AN ECOLOGICAL MODEL APPLICATION TO THE SANTOS ESTUARY, BRAZIL: TESTING AND VALIDATION

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1 WHY MODEL ECOLOGICAL PROCESSES IN SANTOS ESTUARY?

Over the past decades an intense research program has been carried out at the Santos Estuary to study the ecological dynamics of the system. Much of this work has been field data acquisition in monitoring programs and subsequent interpretation. Modelling approaches have been scarce and generally devoted to the study of hydrodynamics in the bay area or sediment transport in the system (Harari and de Camargo 2003). Until now there has been a lack of integrative modelling approaches in the Santos estuary. This is the first attempt at simulating the hydrodynamics of the system coupled to some of its ecological processes. Since the Santos estuary is a highly impacted system (Braga et al. 2000, Medeiros and Bicego 2004a, b, Abessa et al. 2005, Cesar et al. 2007), the need for such a tool is emphasized by the necessity to link human pressures known in the area with the ecological state of the system according to the DPSIR framework (Mateus and Campuzano, this volume). Among the most relevant aspects that such a tool can address, there are: (1) The insights that it can provide into the major physical-ecological interactions in the estuary; (2) Assessing the contribution of isolated Pressures such as the sewage outfall or industrial effluent to the State of the system; (3) Provide a numerical tool to help in the management of the system (Response) by allowing the testing of different scenarios of human Pressures.

This work presents the application of a coupled physical-ecological model within the MOHID system (Leitão et al., this volume) to the Santos estuary. The ecological model, the MOHID WQ model, is an adaptation of the NPZ modelling paradigm (Fasham et al. 1990). Detailed description of the model implementation is provided, with particular emphasis on the characterization of the forcing and modelling options. Model results are compared against field data to assess model performance and validate the results. This model application relies on the assumption that the model correctly reproduces the hydrodynamics of the Santos estuary.

In the DPSIR framework, this work describes the state of the system based on some ecological and water quality parameters. The model is forced with values previously quantified for the Pressures, namely, nutrient and organic matter concentrations in the rivers, the submarine outfall in the bay, the absent sewage drainage networks in the quarters and direct raw sewage inputs from slum quarters around the margins of the estuary. These Pressures, which fall in one of the major groups of estuarine and coastal area pressures, namely pollution, including urban, industrial, agricultural and aquaculture discharges (Borja et al. 2006), express the forcing from the major drivers: human occupation and industry. The outcome of this numerical study is a benchmark model application which can be further developed to study different scenarios of development or actions prompted by responses. Also, the results presented here will enable the quantification of changes induced by responses, when compared with the results from the model runs for different scenarios.

2 MODEL IMPLEMENTATION

The ecological model is coupled with the hydrodynamic model previously described, and so the same assumptions for the physical features of the system apply here. These are: (1) the water-column is homogeneous, i.e., non-stratified over the modelled domain (2D horizontal); (2) the hydrodynamics in the bay are controlled by the tide and the water flow from the main channels, i.e., there are no shelf water currents. The model domain is the same as for the hydrodynamic application and to reduce the run time, the coarse grid was adopted for the present study. The external conditions include river discharges, forcing functions (for example irradiance, air temperature), and boundary conditions (concentrations of each state variable on the open Atlantic boundary). Whenever possible, these values have been taken from available field data. The ecological model runs with a time step of 1 hr. A constant value for each property was defined as the open boundary condition (Table 1).

2.1 Atmospheric forcing

Climatological irradiance levels were calculated by the model for the domain geographical coordinates from the solar constant corrected for cloudiness with mean monthly cloud cover data. Air temperature and relative humidity were also used to force the model over the entire domain (Figure 1), with monthly values taken from field observations made by CODESP meteorological station at Alemoa during 1997 and cloud cover was taken from field observations made at the Ilha da Moela meteorological station at Guarujá during 1999.

2.2 River inputs

The model considers six river inputs inside the model domain. When considering the ecological dynamics of the system, river discharges also need to be characterized by values of nutrients, organic matter components, and other biogenic constituents. For simulations with the ecological model, the discharge of Cubatão+Henry Borden and Mogi+Piaçaguera are characterized by mean monthly concentrations of ammonium, nitrate, nitrite, phosphate and dissolved oxygen (Figure 2) calculated from data collected by CETESB between 2000 and 2005. The COSIPA industrial effluent is characterized by high nutrient loads and a significant flow for an effluent of this kind. According to Gragnani (1996) most of Moji/Piçaguera flow is caught by Cosipa and dumped in the Cosipa channel. Therefore we have modelled a joint discharge of Moji/Piaçaguera and the Cosipa effluent. The Cosipa, contribution is a flow of 2.38 $m^3\ s^{-1}$ and a concentration of 23 $mg\ l^{-1}$ of ammonium and DON, and 4.6 $mg\ l^{-1}$ of both phosphate and DOP. These values have been estimated from field observations and available monitoring studies from Cetesb-Cubatão. The remaining values as well as the values assumed for the other discharges are summarized in Table 2.

