing this as an electronic file, whereas those reading from a printed copy are referred to Appendix 4 and the attached CD for all frames of the simulation.
The simulation shows that the processes controlling the flushing of the Saco da Mangueira depend on the exchange across the restricted entrance to the bay. It can be seen that even after 12.5 days the water at the southern end of the embayment has only received ~30% dilution from waters entering from the estuary, therefore it is clear that mixing is very limited. This area of the Saco da Mangueira is not currently impacted directly from sewage and industrial effluents; however, there are proposals to relocate the main sewage outfall for Rio Grande, and also the area is currently being favoured for a high level of aquaculture (shrimp) fisheries. Any development will require a comprehensive impact assessment to avoid deterioration in the water quality.

Figure 6.5  Modelling Water Residence Times in the Saco da Mangueira (the frames from this animation are presented in Appendix 4)
Chapter 7

Calibration and Validation of WQFLOW-2D

7.1 Introduction

This chapter describes the calibration and validation of the water quality model WQFLOW-2D for the Patos Lagoon System with particular focus on Saco da Mangueira which is a semi-enclosed embayment, adjacent to the city of Rio Grande approximately 10km from the mouth of the estuary. The processes involved in setting-up and testing WQFLOW-2D will be initially considered, followed by details of the results obtained from this research.

General procedures for modelling water quality have been described by many authors, notably Oriob (1983); Chapra (1997); Martin et. al (1998); Jørgensen & Bendoricchio (2000); and Spaulding (2002). There is no prescriptive methodology for modelling water quality, however, the general stages involved can be summarised as follows:

i. Identification of the principal processes and variables affecting the water quality of the study area, and most importantly, the selection of temporal, spatial, and kinetic scales, which will form the basis for the type of model and level of detail required;

ii. Conceptualisation, formulation and computer representation of the model (for this research the model software has already been formulated and employed extensively for both research and commercial projects);

iii. Selection of initial and boundary conditions for the hydrodynamic parameters and water quality state variables, together with loadings for point source inputs such as
effluent discharges. WQFLOW-2D uses the flow field output from TELEMAC-2D;

iv. Calibration of the model through the sensitivity analyses of an appropriate range of kinetic parameter values. This is an iterative process where the most important parameters should ideally be obtained from in-situ measurements, or otherwise extracted from previous studies using similar models;

v. Fine tuning of the kinetic parameters until an optimal agreement between predicted and observed water quality variables is obtained;

vi. Validation against further observations to assess the performance of the model. This may take the form of simulations conducted under different hydrodynamic regimes depending on the characteristics of the study area, or perhaps longer term variations in water quality such as seasonal trends. It is important at this stage to include some measure of the uncertainty in model output.

The strengths and weaknesses of using WQFLOW-2D as a management tool for the Patos Lagoon System will be fully discussed in Chapter 9; however, it is important to note here that agreement between modelled and observed results does not necessarily indicate that all relevant processes have been included or correctly described, and regardless of the accuracy and complexity of the modelled physical, chemical, and biological processes, there will be a level of uncertainty due to natural variation; misspecification of boundary conditions; and the quality and quantity of the measured data. In particular, for multi-dimensional models such as WQFLOW-2D, the accuracy will immediately be limited by the accuracy of the results obtained from the flow model.
7.2 Modelled Parameters and Scales

The physical processes and chemical characteristics of the Patos System have been described in detail in Chapters 2 and 3, with new insight into the circulation patterns and transport timescales of the Saco da Mangueira obtained through hydrodynamic modelling reported in Chapters 5 and 6. The following sections provide details of the model resolution and run parameters, and the reader is referred to Chapter 4 for a description of the model processes and formulations.

7.2.1 Temporal, Spatial and Kinetic Scales

The first time scale considered was the length of the model simulation, which needed to reflect the time a pollutant would be retained in the study area, and hence, the period of accumulation and removal through processes such as flushing; decay, settlement; or chemical transformation. Transport and mixing timescales have been investigated using TELEMAC-2D in Chapter 6 with the conclusion that under observed wind and river flow conditions, water remains within the Saco da Mangueira for ~30 days on average depending principally on the direction and duration of the wind. Chemical reactions between water quality parameters occur on much faster time scales, for example, of the order of 5 days for nitrification (Bowie et al., 1985; Chapra, 1997), so it is clear that the water quality model reaches a state of equilibrium before the hydrodynamic model, and therefore, the flushing time would appear to be an appropriate timescale for model simulations.

Secondly, the resolution of the model was considered in terms of the timestep for the mass balance calculations. The numerical methods for advection and diffusion in WQFLOW-
2D are unconditionally stable and reaction kinetics are generally slow enough for long timesteps to be acceptable; however, for conservation of mass and momentum, a solute should not be advected more than one element per timestep, and the water quality model timestep should typically be two or three times that used for the flow calculation (HR Wallingford, 2000).

The model was evaluated for performance and stability using various combinations of timestep, diffusion coefficient, and advection scheme. Model simulations were conducted to find the optimal timestep using values of 30, 60, 120, and 180s (recall the timestep used for the hydrodynamic simulations was 20s). A timestep of 180s caused the model to become unstable and fail due to near zero concentrations of dissolved oxygen, whereas results were not significantly different for each of the other simulations; therefore a value of 120s was chosen as the initial timestep for the model.

Further simulations were conducted to evaluate the sensitivity of the model to varying values of diffusion coefficient (1, 5, 10, and 50m²/s) and to fine tune the timestep (40, 60, 120s). The tests were conducted for a 31 day period which included a critical phase of strong NE winds with falling water levels giving rapid water movement in the lower estuary. The model failed for the same reason stated above during this critical period for all simulations using a timestep of 120s and a diffusion coefficient of 1m²/s. Model run times were optimised using a timestep of 60s with a diffusion coefficient of either 5 or 10m²/s. Figure 7.1 shows the sensitivity of the model to various diffusion coefficients and a timestep of 60s, for dissolved oxygen at the entrance to Saco da Mangueira.
Finally, a sensitivity analysis was conducted on the choice of advection scheme. There was very little difference between model results using the Standard Method of Characteristics (Option 1) and the Hybrid Characteristics and Centred Scheme (Option 4), however, simulation times were shorter with Option 1, which was therefore selected as the advection scheme for all further water quality simulations.

With respect to spatial scales, model scenarios will focus on the lower estuary and the Saco da Mangueira; however, given that WQFLOW-2D uses the mesh from the flow model, the whole system will be modelled. The higher spatial resolution required for the lower part of the Patos System was accounted for in the space discretisation for TELEMAC-2D (see Chapter 5), therefore, no further modification of the mesh was required at this stage. This approach was possible because the availability of substantial computational power (2GHz processor with 512MB memory) enabled a 31 day model run to be completed in approximately 10.5 hours.
7.2.2 Hydrodynamic Conditions

In the previous section it was established that the e-folding flushing time \( T_f \) of the Saco da Mangueira would be an appropriate time scale for water quality simulations. The selection of suitable flow fields would not only need to reflect the range of flushing conditions, but also include both typical and extreme features of the circulation of the study area. The period chosen for the sensitivity analyses was the 21\textsuperscript{st} July to 20\textsuperscript{th} August 1999, which included the passage of a number of frontal systems typical of the region in Winter, and also provided conditions of rapidly changing water levels in the shallow areas of the lower estuary. Although this was a Winter period, the mean fluvial flow (2759m\textsuperscript{3}/s) was more representative of the annual average flow for the system (2371m\textsuperscript{3}/s), owing to the influence of a moderate La Niña event (characterised by reduced river flows resulting from less rainfall). This period also represented average flushing conditions for the Saco da Mangueira of \( \sim 31 \) days.

Validation of the model was subsequently conducted using a different period (1\textsuperscript{st} October to 1\textsuperscript{st} November 2002) representing mean flushing conditions \( T_f = 33.3 \) days, as well as periods representing fast (1\textsuperscript{st} May to 1\textsuperscript{st} June 2003) and slow (1\textsuperscript{st} September to 1\textsuperscript{st} October 1999) flushing conditions of \( T_f = 22 \) and 44.5 days respectively. In addition, simulations were conducted to validate the model over a longer time period (15\textsuperscript{th} May to 1\textsuperscript{st} September 1999) and under typical minimum and maximum water temperatures (13°C and 25 °C respectively). The validation will be described in Section 7.5.

7.2.3 Initial and Boundary Conditions

The initial and boundary conditions for the water quality variables were prescribed as annual average values calculated from field measurements, and are presented in Table 7.1.
Ideally, the use of monthly or seasonal averages would have been preferable, both in terms of coinciding with average residence times in the Saco da Mangueira, and also for evaluating seasonal variation; however, the quantity of field data on these temporal scales was not considered sufficient. Since the exact mathematical representation of nature is not possible, model predictions can represent only an average effect at some scale, therefore, annual averages were considered appropriate for this study because the model will be used for assessing the ability of management actions to meet certain water quality standards, which are themselves expressed in terms of long-term average levels.

<table>
<thead>
<tr>
<th>State Variable</th>
<th>Initial Value</th>
<th>Boundary Value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Lagoon &amp; Estuary</td>
<td>Saco da Mangueira</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>18.8</td>
<td>18.8</td>
</tr>
<tr>
<td>Salinity (ppt)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Dissolved Oxygen (mg/l)</td>
<td>9.4</td>
<td>9.4</td>
</tr>
<tr>
<td>Fast Dissolved BOD (mg/l)</td>
<td>1.6</td>
<td>3.1</td>
</tr>
<tr>
<td>Ammoniacal Nitrogen (mg/l)</td>
<td>0.059</td>
<td>0.153</td>
</tr>
<tr>
<td>Nitrite (mg/l)</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>Nitrate (mg/l)</td>
<td>0.159</td>
<td>0.130</td>
</tr>
<tr>
<td>Mud (Suspended Solids) (mg/l)</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>Chlorophyll-a (Algal Carbon) (µg/l)</td>
<td>4.6 (227.8)</td>
<td>16.7 (836.7)</td>
</tr>
<tr>
<td>Orthophosphate (mg/l)</td>
<td>0.024</td>
<td>0.081</td>
</tr>
<tr>
<td>Silica (µg/l)</td>
<td>2533</td>
<td>2533</td>
</tr>
</tbody>
</table>

Table 7.1 Initial and Boundary Conditions

Spatially variable conditions were imposed at the riverine and ocean boundaries for salinity, BOD, suspended solids, ammoniacal nitrogen, nitrate, phosphate, silicate, and chlorophyll-a, by assigning concentrations at each open boundary node of the model domain.

The average measured values of the water quality variables for the estuary and lagoon were broadly similar (see Chapter 3), and were therefore imposed as spatially constant initial conditions. In contrast, the average measured concentrations of some of the nutrient variables in the Saco da Mangueira were sufficiently different from those in the lagoon and
estuary to warrant separate initial conditions. Care was taken to exclude data collected close to the domestic and industrial discharges, which would have artificially inflated the background conditions, particularly for phosphate and ammoniacal nitrogen.

### 7.2.4 Point Source Inputs

Pollutant inputs in the vicinity of the Saco da Mangueira originate from domestic and industrial discharges from the city of Rio Grande as described by Almeida et al. (1993), and Tagliani & Saint Pastous Madureira (2001).

![Figure 7.2 Pollutant Inputs and Monitoring Locations](image)

The most significant discharges are presented in Figure 7.2 together with the locations of the proposed inputs for the scenarios investigating the management of water quality in (see Chapter 8).
Chapter 7 - Calibration and Validation of WQFLOW-2D

Three locations were chosen to represent the existing inputs of sewage to the embayment, as follows:

- The main outfall for the city of Rio Grande, which discharges crude sewage from ~80% of the total population (circa. 200,000) at a location close to the shore (Coroa do Boi) just outside the entrance of the bay.

- Urban wastewater from both domestic and industrial discharges described in Chapter 2 (see Figure 2.5, p.39), which are discharged to the north eastern corner of Saco da Mangueira;

- Numerous combined surface water and sewage inputs which mostly discharge along the north eastern shore of Saco da Mangueira. For the purposes of this study these small discharges were combined as one input to the model.

Unfortunately, there have been no field measurements to date which quantify the loadings from these discharges, therefore, pollutant concentrations for domestic effluent were estimated from typical values for crude sewage (USACE, 1987; WRc, 1990; Tebbutt, 1998; Butler & Davis, 1998; Gray, 1999), with a biochemical oxygen demand of 60 grams/head/day. The flow from each discharge was also estimated, and the standard formulation used is known as the average daily flow (ADF), which is 1.5 times the dry weather flow (DWF) defined as the average flow over 7 days without rain, after 7 days of less than 0.25mm rain per day (Tebbutt, 1998):

\[
DWF = PG + I + C + E \quad (7.1)
\]

where,
- \(DWF\) = dry weather flow (m³/day)
- \(P\) = population
- \(G\) = water consumption rate (160 litre/head/day for Brazil)  \(\text{Domestic foul flow}\)
- \(I\) = infiltration (25% of domestic foul flow) (l/s)
Loadings were simply calculated from the flow rate multiplied by the concentration of each parameter, expressed in kg/day for input to the model and are presented in Table 7.2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>East</th>
<th>North</th>
<th>Population</th>
<th>Flow discharge (cubic m)</th>
<th>Suspended solids (g)</th>
<th>FeN (g)</th>
<th>NH4 (g)</th>
<th>NO2 (g)</th>
<th>NO3 (g)</th>
<th>PO4 (g)</th>
<th>SiO4 (g)</th>
<th>Faecal coliforms</th>
</tr>
</thead>
<tbody>
<tr>
<td>Municipal Wastewater Discharge</td>
<td>500</td>
<td>200</td>
<td>25</td>
<td>40</td>
<td>0.1</td>
<td>0.2</td>
<td>10</td>
<td>20</td>
<td>3.0E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Surgical Wastewater Discharge</td>
<td>500</td>
<td>200</td>
<td>25</td>
<td>40</td>
<td>0.1</td>
<td>0.2</td>
<td>10</td>
<td>20</td>
<td>3.0E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Urban Wastewater Discharges</td>
<td>500</td>
<td>200</td>
<td>25</td>
<td>40</td>
<td>0.1</td>
<td>0.2</td>
<td>10</td>
<td>20</td>
<td>3.0E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rural Wastewater Discharges</td>
<td>500</td>
<td>200</td>
<td>25</td>
<td>40</td>
<td>0.1</td>
<td>0.2</td>
<td>10</td>
<td>20</td>
<td>3.0E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total Wastewater Discharges</td>
<td>500</td>
<td>200</td>
<td>25</td>
<td>40</td>
<td>0.1</td>
<td>0.2</td>
<td>10</td>
<td>20</td>
<td>3.0E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer Factories Discharge</td>
<td>500</td>
<td>200</td>
<td>25</td>
<td>40</td>
<td>0.1</td>
<td>0.2</td>
<td>10</td>
<td>20</td>
<td>3.0E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer Factories Discharge</td>
<td>500</td>
<td>200</td>
<td>25</td>
<td>40</td>
<td>0.1</td>
<td>0.2</td>
<td>10</td>
<td>20</td>
<td>3.0E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer Factories Discharge</td>
<td>500</td>
<td>200</td>
<td>25</td>
<td>40</td>
<td>0.1</td>
<td>0.2</td>
<td>10</td>
<td>20</td>
<td>3.0E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer Factories Discharge</td>
<td>500</td>
<td>200</td>
<td>25</td>
<td>40</td>
<td>0.1</td>
<td>0.2</td>
<td>10</td>
<td>20</td>
<td>3.0E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 7.2 Estimated Loadings for Crude Sewage and Fertiliser Discharges to the Saco da Mangueira

The final point source input to the model represented the discharges from three fertiliser factories situated in the industrial district on the southern shore of Saco da Mangueira. There were no data available for these discharges, so loadings were estimated using the programme: Rapid Assessment of Pollution Sources (RAPS), which was originally developed by the World Health Organisation and updated by the University of Plymouth (http://www.ims.plym.ac.uk/giwa/) as part of the Global International Waters Assessment (GIWA, http://www.giwa.net/). The RAPS programme is based on the general export coefficient modelling approach, using coefficients derived from studies in the late 1960’s to calculate loadings for user specified discharges from domestic and industrial point sources.

An annual value of 900,000 tons P2O5 (Baumgarten et al., 1995) of phosphatic fertilisers (triple super phosphates, phosphate rock, H3PO4) was input to RAPS with resulting loadings of 789 kg/d phosphate and 1356 kg/d BOD.
7.2.5 Model Run Parameters

The model parameters consist of run parameters, water quality parameters and other physical parameters. The run parameters manage the processes to be simulated (Chapter 4), and the values used for the sensitivity analysis are listed in Table 7.3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start Time (s): 21/07/99 (relative to start time of flow results 19/04/99)</td>
<td>8035200</td>
</tr>
<tr>
<td>Timestep (s)</td>
<td>60</td>
</tr>
<tr>
<td>Storage Interval: the number of timesteps between output results</td>
<td>120 (2 hourly)</td>
</tr>
<tr>
<td>Initial Time of Day: used with times of sunrise and sunset in the calculation of light intensity to account for diurnal variation of algal growth (hours after midnight)</td>
<td>0</td>
</tr>
<tr>
<td>Time of Sunrise (hours after midnight)</td>
<td>7</td>
</tr>
<tr>
<td>Time of Sunset (hours after midnight)</td>
<td>20</td>
</tr>
<tr>
<td>Calculate Light Limitation: necessary for algal growth</td>
<td>YES</td>
</tr>
<tr>
<td>Initial Conditions: activates a file for each water quality variable describing spatial variation for initial and boundary conditions</td>
<td>YES</td>
</tr>
<tr>
<td>Coliforms: switch to specify the simulation of coliforms</td>
<td>YES</td>
</tr>
<tr>
<td>Reactions: switch to specify the oxygen balance processes</td>
<td>YES</td>
</tr>
<tr>
<td>Ecosystem: switch to specify the processes related to primary production</td>
<td>YES</td>
</tr>
<tr>
<td>Settling: switch to specify the deposition/erosion of particulate matter</td>
<td>YES</td>
</tr>
<tr>
<td>Type of Advection: 1 = standard method of characteristics, 4 = hybrid characteristics and centred scheme</td>
<td>1</td>
</tr>
<tr>
<td>Diffusion Step: diffusion is calculated isotropically</td>
<td>YES</td>
</tr>
<tr>
<td>Diffusion: horizontal diffusivity of water quality variables (m²/s)</td>
<td>3</td>
</tr>
</tbody>
</table>

Table 7.3 Model Run Parameters for the Sensitivity Analyses

The sensitivity of the model with respect to water quality parameters and other physical parameters such as settling velocity is investigated in Section 7.3 below.
7.3 Sensitivity Analysis of the Water Quality Parameters

Following the prescription of initial and boundary conditions, and pollutant inputs, the next stage was to undertake a sensitivity analysis of the kinetic coefficients used in the model to regulate the biochemical interactions between variables. The sensitivity analysis was undertaken in two phases: firstly, a simple investigation of coliform bacteria using the COLIFORMS function of WQFLOW-2D, and secondly an investigation of nutrients and algal processes using the REACTIONS, ECOSYSTEM, and SETTLING components of the model.

7.3.1 Modelling Bacteria

The modelling of coliform bacteria was selected at this stage because it is the most straightforward variable to model in WQFLOW-2D in the sense that it requires just one fixed first order decay rate, $k$, commonly expressed as $T_{90}$ (hours) (see Chapter 4, Section 4.3.11). $T_{90}$ values are commonly used in mathematical models to help predict the microbial impact of sewage discharges on receiving waters, and hence, provide guidance for the design of sewage treatment schemes that focus on achieving bacterial water quality standards for the protection of designated waters for uses such as bathing and shellfish cultivation.

In reality, $T_{90}$ values are highly variable because bacterial dynamics are influenced by a complex combination of physiochemical factors including dilution and dispersion; the action of sunlight intensity and duration (irradiance); death; temperature and salinity; algal toxins; bacteriophages; suspended matter and sedimentation; nutrients; pH; dissolved oxygen; and predation. Of these, it is widely accepted that the effects of sunlight, temperature, salinity and turbidity are the salient factors, and coliforms die most rapidly in warm, clear seawater under conditions of strong sunlight. Accordingly, various model
formulations have been derived from both *in vitro* and *in situ* experiments over recent decades to express bacterial mortality rate as a function of different environmental parameters, e.g. Chamberlain and Mitchell (1978); Mancini (1978); Lantrip (1983); Bowie *et al.* (1985); Thomann & Mueller (1987); Solic & Krstulovic (1992); Canale *et al.* (1993); Auer & Niehaus (1993); Chapra (1997), and these formulations and methods have been comprehensively reviewed by Merrett & Weatherley (2004).

Experiments conducted by a research team at the University of Cardiff (Lin *et al.* 2001; Harris *et al.*, 2002; Kashefipour *et al.*, 2002; Falconer & Lin, 2003) have shown through hydro-environmental modelling investigations and field measurements, that faecal coliform levels vary significantly when a dynamic decay rate dependent on diurnal variations in sunlight intensity, water temperature and irradiance is applied, compared with the traditional use of a constant decay rate, as used by WQFLOW-2D. Further refinements to this work *viz.* the inclusion of sediment-related bacterial processes, have been achieved through a recent study commissioned by the Environment Agency and undertaken by the University of Cardiff and the Centre for Research into Environment and Health (The University of Wales, Aberystwyth). This study resulted in the development of empirical relationships between $T_{90}$ and turbidity for irradiated and dark conditions, which have been incorporated into a hydrodynamic model as real-time variable $T_{90}$ values which vary with the temporally and spatially modelled suspended solid concentrations, and the diurnal pattern of solar radiation (Environment Agency, 2004 unpublished).

A sample of coliform decay rates from *in-situ*, laboratory, and modelling experiments quoted in the literature together with environmental conditions and the equivalent values of $T_{90}$ are given in Table 7.4.
There is clearly a large variation in the range of decay rates for coliforms with $T_{90}$ values generally between 0.5 hrs to several days depending on environmental conditions. Faecal coliform survival is generally extended in cool, freshwater conditions, with high turbidity and during the hours of darkness. It is therefore rather difficult to define an appropriate value for modelling purposes without information from site specific studies.

Although most numerical modelling tools simplify the complex processes involved in the decay of coliform bacteria, such predictions would not be possible using traditional scaled physical models (Falconer & Lin, 2003), therefore, it was considered that the modelling of bacteria would provide valuable information on advection in the study area, and should take the form of a comparative study for water quality management scenarios such as the relocation of sewage outfalls and bacterial loading reduction (see Chapter 8). Model scenarios would result in a range of possible coliform levels as a first order approximation.
that could be compared with levels of bacteria permitted for the system under local, national, and international water quality legislation.

Initial simulations were carried out for the 31 day period from 21\textsuperscript{st} July to 20\textsuperscript{th} August 1999 to investigate model sensitivity to variations in $T_{90}$ of 6, 12, 24, 48, 72 and 120 h. Contours of the maximum concentration of coliforms for each simulation are presented in Figures 7.3a to f, and results plotted as time series in Figures 7.4a to d. The four locations for the time series are shown in Figures 7.2 and 7.3f:

- 'Diamante' in the lower estuary and distant from the direct influence of pollutant inputs (397429E, 6465547N);
- 'Buoy 1' in lower estuary approximately 2km from the entrance to Saco da Mangueira (398812E, 6451486N);
- French Bridge at the entrance to Saco da Mangueira (397398E, 6452461);
- the centre of Saco da Mangueira (394093E, 6450966N).

The results showed the model to be hypersensitive to bacterial mortality with maximum concentrations varying by up to three orders of magnitude for $T_{90}$ values between 6 and 120 h, and the area impacted by high concentrations significantly increasing each time the $T_{90}$ was doubled. This clearly demonstrated the importance of specifying an appropriate mortality rate for the system in terms of determining the impact of wastewater plumes, which is an important requirement for the design of wastewater treatment schemes.
It is also important to note that since the model is depth-averaged, concentrations are likely to be under-predicted for surface waters when saline water is present, on account of the buoyancy of a plume of sewage in reality.