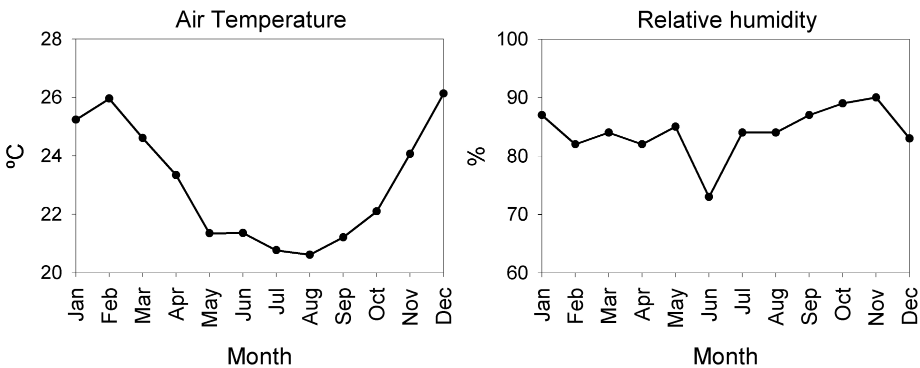

FIGURE 1: *Monthly mean values for air temperature and relative humidity used to force the model.*

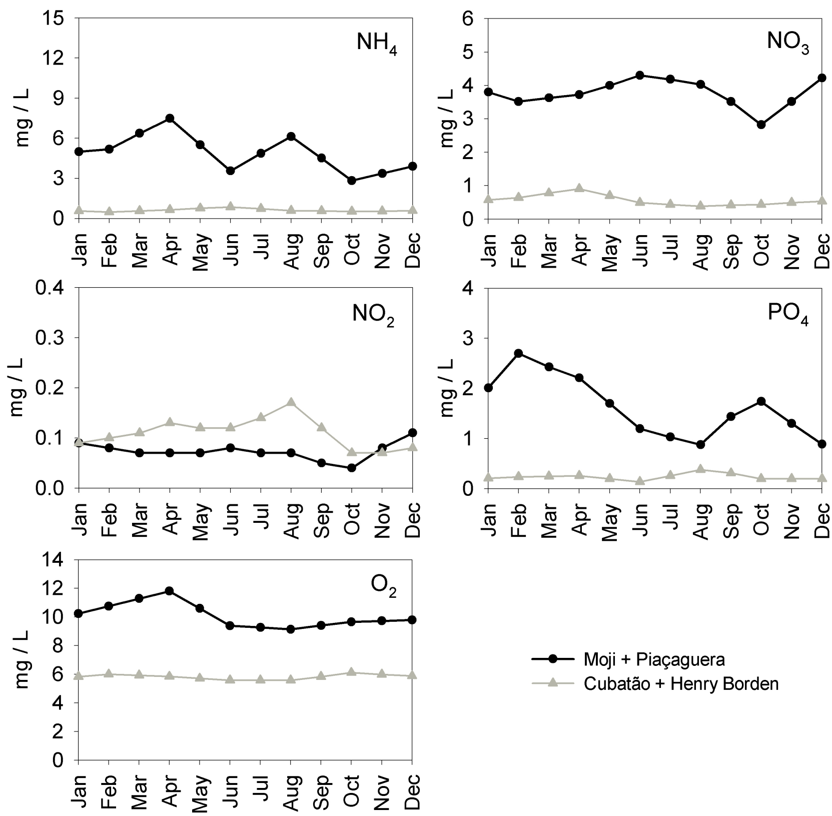

FIGURE 2: *Monthly mean values of water quality parameters assumed for the major river discharges: the joint discharges of Moji + Piaçaguera and Cubatão + Henry Borden.*

TABLE 1: *Initial conditions, river inputs and boundary conditions defined for each variable in the model simulations (unless noted otherwise).*

Properties	Units	Initial conditions	Boundary conditions
Nitrate		0.09	0.095
Nitrite		0.003	0.001
Ammonium	mg N l^{-1}	0.002	0.002
Refractory DON		0.2	0.02
Labile DON		0.02	0.002
PON		0.37	0.0009
Inorganic phosphorus		0.03	0.03
Refractory DOP	mg P l^{-1}	0.028	0.002
Labile DOP		0.0028	0.00028
POP		0.05	0.005
Oxygen	mg O_2 l^{-1}	8	9.56
Phytoplankton	mg C l^{-1}	0.05	0.02
Zooplankton		0.03	0.01
Temperature	ºC	20	20
Salinity	PSU	20	36
Cohesive sediments	mg l^{-1}	100	25

2.3 Sewage nutrient input

As already mentioned, the Santos estuarine system is heavily impacted by human occupation and activities. A significant part of the anthropogenic pressure is in the form of diffuse sewage discharges in several places scattered inside the estuary (Braga et al. 2000, CETESB 2001). Most of these discharges are associated with the slum quarters near (and sometimes over) the water line, and often with absent or provisional sewage drainage systems. Together with the faecal contamination, the discharges into the system also have an associated load of nutrients, both in a mineral and an organic form. To account for this source of eutrophication, the model considers 29 sewage discharge points inside the estuary (Figure 3, left). These comprise the submarine outfall, sewage treatment plants and direct inputs from slum quarters. Each discharge is characterized by flow rate, associated nutrients and dissolved organic matter concentrations. The flow and concentration of sewage treatment plants were calculated from data obtained from SABESP (São Paulo State Basic Sanitation Company) and direct discharges were estimated from the population number calculated for each district by the Brazilian Institute of Geography and Statistics (IBGE 2000), in the municipal data on people living in slums and in measured values of water consumption by neighborhoods (Table 2). This number stands as an estimate based on the households not connected to the municipal sewage system.