The time series presented in Figure 7.4a-d show the level of European Commission Bathing Waters Directive 76/160/EEC (CEC, 1976) mandatory standard for faecal coliforms of 2000 no./100ml at each location. Model results marginally exceed this standard for $T_{90}$ values greater than 24 hrs in the lower estuary, however, bacterial water quality within the Saco da Mangueira is very poor for all values greater than 12 hrs. The levels at French Bridge were at least an order of magnitude higher due to the proximity to the main sewage discharge for the city.
The dotted line in Figure 7.4b indicates the landward component of the wind, and when compared with model results in the main channel of the lower estuary at Buoy 1, it is apparent that the concentration of coliforms decreases when associated with seaward winds, which can be attributed to the combination of fluvial flow and winds from the northerly sectors causing an increase in horizontal dispersion, enhancing mass transport along the major axis of the estuary.

With respect to defining an appropriate \( T_{90} \) for the lower estuary for use in subsequent modelled scenarios, there were not sufficient field data to compare with the model results, however, it was considered that values of 24 and 72 h would be appropriate to reflect the...
general range of environmental conditions typical for the area such as the warm waters of
the bay and estuary (average ~ 19°C), and predominance of freshwater from the Patos
lagoon and river inputs, combined with very high background levels of suspended solids
(~50 mg/l), which tend to enhance the longevity of bacteria by reducing the penetration of
light through the water column. Laboratory experiments to evaluate bacterial mortality
rates typical for the study area are required for a higher level of confidence in future model
predictions, and a programme of bacterial water quality monitoring should be implemented
to assess current levels of pollution in the Saco da Mangueira. Results for the various
management scenarios conducted to evaluate the impact on bacterial water quality by
relocating outfalls and adding sewage treatment are presented in Chapter 8.

7.3.2 Modelling Nutrients and Primary Productivity

The water quality reactions and primary productivity modules within WQFLOW-2D
comprise a system of eighteen state variables, the interactions of which are represented by
numerical equations employing a set of kinetic rate constants. There are a total of 34
kinetic parameters which control the process reactions for the biochemical interaction of
water quality variables; the balance of oxygen and nutrients; and algal growth, which have
been defined in Chapter 4, Section 4.3.

The values of the kinetic parameters are implicitly functions of time and space (Beck,
1983) since they can vary with other variables such as temperature and water movement,
therefore, in reality, values are not constant and will lie within a range according to
laboratory or field measurements. There is a consensus amongst water quality modellers
that model calibration or parameter estimation is largely a process of iteration, and with
large numbers of state variables and water quality parameters, it is not possible to perform
a rigorous calibration and validation. Consequently, it is usual to direct calibration effort
to those parameters to which the model is most sensitive, until an acceptable agreement
with measured water quality variables is achieved, with subsequent fine tuning of other
less critical parameters.

Following this approach, a set of kinetic parameters was compiled from the literature
relating to similar model formulations (since there were no in-situ measurements for the
Patos System), and these are presented in Table 7.5, together with the values used for the
sensitivity tests and final values obtained from the calibration (in bold).

In addition to the values presented in Table 7.5, a typical temperature factor from the
literature of 1.0047°C was used in the expressions for the decay of organic materials and
the nitrification of ammoniacal nitrogen. The light limitation factor was set to a constant
value of 1 to negate the need for spatially or temporally varying sunlight conditions for
which a dataset is required. As described in Chapter 4, chlorophyll-a is represented in the
model by the proportion of carbon in the algal biomass (by dry weight), i.e. algal carbon
(HR Wallingford, 2000). In reality, the amount of carbon in the form of chlorophyll-a
depends on the species of phytoplankton, but is denoted in WQFLOW-2D by a single
representative species. A typical ratio of 0.02 was used, i.e. 1/50 of the algal carbon is
chlorophyll-a.
### Table 7.5  Sensitivity Analysis of the Kinetic Parameters

The procedure used for the sensitivity analyses was to model initially a mid-value for each parameter range, and then to adjust each parameter in isolation to the upper and lower limits of the feasible range. This was generally achieved by multiplying the mid-value by 0.5 and 2, or until an acceptable degree of variation from measured variables was reached.

A general rule of thumb for the required performance of an estuary water quality model is that 70% of nutrient or dissolved oxygen predictions should lie within ±20% of the observations (Bartlett, 1998). However, given that the initial and boundary conditions for

### Parameter/Coefficient

<table>
<thead>
<tr>
<th>Reactions</th>
<th>Reported Range</th>
<th>Values for Sensitivity Analysis (optimum result in bold)</th>
<th>Source of Reported Values (ranges cited from various field and laboratory experiments)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Denitrification Reaction Rate (at 20°C) (day⁻¹)</td>
<td>0.1 - 0.2</td>
<td>0.115; 0.23; 0.46</td>
<td>Di Toro et al., 1978</td>
</tr>
<tr>
<td>Hydrolysis Reaction Rate (at 20°C) (day⁻¹)</td>
<td>0.008 - 4.24 (median = 0.23)</td>
<td>0.115; 0.23; 0.46</td>
<td>Bowie et al., 1985</td>
</tr>
<tr>
<td>Fast BOD Decay Rate (at 20°C)</td>
<td>0.03 - 0.3</td>
<td>0.13; 0.26</td>
<td>Beck, 1978; Bowie et al., 1985</td>
</tr>
<tr>
<td>Nitrification Reaction Rate (at 20°C) (day⁻¹)</td>
<td>0.03 - 0.1</td>
<td>0.0185; 0.037; 0.039; 0.074; 0.1; 0.2</td>
<td>Bowie et al., 1985</td>
</tr>
<tr>
<td>Respiration Rate (at 20°C) (mCW)</td>
<td>0.03 - 0.1</td>
<td>0.0185; 0.037; 0.039; 0.074; 0.1; 0.2</td>
<td>Bowie et al., 1985</td>
</tr>
<tr>
<td>Erosion Rate (kg/m²s)</td>
<td>0.001</td>
<td>0.0005</td>
<td>typical default value for model</td>
</tr>
<tr>
<td>Algae &amp; Detritus Settling Velocities (m/s)</td>
<td>0; 1x10⁻³; 1x10⁻⁷; 1x10⁻⁷; 1x10⁻⁷; 1x10⁻⁷</td>
<td>typical default value for model</td>
<td></td>
</tr>
</tbody>
</table>

### Lesssystem

| Chlorophyll To Carbon Ratio | 0.01 - 0.1 | 0.01; 0.0125; 0.015; 0.02; 0.033 | Di Toro et al., 1978; Beck, 1978; Bowie et al., 1985 |
| Critical Temperature for Production (°C) | 23 | typical default value for model |
| Half Saturation Constant For Nitrate | 0.0014 - 0.4 | 0.005; 0.02; 0.2 | Di Toro et al., 1978; Beck, 1978; Bowie et al., 1985; Chapra, 1997 |
| Half Saturation Constant For Phosphate | 0.001 - 0.1 | 0.001; 0.014; 0.024; 0.024; 0.055 | Di Toro et al., 1978; Beck, 1978; Bowie et al., 1985; Chapra, 1997 |
| Light Extinction Coefficient For Algae (m⁻¹) | 0.5; 0.85; 1.5 | typical default value for model |
| Light Intensity | 1; 3; 5; 10 | typical default value for model |
| Maximum Algal Growth Rate (day⁻¹) | 1 - 3 | 0.5; 1.5; 2.4 | Di Toro et al., 1978; Bowie et al., 1985; Chapra, 1997 |
| Maximum Respiration Rate (at 20°C) (day⁻¹) | 0.015 - 0.25 | 0.02 | Di Toro et al., 1978; Beck, 1978; Bowie et al., 1985; Thomann & Mueller, 1987 |
| Mortality Rate For Algae (day⁻¹) | 0.003 - 0.1 | 0.05; 0.15; 0.25; 0.35; 1 | Bowie et al., 1985 |
| Nitrate To Carbon Ratio In Algae | 0.05 - 0.43 | 0.16 | Beck, 1978; Bowie et al., 1985 |
| Phosphorus To Carbon Ratio In Algae | 0.024 - 0.05 | 0.024 | Bowie et al., 1985; Thomann & Mueller, 1987 |
the model were average values from the water quality field data, with no time series available on a more detailed scale to compare with concurrent model predictions, the most suitable option was to calculate the mean concentration of each output variable, and assess these against the mean observed concentrations at various locations in the estuary and Saco da Mangueira.

The measure chosen to assess the model output against field observations was the Relative Mean Absolute Error (RMAE) (Walstra et al., 2001) which is a dimensionless quantity defined as the mean of the absolute differences between predictions and observations, divided by the mean of the observations. The RMAE values are quantified as Excellent (<0.2); Good (0.2 – 0.4); Reasonable (0.4 – 0.7); Poor (0.7 – 1.0); and Bad (>1.0).

The water quality variables used for the assessment were dissolved oxygen; total biochemical oxygen demand; ammoniacal nitrogen; nitrate; phosphate; and chlorophyll-a. These quantities were extracted from the model output files at the same four locations used during the assessment of coliforms in Section 7.3.1: lower estuary at Diamante (Dia) and Buoy 1 (Buo); the entrance to Saco da Mangueira at French Bridge (Fre) and the centre of Saco da Mangueira (Cen).

A total of sixty-two model simulations were completed for the period 21st July to 20th August 1999, and as an overall introduction to the discussion of the results, the mean concentrations for each variable from the model and observations are presented in Figures 7.5a-f. The simulations have been ordered on the x-axis from left to right starting with the poorest overall calibration. The coloured arrows in Figure 7.5f are denoted in Table 7.6 and indicate groups of simulations for the most important kinetic parameters, which will be discussed with reference to Figures 7.6 to 7.10.
Chapter 7 - Calibration and Validation of WQFLOW-2D

Figure 7.5  Mean Model Results with Mean Measured Concentrations

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Value (Model Run)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Hydrolysis Reaction Rate and Fast BOD Decay Rate</td>
<td>0.115 (82); 0.23 (80); 0.46 (90)</td>
</tr>
<tr>
<td></td>
<td>Reaeration Rate</td>
<td>0.0185; 0.037 (126); 0.039; 0.074; 0.1 (125); 0.2 (124)</td>
</tr>
<tr>
<td></td>
<td>Maximum Growth Rate for Algae</td>
<td>0.5 (109); 1.5 (197); 2 (115); 4 (118)</td>
</tr>
<tr>
<td></td>
<td>Mortality Rate for Algae</td>
<td>0.05 (91); 0.15 (100); 0.25; 0.35 (80); 1 (86)</td>
</tr>
<tr>
<td></td>
<td>Chlorophyll to Carbon Ratio</td>
<td>0.01 (139); 0.0125 (156); 0.015 (197); 0.02 (134); 0.033 (137)</td>
</tr>
<tr>
<td></td>
<td>Light Intensity</td>
<td>1 (80); 3 (85); 5 (197); 10 (87)</td>
</tr>
<tr>
<td></td>
<td>Mud, Algae &amp; Detritus Settling Velocities</td>
<td>0 (108); 1x10^{-8} (115); 1x10^{-7} (114); 1x10^{-6} (113); 1x10^{-5} (112); 1x10^{-4}; 1x10^{-3}</td>
</tr>
</tbody>
</table>

Table 7.6  Kinetic Parameters of Primary Importance
Firstly, the most conspicuous feature illustrated in Figures 7.5e is the calibration of phosphate. It became evident during the sensitivity analyses that mean phosphate predictions in the Saco da Mangueira were very high, giving overall RMAE values > 1, and it was not possible to reduce these levels sufficiently by varying the kinetic parameters controlling algal growth within a realistic range.

The first reason for this discrepancy was considered to be the exclusion from the model of the complex processes controlling the dynamics of phosphorus, which include the adsorption of phosphate onto suspended or deposited matter, and biological cycling. Phosphate adsorption is dependent on the level of dissolved oxygen and enhanced by high phosphorus levels; pH in the range of 3-7; higher temperatures; and low salinities, all of which apply in the Saco da Mangueira. In order to model phosphorus more accurately, these effects would need to be quantified by site specific studies to evaluate the sorption coefficient for phosphorus, which could subsequently be integrated into the model by a framework for sediment oxygen demand.

The most significant source of error of the predicted levels of phosphate in the Saco da Mangueira was considered to be the estimated input of phosphate from the fertiliser plant. Concentrations of phosphate measured from water samples collected adjacent to the main fertiliser factory discharge (395556E, 6451229N) ranged from 0.015 mg/l to 1.028 mg/l with a mean value of 0.375 mg/l (n = 38), whereas levels predicted at the same location using the initial estimated loading from the fertiliser factory ranged from 0.121 mg/l to 1.855 mg/l with a mean value of 0.970 mg/l, indicating that mean predicted concentrations were inflated by a factor of ~2.5. In the absence of measured loadings from the fertiliser plant, a less ideal course of action was taken to gradually reduce the phosphate loading from the fertiliser factory until predicted concentrations in the Saco da Mangueira were
closer to the average observations. This action was successful and also had the effect of improving the model predictions for the other nutrient variables, but highlights the imperative requirement for pollutant loadings to be quantified from field measurements.

Figure 7.6 Modelled Concentrations of Dissolved Oxygen, Nitrate, and Chlorophyll-a with Varying Values of the Maximum Algal Growth Rate
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The model was most sensitive to three of the parameters controlling algal growth, namely, the chlorophyll to carbon ratio; the maximum algal growth rate; and the mortality rate for algae. The most notable results are discussed as follows:

The effects of varying the **Maximum Algal Growth Rate** on concentrations of dissolved oxygen, nitrate, and chlorophyll-a are shown above in Figure 7.6 for the estuary and Saco da Mangueira. The slowest rate of 0.5 /day (pink line) resulted in low concentrations of both dissolved oxygen (<6 mg/l) and chlorophyll-a (<2 mg/l) together with the substantial build-up of nitrate in the Saco da Mangueira. The results for dissolved oxygen clearly show that primary production was not occurring, since the typical diurnal pattern of daytime oxygen production due to photosynthesis, followed by night time oxygen depletion from respiration was not apparent. The fastest algal growth rate of 4 /day (blue line) resulted in mean chlorophyll-a concentrations of 8.70 mg/l and 34.16 mg/l in the estuary and Saco da Mangueira respectively, which were twice as high as observed mean concentrations. A rate of 1.5 /day (black line) was found to give the closest overall match of mean model results with observations.

The effects of varying the **Mortality Rate for Algae** on concentrations of dissolved oxygen, nitrate, and chlorophyll-a are shown in Figure 7.7 for the estuary and Saco da Mangueira. A low rate of 0.05 /day (pink line) resulted in mean levels of chlorophyll-a to be elevated by factors of 3.3 and 1.5 for the Saco da Mangueira and estuary respectively compared with mean observed levels. A rate of 0.15 /day (black line) gave much better results for chlorophyll-a in the estuary, however levels in the Saco da Mangueira remained elevated by a factor of 2.5. A high mortality rate of 1 /day (blue line) caused primary productivity to stop in both the Saco da Mangueira and estuary with a corresponding increase in the concentration of nitrate in the bay. The optimum value was found to be
0.35/day which was later fine-tuned to 0.25/day following further sensitivity tests varying other kinetic parameters.

![Modelled Concentrations of Dissolved Oxygen, Nitrate, and Chlorophyll-a with Varying Values of the Mortality Rate for Algae](image)

**Figure 7.7** Modelled Concentrations of Dissolved Oxygen, Nitrate, and Chlorophyll-a with Varying Values of the Mortality Rate for Algae

The effects of varying the Chlorophyll to Carbon Ratio on the concentration of chlorophyll-a are shown in Figure 7.8 for the estuary and Saco da Mangueira. The model
was clearly sensitive to small changes in this parameter which ranged between 0.033 (blue line) and 0.01 (pink line). The optimum ratio was found to be 0.015 (black line).

![Figure 7.8 Modelled Concentrations of Chlorophyll-a with Varying Values of the Chlorophyll to Carbon Ratio](image)

The effects of varying the **Settling Velocity** on concentrations of dissolved oxygen, nitrate, and chlorophyll-a are shown in Figure 7.9 for the estuary and Saco da Mangueira. Values greater than \(1 \times 10^{-4}\) m/s (blue and pink lines) i.e. >8.6 m/d, caused particles to settle too rapidly giving poor overall correlations with measured data. Settling velocities between \(1 \times 10^{-5}\) m/s and \(1 \times 10^{-8}\) m/s (i.e. 0.86 to 0.001 m/d) gave a much better correlation with measured data and are in the range of typical settling velocities found in natural waters for clay sized particles (0.3 – 1 m/d) and phytoplankton (0.08 – 2 m/d), (Chapra, 1997). Site specific studies to evaluate the factors affecting settling velocities for phytoplankton, suspended sediments and detritus (density, size, shape, turbulence, etc.) should be conducted to give a greater degree of confidence for future modelling studies.
The effects of varying the **Light Intensity** on concentrations of nitrate and chlorophyll-a are shown in Figure 7.10 for the estuary and Saco da Mangueira. The results showed that primary productivity was limited in the lower estuary when the value of light intensity was 1 (green line), and excessive growth occurred in the Saco da Mangueira for values of 5 (blue line) and 10 (pink line). These tests were carried out in the early stages of the
calibration when phosphate input to the Saco da Mangueira proved to be too high. Following a reduction to the input of phosphate from the fertiliser plant, the closest correlation with the average observed concentrations of chlorophyll-a and nitrate for both the estuary and the bay was obtained with a value of 5 (black line).

![Modelled Concentrations of Nitrate, and Chlorophyll-a with Varying Values of the Light Intensity](image)

**Figure 7.10** Modelled Concentrations of Nitrate, and Chlorophyll-a with Varying Values of the Light Intensity

On the time and space scales selected for this project, the model was found to be less sensitive to other kinetic parameters such as the Hydrolysis Reaction Rate; Fast BOD Decay Rate; and Reaeration Rate, however these parameters are known to be important and would need further scrutinisation during future modelling studies conducted on a more detailed time scales, for example, when investigating daily or weekly water quality variations.
The statistics for the final calibration (run 197) are presented in Table 7.7, with results at Diamante, French Bridge, and the centre of Saco da Mangueira shown in Figures 7.11 to 7.13 respectively, together with the mean, standard deviation (vertical bars) and 95th percentile (red line) of the observations. RMAE values averaged over all four test locations were: Dissolved Oxygen = 0.235; Total BOD = 0.651; Ammoniacal Nitrogen = 0.385; Nitrate = 0.287; Phosphate = 0.269; and Chlorophyll-a = 0.145, and overall statistics showed that 42% of predictions were Excellent (RMAE <0.2); 29% were Good (RMAE 0.2 - 0.4); 17% were Reasonable (RMAE 0.4 - 0.7); 8% were Poor (RMAE 0.7 - 1.0); and just 4% were Bad (RMAE >1).

<table>
<thead>
<tr>
<th>Water Quality Variable</th>
<th>Site</th>
<th>Mean Annual Observation</th>
<th>Mean Model Output Concentration</th>
<th>RMAE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dissolved Oxygen (mg/l)</td>
<td>Dia</td>
<td>9.3</td>
<td>7.4</td>
<td>0.205</td>
</tr>
<tr>
<td></td>
<td>Buo</td>
<td>9.3</td>
<td>7.5</td>
<td>0.195</td>
</tr>
<tr>
<td></td>
<td>Fre</td>
<td>9.2</td>
<td>6.5</td>
<td>0.281</td>
</tr>
<tr>
<td></td>
<td>Cen</td>
<td>9.2</td>
<td>6.7</td>
<td>0.261</td>
</tr>
<tr>
<td>Total BOD (mg/l)</td>
<td>Dia</td>
<td>1.6</td>
<td>0.2</td>
<td>0.891</td>
</tr>
<tr>
<td></td>
<td>Buo</td>
<td>1.6</td>
<td>0.2</td>
<td>0.863</td>
</tr>
<tr>
<td></td>
<td>Fre</td>
<td>3.1</td>
<td>2.5</td>
<td>0.192</td>
</tr>
<tr>
<td></td>
<td>Cen</td>
<td>3.1</td>
<td>1.1</td>
<td>0.657</td>
</tr>
<tr>
<td>Ammoniacal Nitrogen (mg/l)</td>
<td>Dia</td>
<td>0.044</td>
<td>0.034</td>
<td>0.241</td>
</tr>
<tr>
<td></td>
<td>Buo</td>
<td>0.044</td>
<td>0.044</td>
<td>0.014</td>
</tr>
<tr>
<td></td>
<td>Fre</td>
<td>0.239</td>
<td>0.529</td>
<td>1.214</td>
</tr>
<tr>
<td></td>
<td>Cen</td>
<td>0.239</td>
<td>0.222</td>
<td>0.072</td>
</tr>
<tr>
<td>Nitrate (mg/l)</td>
<td>Dia</td>
<td>0.163</td>
<td>0.129</td>
<td>0.209</td>
</tr>
<tr>
<td></td>
<td>Buo</td>
<td>0.163</td>
<td>0.126</td>
<td>0.228</td>
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<td></td>
<td>Fre</td>
<td>0.130</td>
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<td></td>
<td>Cen</td>
<td>0.130</td>
<td>0.056</td>
<td>0.570</td>
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<tr>
<td>Phosphate (mg/l)</td>
<td>Dia</td>
<td>0.029</td>
<td>0.016</td>
<td>0.458</td>
</tr>
<tr>
<td></td>
<td>Buo</td>
<td>0.029</td>
<td>0.019</td>
<td>0.342</td>
</tr>
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<td></td>
<td>Fre</td>
<td>0.149</td>
<td>0.177</td>
<td>0.189</td>
</tr>
<tr>
<td></td>
<td>Cen</td>
<td>0.149</td>
<td>0.162</td>
<td>0.086</td>
</tr>
<tr>
<td>Chlorophyll-a (μg/l)</td>
<td>Dia</td>
<td>4.12</td>
<td>4.34</td>
<td>0.052</td>
</tr>
<tr>
<td></td>
<td>Buo</td>
<td>4.12</td>
<td>4.21</td>
<td>0.022</td>
</tr>
<tr>
<td></td>
<td>Fre</td>
<td>16.81</td>
<td>9.51</td>
<td>0.434</td>
</tr>
<tr>
<td></td>
<td>Cen</td>
<td>16.81</td>
<td>18.01</td>
<td>0.072</td>
</tr>
</tbody>
</table>

Table 7.7 Final Calibration Statistics
Chapter 7 - Calibration and Validation of WQFLOW-2D

Figure 7.11 Calibration at Diamante (Lower Estuary)
Figure 7.12  Calibration at French Bridge
Figure 7.13  Calibration at the Centre of Saco da Mangueira
Modelled concentrations of dissolved oxygen generally remained between 6 and 8 mg/l, which was slightly lower than the observed levels of between 7 and 10 mg/l. This discrepancy may have been due to an anomaly between the in-situ and laboratory measurements for equivalent samples where available. The in-situ readings were on average ~2.5mg/l less than the laboratory results used for the model, therefore there is some uncertainty with respect to the true concentration of dissolved oxygen.

Results for total BOD were under-predicted in the estuary, and to a lesser extent in the Saco da Mangueira, but predictions were excellent at French Bridge (close to the main sewage outfall for Rio Grande). This would indicate that there were other unquantified sources of BOD outside the influence of the main sewage discharge that were not included in the model. For example, BOD not simulated very successfully may be in part due to bottom decomposition being more pronounced in shallower systems (Chapra, 1997) since micro-organisms attached to the bed are generally more effective decomposers than those in the water column, so that shallower systems tend to exhibit higher BOD removal rates than deeper water. Sources of BOD at the bed are likely to have been underestimated in the model and field measurements are required to quantify this contribution.