Reference flow and concentrations for areas where data were not available were taken from Metcalf and Eddy (2005) values for high-strength wastewater (Table 3). The partition between the different pools of nutrients (organic and mineral) was also based on Metcalf and Eddy

(2005). All discharges are characterized by a cohesive sediment concentration of 120 mg l^{-1}, a salinity of 0.5 and a temperature of 24 °C. Together with the sewage discharges originating from the poor or non-existent sewage system in some areas of Santos, the submarine outfall in the bay is another large source of nutrients. The effluent characteristics used in this simulation are presented in Figure 4.

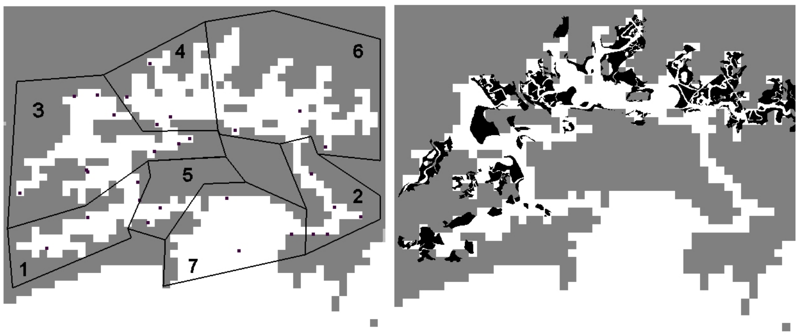

FIGURE 3: *Left: Sewage discharge points associated with the outfall, sewage treatment plants, and the slum quarters and absent sewage drainage networks. The model domain is divided in seven integration boxes to allow the calculation of the exchange fluxes of properties inside the estuarine area between the boxes. Legend for the boxes: São Vicente Channel and Piaçabuçu river (1), Santos channel (2), Boturoca and Mariana river and Pompeba large (3), Largo do Canéu or Cubatão area (4), Lower São Vicente Channel (5), Bagres and Barnabé Island area (6), and Santos bay (7). Right: Mangrove areas used in the model to account for the shading effect.*

2.4 Mangrove shading effect

Considering the large mangrove areas inside the estuaries, the model accounts for the shading effect of mangrove trees. Because a considerable fraction of the mangrove forest is in permanently flooded areas, they strongly reduce the amount of light reaching the water surface. The spatial distribution of mangrove areas (Figure 3, right) was taken from aerial survey photographs and satellite images. This model feature is based on three simple assumptions: (i) the shading effect is quantified as a 50% reduction of the irradiance that reaches the surface, (ii) the mangrove is a climax community, implying that the shading effect is constant, and (iii) there are no net nutrient fluxes between mangrove and water column. The latter assumption is based on studies made in the nearby mangrove forest at Cananeia, where it was observed that the mangrove forest does not export significant amounts of nitrogen to the adjacent lagoon (Carmouze et al. 1998). Apparently, the simultaneous processes of release and incorporation of ammonium explains this occurrence. The explicit modelling of mangrove dynamics would require a complex biochemical reaction model. This, in turn, would make the modelling exercise computationally heavy and compromise the simplicity that management models aim for.

TABLE 2: *Sewage discharge areas and characterization of the respective effluent. Discharges include the outfall, sewage treatment plants (STP), slum quarters and quarters beyond sewage drainage. Values calculated according to measured mean concentrations of N and P of the effluent marked with *. The remaining values were estimated.*

Sewage discharge area	Inhabitants	Flow ($m^3\ s^{-1}$)	N (kg day^{-1})	P (kg day^{-1})
Quietude and Vila Nova	36006	0.057	310.4	44.8
Antartica and Ponte Nova	38120	0.060	356.6	57.8
Sítio Campo	10533	0.011	89.5	12.6
Jd Rio Branco, Mangue Seco and Quarentenário	12356	0.011	148.3	30.9
STP Humaitá*	23018	0.040	97.1	17.5
Trevo*	21522	0.020	258.3	53.8
STP Samaritá	26940	0.040	78.7	8.1
Vale verde and Vl Esperança	7792	0.007	66.2	9.4
Vl Esperança e Vl Natal	8557	0.008	72.7	10.3
Nova Republica e Bolsão	5583	0.005	67.0	14.0
São José e Vila Nova	9555	0.009	81.2	11.5
Vila Pescadores	8340	0.008	100.1	20.9
Vila Criadores	800	0.001	9.6	2.0
Caneleira/Butantã/ Jd São Manoel/Alemoa	9751	0.009	117.0	24.4
Vila Gilda / Sá Catarina / Joquey (Sambaiatuba)	34239	0.032	410.9	85.6
Pompeba / Piçarros / Caxeta and Joquey	13950	0.013	167.4	34.9
Vl Pantanal	3600	0.003	43.2	9.0
Explanada do Barreiros	9215	0.009	78.3	11.1
México 70	28980	0.027	347.8	72.5
Bitaru (Rio d`avó)	15300	0.018	183.6	38.3
Morro José Menino	1233	0.001	14.8	3.1
Ilha diana	175	0.000	2.1	0.4
V. Carvalho (Caixao/ Acaraú/Sta Madalena) and V. Carvalho c/ rede	90242	0.084	1082.9	225.6
Prainha	7552	0.007	90.6	18.9
V. Carvalho (Conceiçãozinha)	7774	0.007	93.3	19.4
Sto Antonio / Sta Clara / Engenho / Flores / Cachoeira / Mangue Seco e Primavera	20782	0.019	249.4	52.0
Sta Cruz	5018	0.003	60.2	12.5
Goes	300	0.000	3.6	0.8
Sta rosa e Vl Ligia	7359	0.007	88.3	18.4
STP Cubatao *	31493	0.200	546.5	113.8
Santos outfall*	520950	2.500	12313.7	1883.5
TOTAL	1,017,035	3.22	16,151	2,673

2.5 The role of benthonic OM mineralization

A simple benthic model is coupled to the pelagic model to account for nutrient diagenesis in the sediment. A fixed mineralization rate of 0.1 d^{-1} is assumed and PON and POP are converted to ammonium and phosphate, respectively, and released to the water column. The stoichiometric balance of oxygen consumption is considered in this process.

2.6 Spin-up

The model is run for a period of one year (July 2004 - July 2005) as a spin up period. Given the control of suspended sediment concentration on the ambient light, special attention was paid to the description of cohesive sediments, both in the water column and in the sediments of the estuary. The methodology adopted for modelling cohesive sediment dynamics consisted of starting the simulations with a layer of 10 kg m^{-2} of cohesive sediments in the entire domain and a constant concentration of 100 mg l^{-1} in the water column. Based on previous modelling experiments, a one year spin-up was considered a reasonable time to achieve a reasonable cohesive sediment pattern inside the estuary with deposition and erosion areas already defined.

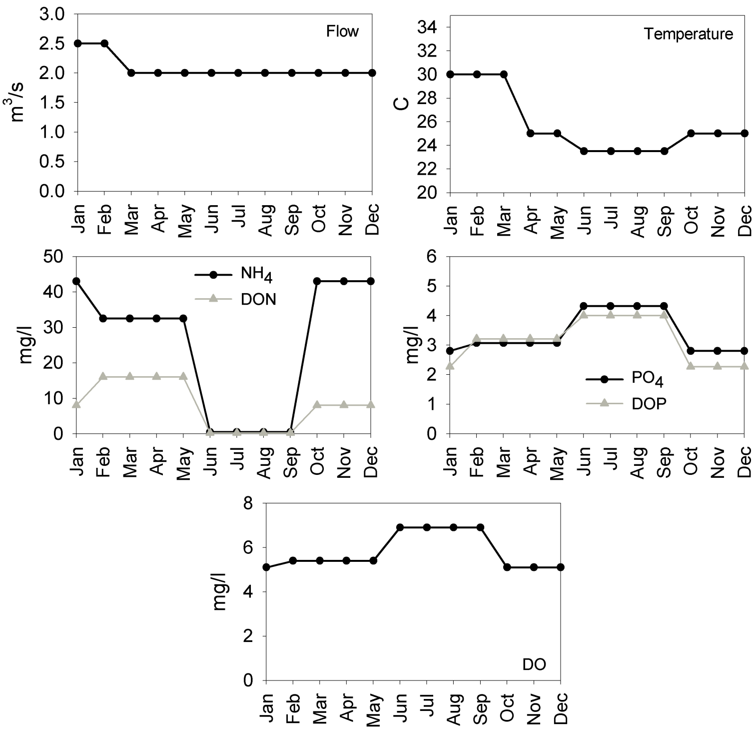

FIGURE 4: *Monthly mean values used to characterize the outfall effluent discharge in Santos bay.*

2.7 Model calibration and validation

Models can be calibrated with field data by adjusting model parameter values until an acceptable simulation is achieved, i.e., reproduce the main features of the modelled system as reflected in the data. Once this is achieved, another simulation is performed and validated with an independent set of data (Thomann and Muller 1982, 1987). If the second simulation is also acceptable then the model is considered valid. This approach has been used in this model application.

The model has been previously calibrated with available data (Braga et al. 2000, Bosquilha 2002, Lima 2003). Due to the scarcity of available field data, the calibration process focused on reproducing the major features of the system and the range of variability as inferred from in situ data. Once this was achieved, the model was then validated with data from two monitoring campaigns in the estuary made during the Ecomanage project. The monitoring program was designed to quantify the spatial. differences in the estuary (eight stations distributed all over the estuary) as well as the seasonal differences by running a campaign in winter (August 2005) and summer (March 2006). The model was validated using the field data for temperature, dissolved oxygen, nutrients (ammonia and phosphate), and chlorophyll.