Predictions of ammoniacal nitrogen were good to excellent at all locations apart from French Bridge where concentrations tended to be over-predicted by a factor of ~2. It was not possible to reduce these levels sufficiently by varying the nitrification reaction rate within a realistic range, therefore, it was concluded that the estimated input of ammoniacal nitrogen from the sewage discharge may have been too high, which highlights the imperative requirement for pollutant loadings to be quantified from field measurements.
Predictions of nitrate were also good to excellent at all locations apart from the centre of Saco da Mangueira where concentrations tended to be under-predicted by a factor of ~2, but still remained within the range of observed values. The overall model results for nitrogenous compounds were in good agreement with the observed data. This adds further support to the results of previous studies that suggested the whole of the Patos System is hypernutrified and likely to have a trophic status ranging from mesotrophic to eutrophic, which has been evidenced by the occurrence of persistent algal blooms studied by, for example, Yunes et al. (1995 and 1996).

Mean predicted levels of phosphate were closely correlated with the observed mean concentrations and remained within the range of observations throughout the simulation at all locations. Both modelled and observed concentrations in the Saco da Mangueira were around 0.15 mg/l which is five times higher than elsewhere, although levels of phosphate have been recorded of at least an order of magnitude higher than those expected in uncontaminated waters (0.031 mg/l) (Aminot & Chaussepied, 1983; Day et al., 1987; Pomeroy et al., 1965), and this is without doubt due to the wastewater discharges from the fertiliser factories which border the embayment.

Mean predicted levels of chlorophyll-a were also closely correlated with the observed mean concentrations and remained within the range of observations throughout the simulation at all locations. The diurnal patterns of photosynthesis and respiration are clearly identified in the Saco da Mangueira (Figure 7.13), where levels of dissolved oxygen and chlorophyll-a increase during photosynthetic daylight hours with a corresponding decrease in concentrations of nitrate, with the reverse occurring during the hours of darkness due to the process of respiration. This pattern was not shown by the time series of phosphate which would indicate that this is not the limiting nutrient for the bay,
which is clear from the excess of phosphate present due to discharges from the fertiliser factories.

The maximum levels of various water quality variables and minimum levels of dissolved oxygen reached during the final calibration are presented below in Figures 7.14a-f, and give a good indication of the general areas where highest concentrations are expected to occur.

![Figure 7.14 Maximum Levels of Water Quality Parameters During Calibration](image-url)
The distribution of salinity gives an indication of the difference in the advective characteristics of the estuary compared to the Saco da Mangueira and other shallow areas to the north of Rio Grande. These shallow areas are where the majority of the point source domestic and industrial inputs discharge, and as a consequence of reduced dilution and dispersion, high levels of nutrients and primary productivity (>10 mg/l chlorophyll-a) occur with corresponding low values of dissolved oxygen.

The results of the final calibration at Diamante (black lines), French Bridge (pink lines), and the centre of Saco da Mangueira (blue lines) are compared with water quality standards (green lines) in Figure 7.15. It is clear that water quality in the estuary is generally consistent with that expected for non-polluted estuaries. However, in the Saco da Mangueira, levels of dissolved available inorganic nitrogen and chlorophyll-a exceed the levels considered indicative of eutrophic conditions (0.168mg/l and 10 mg/l respectively), by an average factor of ~2, and for phosphate the average levels are ~5 times higher than elsewhere, and these results are consistent with the results given for field measurements described in Chapters 2 and 3.
Figure 7.15  Calibration Results Compared with Water Quality Standards
7.4 Model Validation

The water quality model has been calibrated using annual average conditions for the water quality variables, and water temperature (18.8°C), with hydrodynamic conditions representing the average length of time that water is expected to reside within the Saco da Mangueira. However, in order to assess the robustness of the model under a range of typical physical and chemical conditions, validation simulations are required. From Chapter 3 it was established that the water quality field measurements had low sampling frequencies on a seasonal scale particularly for the riverine inputs, and the available data could not be confirmed as being representative on this scale.

Therefore, validation simulations were conducted for three independent periods representing hydrodynamics for fast, mean, and slow flushing conditions ($T_f$), to confirm whether the model could continue to predict concentrations within the range of water quality measurements using the calibrated kinetic parameters. The validation periods were:

- 1st October to 1st November 2002 (Mean flushing $T_f = 33.3$ days);
- 1st May to 1st June 2003 (Fast flushing $T_f = 22$ days);
- 1st September to 1st October 1999 (Slow flushing $T_f = 44.5$ days).

An additional simulation was conducted to validate the model over a longer time period (15th May to 1st September 1999), together with two final simulations over this time period using average Summer and Winter water temperatures of 25°C and 13°C respectively. These additional simulations were not designed to represent true seasonal variation in water quality since the input variables were based on annual mean concentrations;
Chapter 7 - Calibration and Validation of WQFLOW-2D

however, it was important to evaluate whether model predictions remained within the range of measured concentrations when subjected to minimum and maximum water temperatures typical of the study area.

<table>
<thead>
<tr>
<th>Water Quality Variable</th>
<th>Site</th>
<th>Mean Annual Obs.</th>
<th>Mean Flushing (T&lt;sub&gt;r&lt;/sub&gt; = 33.3 days)</th>
<th>Slow Flushing (T&lt;sub&gt;r&lt;/sub&gt; = 44.5 days)</th>
<th>Fast Flushing (T&lt;sub&gt;r&lt;/sub&gt; = 22 days)</th>
<th>Mean Annual Temperature (18°C)</th>
<th>Mean Winter Temperature (13°C)</th>
<th>Mean Summer Temperature (25°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mean Output</td>
<td>RMAE</td>
<td>Mean Output</td>
<td>RMAE</td>
<td>Mean Output</td>
<td>RMAE</td>
<td>Mean Output</td>
</tr>
<tr>
<td>Dissolved Oxygen (mg/l)</td>
<td>Dia</td>
<td>9.3</td>
<td>7.4</td>
<td>0.212</td>
<td>7.3</td>
<td>0.217</td>
<td>7.3</td>
<td>0.225</td>
</tr>
<tr>
<td></td>
<td>Fre</td>
<td>9.2</td>
<td>6.6</td>
<td>0.268</td>
<td>6.7</td>
<td>0.291</td>
<td>6.5</td>
<td>0.284</td>
</tr>
<tr>
<td></td>
<td>Cen</td>
<td>9.2</td>
<td>6.8</td>
<td>0.274</td>
<td>6.7</td>
<td>0.265</td>
<td>6.8</td>
<td>0.300</td>
</tr>
<tr>
<td>Total BOD (mg/l)</td>
<td>Dia</td>
<td>1.6</td>
<td>0.2</td>
<td>0.883</td>
<td>0.2</td>
<td>0.884</td>
<td>0.2</td>
<td>0.881</td>
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<td>1.8</td>
<td>0.399</td>
<td>2.7</td>
<td>0.108</td>
<td>1.8</td>
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<tr>
<td></td>
<td>Cen</td>
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<td>0.9</td>
<td>0.704</td>
<td>1.2</td>
<td>0.610</td>
<td>0.9</td>
<td>0.696</td>
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<tr>
<td>Ammonium (mg/l)</td>
<td>Dia</td>
<td>0.044</td>
<td>0.031</td>
<td>0.309</td>
<td>0.028</td>
<td>0.369</td>
<td>0.037</td>
<td>0.160</td>
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<tr>
<td></td>
<td>Fre</td>
<td>0.239</td>
<td>0.383</td>
<td>0.603</td>
<td>0.584</td>
<td>1.442</td>
<td>0.387</td>
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<td>0.188</td>
<td>0.213</td>
</tr>
<tr>
<td>Nitrate (mg/l)</td>
<td>Dia</td>
<td>0.163</td>
<td>0.122</td>
<td>0.253</td>
<td>0.114</td>
<td>0.305</td>
<td>0.134</td>
<td>0.182</td>
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<tr>
<td></td>
<td>Fre</td>
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<td>0.123</td>
<td>0.055</td>
<td>0.131</td>
<td>0.012</td>
<td>0.140</td>
<td>0.079</td>
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<tr>
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<td>Cen</td>
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<td>0.602</td>
<td>0.067</td>
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<tr>
<td>Phosphate (mg/l)</td>
<td>Dia</td>
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<td>0.014</td>
<td>0.514</td>
<td>0.012</td>
<td>0.574</td>
<td>0.019</td>
<td>0.340</td>
</tr>
<tr>
<td></td>
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<td>0.130</td>
<td>0.126</td>
<td>0.203</td>
<td>0.362</td>
<td>0.137</td>
<td>0.079</td>
</tr>
<tr>
<td></td>
<td>Cen</td>
<td>0.149</td>
<td>0.130</td>
<td>0.128</td>
<td>0.180</td>
<td>0.207</td>
<td>0.140</td>
<td>0.059</td>
</tr>
<tr>
<td>Chlorophyll-a (µg/l)</td>
<td>Dia</td>
<td>4.12</td>
<td>4.35</td>
<td>0.055</td>
<td>4.71</td>
<td>0.143</td>
<td>3.75</td>
<td>0.089</td>
</tr>
<tr>
<td></td>
<td>Fre</td>
<td>16.81</td>
<td>7.81</td>
<td>0.535</td>
<td>11.09</td>
<td>0.340</td>
<td>7.32</td>
<td>0.564</td>
</tr>
<tr>
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<td>Cen</td>
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<td>13.95</td>
<td>0.170</td>
<td>18.98</td>
<td>0.129</td>
<td>14.56</td>
<td>0.134</td>
</tr>
</tbody>
</table>

Table 7.8 Validation Statistics

The statistics for the six validation simulations are presented in Table 7.8 above and Figure 7.16, and results are shown as time series at Diamante (Figures 7.17 and 7.20), French Bridge (Figures 7.18 and 7.21), and the centre of Saco da Mangueira (Figures 7.19 and 7.22), together with the mean, standard deviation (vertical bars) and 95 percentile (red lines) of the observations.

RMAE values averaged over all four test locations for the three validation runs conducted under varying hydrodynamic conditions were: Dissolved Oxygen = 0.244; Total BOD = 0.678; Ammoniacal Nitrogen = 0.402; Nitrate = 0.276; Phosphate = 0.250; and
Chlorophyll-a = 0.201, which were consistent with the results for the final calibration, as were the mean output concentrations, with at least 70% of predictions for all three simulations relating to Good to Excellent correlations, and >87% producing at least Reasonable correlations with measured data. Again, the poorest predictions were for BOD in the estuary and the Saco da Mangueira, and ammoniacal nitrogen at French Bridge.

![Figure 7.16 Validation Statistics](image)

The results presented in Figures 7.17 to 7.19 below indicate that the model is able to predict concentrations within the range of observations under varying hydrodynamic conditions typical of the area. Nutrient levels remained within the observed range of concentrations apart from an occasional over-prediction of ammoniacal nitrogen under conditions of slow flushing in the estuary. It is noted that output concentrations from the ‘slow flushing’ simulation (blue lines) are consistently higher than for other simulations, and this can be attributed to the longer time available for concentrations to build up.
Figure 7.17  Varying Flushing Characteristics at Diamante (Lower Estuary)
Figure 7.18  Varying Flushing Characteristics at French Bridge
Figure 7.19  Varying Flushing Characteristics at the Centre of Saco da Mangueira
The results for varying water temperature are presented in Figures 7.20 to 7.22, with the green lines representing the mean annual temperature of 18.8°C; the blue lines indicating 13°C; and the pink lines showing 25°C. Results were generally within the observed range, with RMAE values consistent with those calculated for the calibration and initial validation simulations (see Figure 7.16). RMAE values averaged over all four test locations for the three validation runs conducted under varying conditions of water temperature were: Dissolved Oxygen = 0.290; Total BOD = 0.712; Ammoniacal Nitrogen = 0.504; Nitrate = 0.253; Phosphate = 0.334; and Chlorophyll-a = 0.293, with at least 70% of predictions for mean and minimum temperature scenarios relating to Good to Excellent correlations, and >83% producing at least Reasonable correlations with measured data. However, the model predictions under maximum Summer conditions of water temperature (25°C) correlated slightly less well with the observations, even though at least 41% of predictions related to Good to Excellent correlations, and >79% produced at least Reasonable correlations.

Predicted dissolved oxygen concentrations were generally ~2 mg/l lower in the Summer and ~2 mg/l higher in the Winter compared with levels predicted under mean annual water temperatures, and this is consistent with the field measurements (see Figure 3.16, p. 75), and is attributed to the reduction in the solubility of oxygen with increasing temperature. A corresponding decrease in the concentrations of ammoniacal nitrogen and chlorophyll-a of the order of 0.1 mg/l and 1 µg/l respectively, and a slight increase in nitrate of ~0.3 mg/l, are apparent in the lower estuary (Figure 7.20) under summer conditions, and these patterns are even more pronounced by a factor of ~2 in the Saco da Mangueira (Figure 7.22), and are also consistent with field data.
Figure 7.20 Validation at Diamante (Lower Estuary)
Figure 7.21 Validation at French Bridge
Figure 7.22  Validation at the Centre of Saco da Mangueira
In conclusion, these calibration and validation exercises have demonstrated that WQFLOW-2D appears to consistently simulate concentrations of most of the water quality variables studied within the range of observed concentrations both within the Saco da Mangueira and in the lower Patos Estuary, and under a range of hydrodynamic conditions typical for the area. The model is therefore considered fit for purpose as a management tool for investigating mean water quality conditions. Further calibration will be necessary to conduct modelling studies requiring a higher temporal resolution.
Chapter 8

Scenarios for the Management of Water Quality

8.1 Introduction

The water quality model has been calibrated using mean annual observed data for water quality parameters (dissolved oxygen, ammonia, nitrate, phosphate, chlorophyll-a, and coliform bacteria), and hydrodynamics representing the average flushing time of Saco da Mangueira of ~31 days (21st July to 20th August 1999). The model has also been validated under varying conditions of wind and river flow representing fast flushing of ~22 days (May 2003) and slow flushing of ~45 days (September 1999), as well as longer term simulations (19th April to 1st October 1999) using different water temperatures to quasi-simulate seasonal variation.

The use of hydrodynamic and ecological models provide the potential for investigating solutions and environmental impacts from engineering works, such as (i) development of the shoreline and dredging for navigational access or (ii) to improve the flushing of waters with restricted exchange to help mitigate problems produced by the input of excess nutrients or other pollutants.

This Chapter describes the results of a series of modelled management scenarios investigating the flushing characteristics and the water quality of the lower estuary and Saco da Mangueira by comparing different loadings from discharges of industrial and domestic effluents at several locations and under a range of hydrodynamic conditions.
8.2 Modelled Scenarios

Three sets of hypothetical scenarios were modelled as follows:

a. The impact on the water exchange at the entrance to the Saco da Mangueira was investigated by initially widening the entrance, and secondly, by creating a deep channel from the entrance to the main Access Channel of the estuary.

b. The impact on the water quality in the Saco da Mangueira was investigated by altering the pollutant loadings and outfall locations of the main domestic sewage discharges of Rio Grande and comparing the results with the water quality from current outfall locations and treatment:

   i. The main Rio Grande outfall was extended by 2 km to the 10m depth contour of the access channel of the estuary;

   ii. The main Rio Grande outfall was relocated to the southern end of the Saco da Mangueira;

   iii. The pollutant loadings were reduced to represent secondary treated effluent;

   iv. The sewage outfalls were removed.

c. The impact on the water quality of the Saco da Mangueira was investigated by removing the discharge from the fertiliser plant.
8.3 Modifying the width and bathymetry of the entrance to Saco da Mangueira to investigate flushing characteristics

The modifications made to the model geometry at the entrance to Saco da Mangueira are presented in Figure 8.1. Panel 8.1a shows the existing bathymetry with north to south, and east to west sections below. Panel 8.1b shows the bathymetry interpolated by the MATISSE software following removal of the peninsula of land to increase the width of the entrance from 195m to 950m. This increased the cross-sectional area at the entrance by a factor of 4. Panel 8.1c shows the bathymetry for an 8m channel perpendicular to the existing entrance connecting to the 10m depth contour of the main channel of the estuary.

Figure 8.1 Modifying Bathymetry at the Entrance to Saco da Mangueira
TELEMAC-2D was run for 31 days from 1st May to 1st June 2003 with a unit tracer in the Saco da Mangueira (as described in Chapter 6) to generate results for the calculation of the e-folding flushing time for each scenario, and results for the east (U) and north (V) components of velocity were extracted at 15 minute intervals. The east component for each modelled scenario is shown as a time series in Figure 8.2, and maximum flows in the vicinity of the entrance and the lower estuary are presented as contours in Figure 8.3a to f.

Figure 8.2 Modelled Flows Across the Entrance to Saco da Mangueira (Positive values indicate flow from West to East)

From Figure 8.2 the current velocities across the entrance under existing conditions (green line) ranged from -1.07 m/s to 0.8 m/s, with positive values indicating flow from west to east, whereas for the entrance widening scenario (blue line) the velocities were reduced significantly and ranged between -0.15 m/s and 0.17 m/s. The scenario incorporating an 8m channel (red line) also caused a reduction in current velocities at the entrance which ranged from -0.67 m/s to 0.58 m/s.
Figure 8.3  Maximum Flows for Modelled Scenarios for Widening the Entrance to Saco da Mangueira

From Figure 8.3 it is evident that the effects on current velocity from the modelled scenarios were apparent in the near-field only, and did not affect water movement at distances greater than ~1 km from the entrance to the Saco da Mangueira. Widening the entrance simply slowed water movement to compensate for the additional volume exchange across the entrance, although current speeds were increased by a factor of ~3 in the areas immediately to the east and west of the entrance (Figure 8.3b), which may provide improved local dispersion of pollutants discharged from the main outfalls of Rio Grande which are currently located in this area. It should be noted that any modifications
to the bed will also have an impact on the patterns of sediment movement in the area and this would need to be quantified.

With respect to the flushing characteristics of Saco da Mangueira, the concentrations of total tracer extracted at daily intervals and expressed as percentages of the total initial concentration of tracer in the bay, are presented in Figure 8.4.

![Figure 8.4 Flushing Times for Modelled Scenarios for Widening the Entrance to Saco da Mangueira](image)

It can been seen that widening the entrance caused a slight decrease in the e-folding flushing time from 22 days to 21.2 days, whereas the 8m channel caused the e-folding flushing time to increase to 31.7 days. Further long-term water quality and sediment transport simulations are required together with a cost benefit analysis to assess whether the slight improvement in water exchange and localised increase in current velocities would justify the cost of the engineering required to widen the entrance of the bay.
8.4 Water Quality Scenarios

The impact on the water quality in the Saco da Mangueira and lower Patos lagoon estuary was investigated by altering the pollutant loadings and outfall locations of the main domestic sewage discharges of Rio Grande and comparing the results with the water quality from current outfall locations and treatment as described in Section 8.2. The different outfall locations are represented by the yellow triangles in Figure 8.5.

![Figure 8.5](image)

Figure 8.5 Locations of Sewage Outfalls for Model Scenarios

A total of 24 simulations were completed for three outfall locations: the existing location of the main Rio Grande discharge; the outfall relocated to the southern end of Saco da Mangueira; and the outfall extended by 2 km to the 10m depth contour of the access channel of the estuary. The hydrodynamics were for both slow and fast flushing conditions, pollutant loadings were for crude and secondary treated effluent, and coliform bacteria $T_{90}$ values were 24 and 72 hours. For comparative purposes an additional three scenarios were completed under fast and slow flushing conditions without any sewage
outfalls, and without the discharge from the fertiliser plant. The scenarios are listed in Table 8.1.

<table>
<thead>
<tr>
<th>Model Run</th>
<th>Period</th>
<th>Flushing Time (days)</th>
<th>$T_{90}$</th>
<th>Outfall Location</th>
<th>Sewage Treatment</th>
</tr>
</thead>
<tbody>
<tr>
<td>161</td>
<td>Sep 1999</td>
<td>44.5</td>
<td>72</td>
<td>Existing outfall (Coroa do Boi)</td>
<td>Untreated</td>
</tr>
<tr>
<td>163</td>
<td>Sep 1999</td>
<td>44.5</td>
<td>72</td>
<td>Relocated to the southern end of Saco da Mangueira</td>
<td>Untreated</td>
</tr>
<tr>
<td>165</td>
<td>Sep 1999</td>
<td>44.5</td>
<td>72</td>
<td>Main Rio Grande outfall extended by 2 km to the 10m depth contour of the estuary</td>
<td>Untreated</td>
</tr>
<tr>
<td>162</td>
<td>May 2003</td>
<td>22</td>
<td>72</td>
<td>Existing outfall (Coroa do Boi)</td>
<td>Untreated</td>
</tr>
<tr>
<td>164</td>
<td>May 2003</td>
<td>22</td>
<td>72</td>
<td>Relocated to the southern end of Saco da Mangueira</td>
<td>Untreated</td>
</tr>
<tr>
<td>166</td>
<td>May 2003</td>
<td>22</td>
<td>72</td>
<td>Main Rio Grande outfall extended by 2 km to the 10m depth contour of the estuary</td>
<td>Untreated</td>
</tr>
<tr>
<td>177</td>
<td>Sep 1999</td>
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<td>24</td>
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<td>Untreated</td>
</tr>
<tr>
<td>178</td>
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<td>24</td>
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<td>Untreated</td>
</tr>
<tr>
<td>179</td>
<td>Sep 1999</td>
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<td>24</td>
<td>Main Rio Grande outfall extended by 2 km to the 10m depth contour of the estuary</td>
<td>Untreated</td>
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<tr>
<td>184</td>
<td>May 2003</td>
<td>22</td>
<td>24</td>
<td>Existing outfall (Coroa do Boi)</td>
<td>Untreated</td>
</tr>
<tr>
<td>185</td>
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<td>24</td>
<td>Relocated to the southern end of Saco da Mangueira</td>
<td>Untreated</td>
</tr>
<tr>
<td>186</td>
<td>May 2003</td>
<td>22</td>
<td>24</td>
<td>Main Rio Grande outfall extended by 2 km to the 10m depth contour of the estuary</td>
<td>Untreated</td>
</tr>
<tr>
<td>170</td>
<td>Sep 1999</td>
<td>44.5</td>
<td>72</td>
<td>Existing outfall (Coroa do Boi)</td>
<td>2° Treated</td>
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<tr>
<td>172</td>
<td>Sep 1999</td>
<td>44.5</td>
<td>72</td>
<td>Relocated to the southern end of Saco da Mangueira</td>
<td>2° Treated</td>
</tr>
<tr>
<td>174</td>
<td>Sep 1999</td>
<td>44.5</td>
<td>72</td>
<td>Main Rio Grande outfall extended by 2 km to the 10m depth contour of the estuary</td>
<td>2° Treated</td>
</tr>
<tr>
<td>171</td>
<td>May 2003</td>
<td>22</td>
<td>72</td>
<td>Existing outfall (Coroa do Boi)</td>
<td>2° Treated</td>
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<tr>
<td>173</td>
<td>May 2003</td>
<td>22</td>
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<td>Relocated to the southern end of Saco da Mangueira</td>
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<tr>
<td>175</td>
<td>May 2003</td>
<td>22</td>
<td>72</td>
<td>Main Rio Grande outfall extended by 2 km to the 10m depth contour of the estuary</td>
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</tr>
<tr>
<td>181</td>
<td>Sep 1999</td>
<td>44.5</td>
<td>24</td>
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<td>180</td>
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<tr>
<td>182</td>
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<td>24</td>
<td>Main Rio Grande outfall extended by 2 km to the 10m depth contour of the estuary</td>
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<td>189</td>
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<td>Main Rio Grande outfall extended by 2 km to the 10m depth contour of the estuary</td>
<td>2° Treated</td>
</tr>
<tr>
<td>168</td>
<td>Sep 1999</td>
<td>44.5</td>
<td>72</td>
<td>No Outfalls</td>
<td>Untreated</td>
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<td>169</td>
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<td>22</td>
<td>72</td>
<td>No Outfalls</td>
<td>Untreated</td>
</tr>
<tr>
<td>194</td>
<td>May 2003</td>
<td>22</td>
<td>72</td>
<td>Existing outfall (Coroa do Boi), No Fertiliser Discharge</td>
<td>Untreated</td>
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Table 8.1  Modelled Pollutant Input Scenarios
Pollutant concentrations for the domestic effluent discharges subjected to secondary treatment were estimated from typical values in the literature (USACE, 1987; WRc, 1990; Tebbutt, 1998; Butler & Davis, 1998; Gray, 1999): with biochemical oxygen demand reduced from 200 mg/l in crude sewage to 20 mg/l in secondary treated sewage; suspended solids reduced from 500 mg/l to 30 mg/l; fast organic nitrogen reduced from 25 mg/l to zero; ammoniacal nitrogen reduced from 40 mg/l to 5 mg/l; nitrate increased from 0.2 mg/l to 20 mg/l; phosphate reduced from 10 mg/l to 6 mg/l; and a reduction in faecal coliforms from $3 \times 10^7$ no./100ml to $3 \times 10^5$ no./100ml. During the conventional secondary treatment processes sewage is aerated and bacteria assist in the reduction of BOD and the nitrification of ammonia, hence the increase in nitrate in the final effluent.