3 MODEL RESULTS

Any ecological model, irrespective of the level of detail and complexity, produces a considerable volume of results that may vary in relevance depending on the objectives of the model implementation. For the sake of clarity, we have focused on a few state variables (phytoplankton biomass, oxygen concentration, nitrate, phosphate and organic matter),on rates in the form of mass fluxes and on some dimensionless variables such as limitation factors To reduce the bulk of results, only some stations will be discussed. These have been chosen such as to represent distinct areas of the estuary. Also, the model domain has been aggregated into seven regions, or boxes (Figure 3, box labels in the legend). Integration boxes try to capture areas in the system with similar conditions (both biotic and abiotic). This concept is used to allow the assessment of the temporal evolution over larger areas of the system and to calculate net mass fluxes between adjacent boxes, averaging out temporal and spatial variability. These results are then used to plot annual budgets.

3.1 Temperature

Model results for water temperature show the typical seasonal pattern of tropical estuarine systems, namely, high temperatures during the entire year with an increase in the austral summer months (Figure 5 and Figure 6), reaching 32 ^{o}C in some areas. A spatial pattern can also be seen in the results (Figure 6), with higher temperatures in shallow areas inside the estuary, and lower temperatures in the coastal areas. Only the influence of the Cubatão River and Henry Borden is noticeable by the cool water plume associated with the discharge. Spatial differences are not noticeable when comparing the stations (Figure 5) because they are located in the main (deeper) channels where the residence time of water is significantly lower than in the inner, more stagnant and shallower areas.

3.2 Cohesive sediments

The concentration of cohesive sediments in the water column shows a large spatial and temporal variation. The significant difference between the inner areas and the mouth of the estuary is evident in Figure 5, with concentration at P5 (innermost station) peaking above 100 mg l^{-1}, while barely reaching 20 mg l^{-1} at P1. Higher values are observed during the rainy summer months (Figure 6), while in the drier winter months lower concentrations are observed in the entire system. The timing and level of the higher values of suspended sediment in the water column agree with field data where SST maximum values of around 180 mg l^{-1} are reported in January (Moser et al. 2002).

As the major source of sediment input into the system, river discharges have a significant influence on the horizontal patterns. Sediment concentrations are usually higher in the inner parts of the estuary, where rivers are located (Figure 6). This is particularly evident in summer months near Cubatão River, the largest contributor of sediments to the system. Sediment resuspension also contributes to the concentration in the water column, especially in shallow areas where the currents are more intense, i.e., higher bottom stress. This contribution is seen in the marked spring and neap tide cycles in the model results (time series).

3.3 Light

Suspended matter determines the underwater light climate in the water column by reducing down welling light. As a consequence, available light for photosynthesis is mostly controlled by the amount of cohesive sediments in the water column. This implies that the general pattern of irradiance in the water-column closely follows the pattern of cohesive sediment distribution, as shown in Figure 6. Despite the higher concentration of sediments in the water column during summer, irradiance levels are still higher because the irradiance reaching the surface is also higher during this period. In some places the values are >250 watt m^{-2}. Because the model is a 2D application, light is integrated over the entire water column, meaning that in deeper areas less light is available. This explains why in some areas the irradiance is quite low, even when cohesive sediment concentration is also low, and vice-versa. This effect is seen in the bay area (lower irradiance, lower sediment concentrations) and in the inner shallow areas (higher irradiance, higher sediment concentrations), both with values ranging from 0 and 100 watt m^{-2}.

3.4 Nutrients

Model output for ammonium and phosphate concentrations at all stations is plotted in Figure 7. The results show a similar spatial and temporal pattern characterized by: (1) slight seasonal fluctuations, (2) a marked fortnightly frequency induced by the spring-neap cycle, (3) a strong horizontal gradient caused by high concentrations in the inner estuarine area (e.g., stations P4 and P5) where ammonium and phosphate reach the highest levels, $\sim$1.1 mg l^{-1} and $\sim$0.8 mg l^{-1}, respectively. At the outer stations (P1 and P8) these values are always <0.3 mg l^{-1}. These patterns can in part be explained by the river inputs (especially Cubatão) and their seasonality mostly driven by the presence of a rainy season. The rivers account for an increase in the nutrient loads to the system, thus, enriching the inner areas where river discharges are located.

Nutrients are consumed and converted by primary producers as soon as the light conditions allow it, which is possible in inner areas of the estuary close to the nutrient sources. Since there are no outside sources of nutrients as relevant as rivers (the influence of the oceanic boundary conditions is negligible), nutrient concentrations decrease from the inner areas to the oceanic area by consumption and dilution (Figure 9). Nutrient concentrations are slightly higher in the São Vicente channel (when compared to the Santos channel), probably as a result of the many direct sewage discharges in this channel and the less energetic hydrodynamic regime which reduces the dilution, when compared to the Santos channel. The influence of the submarine outfall is noticeable in the spatial distribution of the ammonium concentration, demonstrating the contribution of this nutrient input to the nutrient levels in the bay.