The water quality variables used for the assessment were faecal coliform bacteria; dissolved available inorganic nitrogen; dissolved available inorganic phosphorus; chlorophyll-a; and dissolved oxygen. These quantities were extracted from the model output files and are presented as time series for fast and slow flushing conditions respectively: at Diamante in the lower estuary (Figures 8.6 and 8.7); the entrance to Saco da Mangueira (Figures 8.8 and 8.9); and the centre of Saco da Mangueira (Figures 8.10 and 8.11). Figures 8.6 to 8.11 also show the water quality standards (black lines) for each variable where applicable so that the impact of each scenario with respect to the average concentrations expected for fast and slow flushing conditions may be discussed in context.

Contours of the maximum concentration of each water quality variable (minimum for dissolved oxygen) throughout the lower estuary and Saco da Mangueira for each simulation are presented in Figures 8.12 to 8.24 and will be discussed in subsequent sections.
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Figure 8.6  Modelling Results for Outfall Scenarios at Diamante (Lower Estuary) - Fast Flushing

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Dissolved Oxygen (mg/l) and Salinity (dotted line, right hand axis) (g/kg)

b. Dissolved Available Inorganic Nitrogen (mg/l)

c. Chlorophyll-a (µg/l)

d. Phosphate (mg/l)

e. Faecal Coliforms (no./100ml) T90 = 72 hrs

f. Faecal Coliforms (no./100ml) T90 = 24 hrs

Figure 8.7 Modelling Results for Outfall Scenarios at Diamante (Lower Estuary) - Slow Flushing
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Dissolved Oxygen (mg/l) and Salinity (dotted line, right hand axis) (g/kg)

Dissolved Available Inorganic Nitrogen (mg/l)

Chlorophyll-a (µg/l)

Phosphate (mg/l)

Faecal Coliforms (no./100 ml) T90=72 hrs

Faecal Coliforms (no./100 ml) T90=24 hrs

Figure 8.8 Modelling Results for Outfall Scenarios at French Bridge - Fast Flushing
Figure 8.9  Modelling Results for Outfall Scenarios at French Bridge - Slow Flushing
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Figure 8.10 Modelling Results for Outfall Scenarios at the Centre of Saco da Mangueira - Fast Flushing

- Fast Flushing
Figure 8.11  Modelling Results for Outfall Scenarios at the Centre of Saco da Mangueira
- Slow Flushing
In the lower estuary (Figures 8.6 and 8.7) the scenarios appear to result in very little change to the existing water quality with respect to levels of dissolved oxygen and chlorophyll-a, which maintain average concentrations of 7.2 mg/l and ~3 μg/l respectively.

By adding secondary treatment to the existing outfall, concentrations of DAIN are reduced by an average of 0.01 mg/l, and further reduced by 0.01 mg/l for the other scenarios including removing the outfall completely, giving overall mean levels of 0.161 mg/l. Patterns of DAIP are similar to DAIN with concentrations reducing to 0.015 mg/l when the main outfall is moved or removed. The main impact on water quality is shown by the results for faecal coliforms (Figures 8.6e and 8.7e), with all scenarios reducing the mean concentration to below the 2000 no./100 ml Mandatory Standard of the EC Bathing Waters Directive 76/160/EEC, including the scenarios using a longer T₉₀ of 72 hrs.

At the entrance to the Saco da Mangueira (Figures 8.8 and 8.9) and in the centre of the bay (Figures 8.10 and 8.11) there are clear reductions in the levels of DAIN, chlorophyll-a and faecal coliforms with respect to both the existing situation and water quality standards when the outfall receives secondary treatment or is moved to the estuary, although levels of faecal coliforms still continue to exceed 2000 no./100 ml when the outfall is moved but not treated. In contrast, when the outfall is moved to the western end of the Saco da Mangueira there are significant increases in the mean levels of DAIN (0.824 mg/l) and chlorophyll-a (56.4 μg/l) in the bay for an untreated effluent, with a corresponding decrease in dissolved oxygen. The average level of chlorophyll-a remains high at 27.3 μg/l even when the discharge receives secondary treatment. Average concentrations of phosphate remain elevated in the bay between 0.096 mg/l and 0.33 mg/l under all scenarios with maximum levels resulting from a crude discharge in the western end of the bay.
Figure 8.12  Maximum Faecal Coliforms (T90 = 72 hrs) (Untreated Sewage)

Figure 8.13  Maximum Faecal Coliforms (T90 = 24 hrs) (Untreated Sewage)
Figure 8.14  Maximum Faecal Coliforms (T90 = 72 hrs) (Secondary Treated Sewage)

Figure 8.15  Maximum Faecal Coliforms (T90 = 24 hrs) ( Secondary Treated Sewage)
8.4.1 Faecal Coliform Bacteria

Contours of the maximum concentration of faecal coliforms for each scenario are presented in Figures 8.12 and 8.13 for untreated effluent and Figures 8.14 and 8.15 for treated effluent respectively. The blue areas indicate reductions of at least 4 decimal orders of magnitude from crude sewage which would be necessary to comply with the EC Bathing Waters Directive Mandatory Standard. The final concentrations depend largely on the value of $T_{90}$ as discussed in the previous Chapter, but it is clear that the overall faecal coliform impact in the lower estuary and Saco da Mangueira is reduced by moving the main sewage outfall of Rio Grande to either the main channel of the estuary or to the western end of the bay. There would be some local deterioration close to each new outfall, which would need to be taken into account with respect to the use of the receiving waters.

8.4.2 Dissolved Available Inorganic Nitrogen

Contours of the maximum concentration of DAIN for each scenario are presented in Figures 8.16 and 8.17. It is evident that moving the outfall to the western end of the Saco da Mangueira and not treating the effluent causes a significant increase in levels of DAIN in the bay compared with the current discharge location as shown in Figure 8.11. The waters of the bay are currently hypernutrified, and this situation is likely be exacerbated by an untreated discharge at any location in the bay. The impact is less with a treated discharge to Saco da Mangueira, however, moving the discharge to the main channel of the estuary removes the impact to the bay and would reduce the risk of eutrophication.
Figure 8.16  Maximum DAIN (Untreated Sewage)

Figure 8.17  Maximum DAIN (Secondary Treated Sewage)
8.4.3 Dissolved Available Inorganic Phosphorus

Contours of the maximum concentration of DAIP for each scenario are presented in Figures 8.18 and 8.19 for untreated and treated effluent respectively, and in Figure 8.20 for removal of the discharge from the fertiliser factory. The blue areas indicate areas where the maximum concentration is less than 0.031 mg/l, which is considered typical of non-polluted estuaries (Aminot & Chaussepied, 1983; Day et al., 1989; Pomeroy et al., 1965).

Both scenarios of outfall relocation result in a slight reduction in maximum phosphate levels expected in the estuary compared to the current outfall location, and moving the outfall to the channel of the estuary and treating the effluent reduces maximum concentrations in the bay by ~35% to 0.117 mg/l and 0.175 mg/l for fast and slow flushing conditions respectively. However, maximum phosphate levels within the Saco da Mangueira are increased by up to ~120% to 0.602 mg/l under slow flushing conditions when the outfall is relocated to the southern end of the bay and not treated, and this increase is reduced to ~80% (0.493 mg/l) when secondary treatment is applied.

Removing the discharge from the fertiliser factory (Figure 8.20) only marginally reduces the concentration of phosphate at the entrance to the bay due to the influence of the sewage inputs in this area, and levels within the bay appear to remain an order of magnitude higher than that expected in uncontaminated waters. This situation should be investigated further when the relative magnitudes of inputs from domestic and industrial sources and sediments have been quantified from field measurements and background levels have been re-evaluated.
Figure 8.18  Maximum DAIP (Untreated Sewage)

Figure 8.19  Maximum DAIP (Secondary Treated Sewage)
8.4.4 Chlorophyll-a

Contours of the maximum concentration of chlorophyll-a for each scenario are presented in Figures 8.21 and 8.22. The blue areas indicate areas where the maximum concentration is less than 10 μg/l (according to the CSTT Guidelines reported in MPMMG (1997), if the nitrogen level significantly exceeds 0.168 mg/l DAiN in the presence of >0.062 mg/l DAIP, the water is hypernutrified, and regular exceedence of 10 μg/l Chl-a implies eutrophic conditions).

It is clear from Figures 8.21 and 8.22 that maximum levels of chlorophyll-a are not reduced significantly from the existing levels when the main sewage outfall is treated, moved, or removed. Maximum levels in the Saco da Mangueira resulting from an untreated outfall situated at the southern end are increased by a factor of ~4 compared with the existing situation and by a factor of ~2 if this new discharge receives secondary treatment.
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Figure 8.21 Maximum Chlorophyll-a (Untreated Sewage)

Figure 8.22 Maximum Chlorophyll-a (Secondary Treated Sewage)
In summary, the results from the water quality management scenarios indicate that when compared with the water quality predicted for the existing outfall locations and treatment, the following overall impacts to the Saco da Mangueira and lower estuary are predicted:

- **Applying secondary treatment to the existing outfall** is predicted to give small percentage reductions to average levels in the estuary of up to 4% DAIN; 0.3% Chl-a; and 6% DAIP. An increase of 3% to the maximum level of chlorophyll-a is predicted in the Saco da Manguiera under fast flushing conditions.

- **Moving the crude outfall to the main channel** of the estuary is predicted to give percentage reductions to the average levels in the estuary of up to 8% DAIN; 2% Chl-a; and 15% DAIP, and in the Saco da Mangueira: 62% DAIN; 50% Chl-a; and 31% DAIP. **If this discharge receives secondary treatment** the reductions are of the order of: 9% DAIN; 2% Chl-a; and 16% DAIP in the estuary, and 81% DAIN; 59% Chl-a; and 36% DAIP in the Saco da Mangueira. The principal improvement to water quality by applying secondary treatment is the significant reduction in faecal coliforms in both the estuary and Saco da Mangueira.

- **Relocating the main outfall to the southern end of the Saco da Mangueira** is predicted to give percentage reductions to average levels in the estuary of up to 9% DAIN; and 15% DAIP, with a 2% increase in Chl-a, and in the Saco da Mangueira there are predicted increases to average levels of up to 37% DAIN; 97% Chl-a; and 84% DAIP. **If this discharge receives secondary treatment** the reductions are of the order of 10% DAIN and 16% DAIP in the estuary, and in the Saco da Mangueira a 66% reduction in DAIN, but increases of 44% and 46% for Chl-a and DAIP respectively.
Chapter 9

Conclusions and Recommendations

Coastal lagoons and shallow bay systems throughout the world are important ecosystems for the settlement and development of human activities such as agriculture, industry, fisheries, and recreation. Consequently, environmental degradation of the aquatic environment in these areas is common on account of uncontrolled inputs of sewage from industrial or domestic origin and irrigation waters, which have high nutrient and bacterial concentrations, causing eutrophication and associated water quality problems. Regulatory authorities often find it difficult to determine the best solution for discharges of wastewater when the receiving waters have complicated geography and conflicting water uses, therefore, the development of multi-dimensional water quality models, and an understanding of their limitations, are important predictive tools for helping managers to take suitable decisions to improve the use and/or environmental quality of a system. The overall aim of this research was to set-up and evaluate the use of TELEMAC-2D and WQFLOW-2D models as predictive management tools for the Patos Lagoon System. The conclusions of the work are presented here together with recommendations for future work.