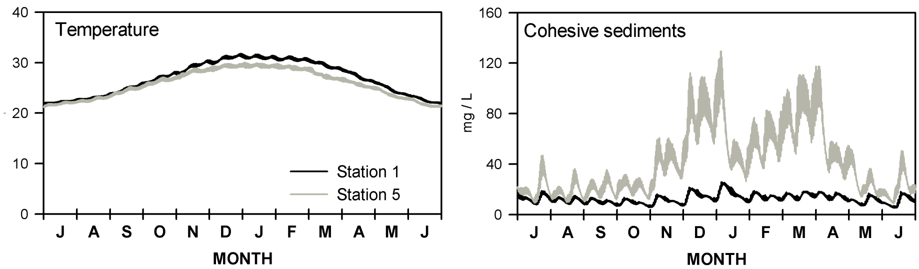

FIGURE 5: *Model results for temperature and cohesive sediment at stations P1 and P5.*

TABLE 3: *Reference flow and concentration values for a high-strength sewage wastewater (Metcalf and Eddy 2005).*

Property	Value
Flow	240 liters per capita*day
Ammonium	45 mg l^{-1}
Dissolved Organic Nitrogen	25 mg l^{-1}
Phosphate	8 mg l^{-1}
Dissolved Organic Phosphorus	4 mg l^{-1}

3.5 Phytoplankton

Being the main driver for primary production, ambient light in the water is the determinant for phytoplankton activity. Any process that affects light penetration in the water can, therefore, influence phytoplankton dynamics in the system. Other factors, such as nutrient availability,water temperature, residence time and grazing pressure, also control the phytoplankton population at any given place and time. This implies that these factors must be taken into consideration when trying to explain the dynamics of producers in any system. The model results show strong fluctuations in phytoplankton biomass (Figure 8 and Figure 9), but without a marked seasonal pattern. This is most obvious by looking at the oscillations seen in station P6 and P7 in Figure 8 where higher values (>3 mg C l^{-1}) are observed between January and May (austral summer and autumn).

The noticeable discrepancy between São Vicente and Santos channels can be partly explained by the different availability of nutrients and light in the two channels. Santos channel has systematically lower concentrations of nutrients given the lesser number of direct discharges in this area, but also because of the short residence time, when compared to São Vicente channel. The residence time controlled by the higher current velocities in this channel is not favorable to the formation of blooms. Contrary to this, the inner (and most stagnant) areas in the São Vicente channel increase retention, thus favoring bloom formation as seen in Figure 9. Also, because of the depth, light availability is usually lower in the Santos channel (Figure 6), imposing a strong limitation on phytoplankton growth.

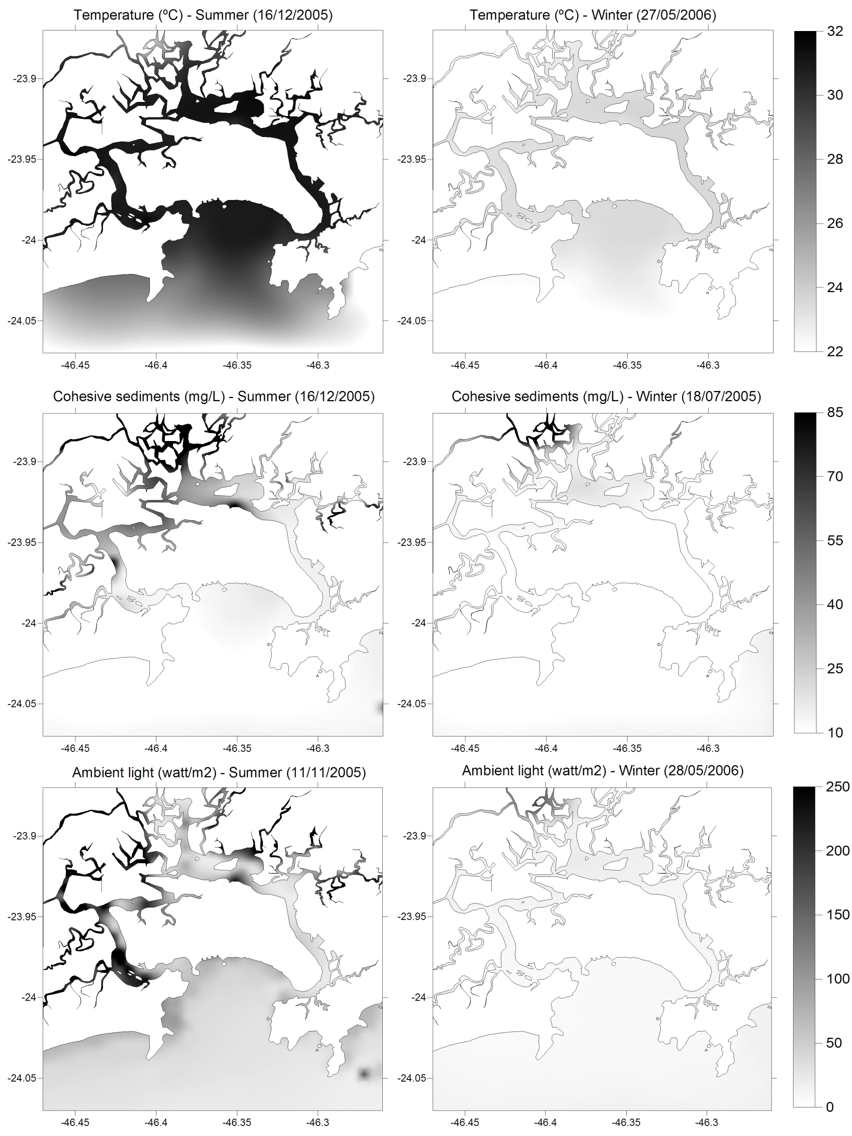

FIGURE 6: *Model results for temperature, cohesive sediments, and irradiance in the water column. Some scales have been expanded to enhance the spatial pattern.*

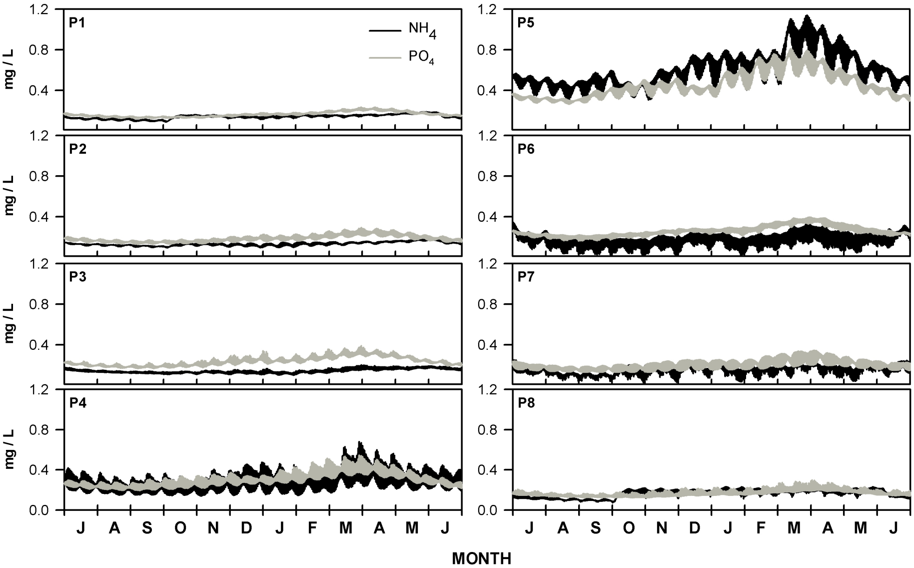

FIGURE 7: *Model results for temperature, cohesive sediments, and irradiance in the water column. Some scales have been expanded to enhance the spatial pattern.*