9.1 Conclusions

The conclusions from this research are summarised as follows:

- TELEMAC-2D has been calibrated and validated to simulate the hydrodynamics of the Patos Lagoon system. The calibration resulted in the model being able to
reproduce up to 71% of observed hourly water elevations and 88% of observed hourly current velocities over a 31 day period of simulation from 21st July 1999 to 21st August 1999. During the validation of the model, up to 93% of water elevations at 5 stations throughout the lagoon were reproduced during a 15 day simulation from 19th April to 4th May 1999, and a longer simulation of 165 days from 18th April to 1st October 1999 reproduced up to 68% of observed water elevations.

- The hydrodynamic simulations indicated a very weak circulation in the Saco da Mangueira with maximum current velocities of ~0.15 m/s, compared with velocities of up 1.9 m/s in the estuary.

- The hydrodynamic simulations conducted to evaluate transport and mixing time scales demonstrated that water exchange between the Saco da Mangueira and the Patos Estuary is principally controlled by wind direction and duration rather than river flow. Flushing was found to be limited, with e-folding exchange rates ranging from 21 to 45 days under observed conditions of wind and river flow. The fastest flushing of the bay occurred during times of low river flow and long periods of wind from the SW sector, whereas high river flows and winds from the NE enhanced the flushing of the Patos lagoon but restricted that of the Saco da Mangueira, due to its orientation relative to the Patos lagoon estuary. An analysis of annual and inter-annual patterns of wind and river flow indicated that water exchange between the bay and estuary was more rapid during Autumn and Winter with respect to wind, whereas river flows were more important during Summer and Autumn given favourable wind conditions.
The water quality modelling undertaken in this research represents the first reported application of WQFLOW-2D to the Patos lagoon and estuary system, and the first water quality modelling exercise of any kind reported to date for the Saco da Mangueira.

The calibration and validation processes demonstrated that WQFLOW-2D could simulate mean observed concentrations of water quality variables consistently, with >87% of predictions producing at least Reasonable RMAE correlations with measured data both within the Saco da Mangueira and in the lower Patos Estuary under a range of hydrodynamic conditions.

The hydrodynamic and tracer simulations conducted to investigate engineering solutions for the improvement of water exchange between the Saco da Mangueira and estuary indicated no significant improvements when either the entrance is quadrupled in width or when a deeper channel (8m) is provided to connect the entrance with the main access channel of the estuary. Localised increases in current velocities were generated by widening the entrance which may provide improved dispersion of pollutants currently discharged in this area.

Scenarios for the management of water quality involving the relocation and secondary treatment of the main sewage outfall of Rio Grande to the southern end of Saco da Mangueira resulted in reduced levels of bacteria in the estuary, however, even with secondary treatment, the levels of nutrients and chlorophyll-a in the bay remain high (>10 µg/l), with an increased risk of eutrophication and the occurrence of nuisance and toxic algal blooms, depleted dissolved oxygen, and loss of submerged aquatic vegetation and benthic fauna.
Scenarios for the management of water quality involving the relocation and secondary treatment of the main sewage outfall of Rio Grande to deeper water in the main access channel of the estuary resulted in a reduction in the levels of bacteria and nutrients in the Saco da Mangueira to a less polluting level even without secondary treatment, however, removal or treatment of the discharges from the fertiliser factories would also be necessary to reduce phosphate to a level which would reduce the risk of eutrophication and associated degradation in water quality. This scenario would be the recommended option for managers.

It is clear that the growth of phytoplankton in Saco da Mangueira is significant even without direct discharges to the embayment.

**9.2 Is TELEMAC a Suitable Predictive Tool for the Patos System?**

It is considered that TELEMAC-2D is fit for purpose to simulate the hydrodynamics of the Patos Lagoon system under a variety of physical conditions typical of the region. Further information is required to confirm the predicted circulation and flushing characteristics of the Saco da Mangueira particularly with respect to identifying any gravitational circulation resulting from thermal or saline stratification as prescribed below in the recommendations.

Based on the data available for the calibration and validation it is considered that WQFLOW-2D may be applied to the Patos lagoon system for use as a comparative tool to evaluate the predicted performance of engineering schemes designed to improve the water quality with respect to nutrients and bacteria. The results presented in this research are considered to represent a first order approximation and further data are required to improve the confidence placed on the predictions as recommended below.
9.3 Recommendations

The recommendations from this research are mainly concerned with the collection of input data (loadings from rivers, land runoff, and point source discharges), and process data (kinetic rate constants) for the water quality model so that uncertainties and errors may be more accurately quantified. Recommendations are summarised as follows:

- Surveys to quantify the circulation patterns and vertical structure of the water column within the Saco da Mangueira are required to confirm the features revealed by the TELEMAC-2D results and to provide information on the dilution and dispersion characteristics of the bay.

- Field measurements are required from the final effluents of the main continuous and intermittent pollutant sources together with rates of discharge to give loadings of the main water quality parameters. This will give a higher level of confidence in model predictions.

- A long-term programme of monthly water and sediment quality surveys for a period of at least 1 year in the Saco da Mangueira and waters surrounding Rio Grande is required to extend the existing information and give a higher level of confidence in model predictions and also enable seasonal simulations to be conducted. Variables should include temperature, salinity, turbidity, pH, chlorophyll-a, total suspended matter, ammoniacal nitrogen, nitrate, phosphate, total nitrogen and phosphorus, dissolved oxygen, BOD, sediment oxygen demand (SOD); nitrite, silicate, and bacteria (faecal coliforms and faecal streptococci). Data on the levels of nutrients and pollutants in the bed sediments would give a
better understanding of the magnitude of this source, and combined with information on the likely rates of chemical interaction between sediment and water column, would enable the evaluation of possible exacerbation of eutrophication caused by release from sediments.

- A programme of in-situ kinetic experiments should be conducted to ascertain appropriate kinetic parameters for the water quality model including measurements of primary productivity to deduce the rate of oxygen evolution and hence a carbon or chlorophyll fixation rate; the processes controlling the dynamics of phosphorus such as the adsorption of phosphate onto suspended or deposited matter; and settling velocities for phytoplankton, suspended sediments and detritus.

- Laboratory experiments to evaluate bacterial mortality rates typical for the study area are required for a higher level of confidence in future model predictions for water quality management decisions.

- Development of the water quality model to include interactions between variables and suspended sediments such as sorption of phosphorus and nitrogen, and bacterial dynamics;

- Simulations of sediment transport and associated water quality focussing on the entrance to the Saco da Mangueira are required together with a cost benefit analysis to assess whether any improvement in water exchange and localised increase in current velocities would justify the cost of the engineering required to widen the entrance of the bay.
Appendix 1 - Water Quality Standards and Nutrient Enrichment

Criteria
## Appendix I  Water Quality Standards and Nutrient Enrichment Criteria

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<td>pH</td>
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<td>CEC (1976) (76/160/EEC)</td>
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<td>Guideline Standard for Bathing Waters</td>
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<td>European Commission (2002)</td>
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<td>(91/676/EEC)</td>
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<td>FEPAM Class B</td>
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<td>FEPAM Class B</td>
<td></td>
<td>Brackish Waters for primary water contact sports; and the protection of aquatic communities</td>
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<td>Brackish Waters for the protection of aquatic communities; primary and secondary water contact sports; and navigation.</td>
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<td><strong>Day et al. (1989)</strong></td>
<td>Maximum level for an uncontaminated estuary</td>
<td>5 μM N-H₄⁺ (0.070 mg/l)</td>
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<td><strong>DoE, MAFF &amp; Welsh Office (1993)</strong></td>
<td>Winter (February) values of Nitrate (salinity adjusted) significantly above background</td>
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<td><strong>Environment Agency (1997)</strong></td>
<td>Winter maximum elevated by &gt; 50% above background</td>
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<td><strong>European Environment Agency (1999)</strong></td>
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<td><strong>Liss, 1976</strong></td>
<td>Maximum level for an uncontaminated estuary</td>
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"Trigger Levels" for Environmental Impact from Nutrients
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<th>Notes</th>
<th>Water Quality Parameter</th>
</tr>
</thead>
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<td>MPMMG (1997) - CSTT Guidelines</td>
<td>If the nitrogen level significantly exceeds 12 ( \mu \text{M} ) N in the presence of &gt;0.2 ( \mu \text{M} ) P, the water is hypernutrified, and regular exceedence of &gt;10 ( \mu \text{g/l} ) Chl-a implies eutrophic conditions</td>
<td>pH, Biochemical Oxygen Demand (BOD), Dissolved Oxygen (DO), Ammoniacal Nitrogen, Nitrate, Nitrite, Dissolved Available Inorganic Nitrogen (DAIN), Dissolved Available Inorganic Phosphorus (DAIP), Silicate, Chlorophyll-a, Total Coliforms (no./100ml), Faecal Coliforms (no./100ml), Faecal Streptococci (no./100ml)</td>
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<tr>
<td>North Sea Status Report</td>
<td>Definition of hypernutrification. Implied level above which algal proliferation commences</td>
<td>7 mg/l (median)</td>
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<tr>
<td>OSPAR Commission (2002)</td>
<td>DAIN &gt;50% above salinity related background; Winter concentrations. DAIP &gt;50% above salinity related background</td>
<td>12 ( \mu \text{M/l} ) (168 ( \mu \text{g/l-N} ))</td>
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<tr>
<td>Pomeroy et al. 1965</td>
<td>Maximum level for an uncontaminated estuary</td>
<td>1 ( \mu \text{M} ) (0.031 mg/l)</td>
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</tbody>
</table>

Guidelines: HM N in the presence of >0.2 \( \mu \text{M} \) P, the water is hypernutrified, and regular exceedence of >10 \( \mu \text{g/l} \) Chl-a implies eutrophic conditions. If the nitrogen level significantly exceeds 12 \( \mu \text{M} \) N in the presence of >0.2 \( \mu \text{M} \) P, the water is hypernutrified, and regular exceedence of >10 \( \mu \text{g/l} \) Chl-a implies eutrophic conditions. The North Sea Status Report defines hypernutrification as the implied level above which algal proliferation commences.

North Sea Status Report: Definition of hypernutrification. Implied level above which algal proliferation commences.

OSPAR Commission (2002): DAIN >50% above salinity related background; Winter concentrations. DAIP >50% above salinity related background.

Pomeroy et al. 1965: Maximum level for an uncontaminated estuary.
Appendix 2 - Model Simulation of the Circulation in Saco da Mangueira
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T = 6 d 3 hrs

T = 6 d 6 hrs

T = 6 d 9 hrs

T = 6 d 12 hrs

T = 6 d 15 hrs

T = 6 d 18 hrs

T = 6 d 21 hrs

T = 7 d 0 hrs

252
Appendix 2 - Model Simulation of the Circulation in Saco da Mangueira
Appendix 2 - Model Simulation of the Circulation in Saco da Mangueira
Appendix 2 - Model Simulation of the Circulation in Saco da Mangueira
Appendix 3 - Model Simulation of the Flushing of Saco da Mangueira Under Various Wind Conditions
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Modelling Water Residence Times in Saco da Mangueira - Comparison of Artificial and Observed Wind Forcing during May 1999

02/05/1999

03/05/1999

04/05/1999

05/05/1999

06/05/1999

07/05/1999

08/05/1999
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Appendix 4 - Model Simulation of the Flushing of Saco da Mangueira
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