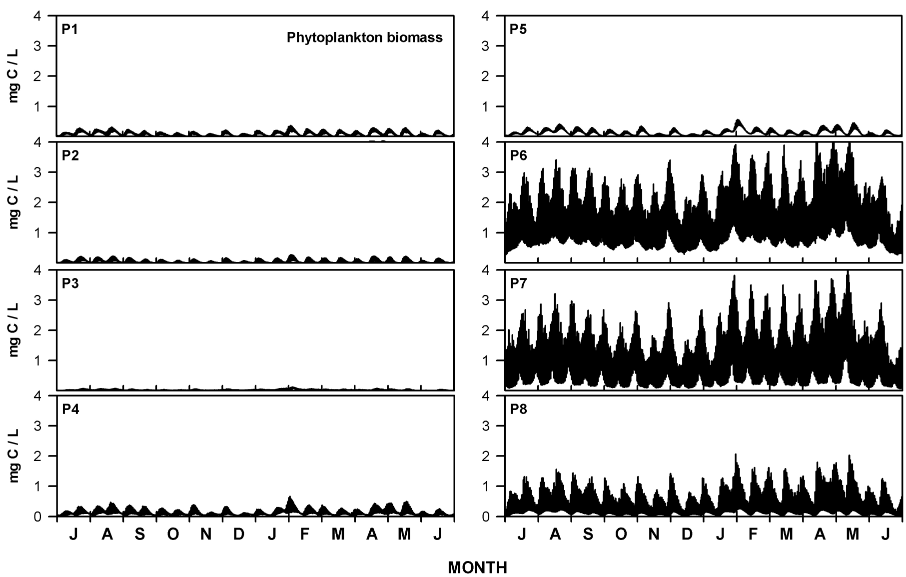

FIGURE 8: *Model results phytoplankton concentration at the monitoring points.*

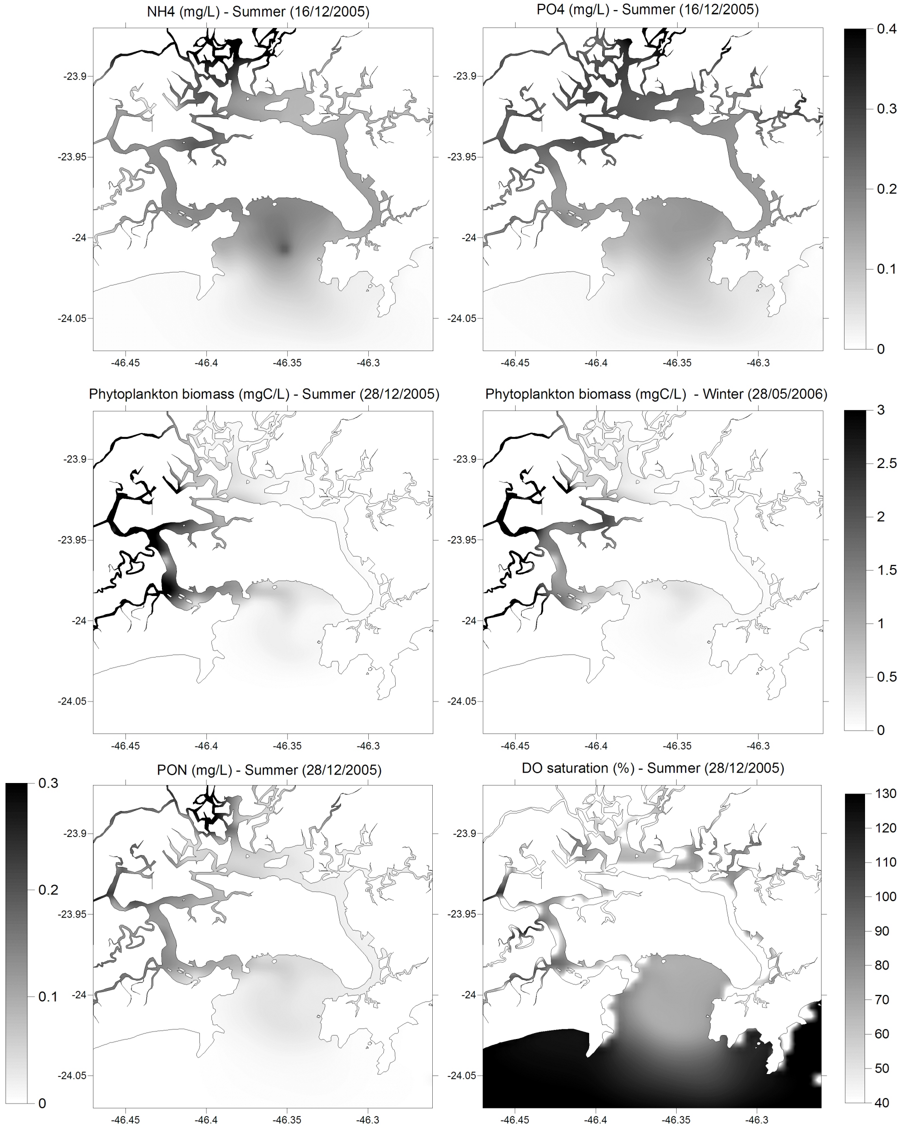

FIGURE 9: *Model results for ammonium, phosphate, phytoplankton biomass, particulate organic nitrogen (PON), and dissolved oxygen saturation.*

Model output allows a detailed assessment of the temporal variation in resource limitation. Overall, the major limitation in the estuary is imposed by light, as seen in Figure 10 for three integration boxes, followed by temperature to a much lesser degree. This limitation is mainly attributed to the high concentrations of cohesive sediments in the inner shallow areas of the estuary and to the depth of the deeper channels and outer area. Despite the high sediment concentrations in the water-column observed in some inner areas, light limitation is lower in these areas when compared with the outer areas. This is illustrated in Figure 10, where Santos channel (box 2) shows a higher limitation by light than the Cubatão area (box 4) located in the upper estuary. No limitation occurs for nutrients and the strong nutrient gradient in the estuary does not translate into an increase in nutrient limitation towards the nutrient-poor outer areas.

Due to the large freshwater contribution, the highest concentrations of dissolved inorganic nutrients are found in the inner areas of the estuary. However, these more eutrophic conditions do not necessarily result in higher phytoplankton biomass since the high sediment concentration in the water and the consequent high light attenuation lead to light limitation of the primary production. A similar mechanism has been reported for the nearby estuarine system of Cananéa-Iguape (Berrera-Alba et al. 2007).

Temperature limitation is almost horizontally homogeneous. Higher limitation is seen in winter and limitation also increases in high summer. This happens because ambient water temperature goes below or above the optimal temperature range. Finally, the model results for zooplankton biomass (Figure 11) suggest that grazing pressure may play a significant role in the control of phytoplankton populations in the more inner areas. As seen for Stations P4 and P5, zooplankton biomass is sometimes higher than phytoplankton biomass. Despite the high concentration of zooplankton at these stations (when compared to phytoplankton), the phytoplankton does not seem to be affected, suggesting high production rates.

3.6 Organic matter

In the present model setting, resuspension from the sediments, detrital material and river discharges are the sources of organic matter. So, in areas where resuspension is frequent (assuming there is PON in the sediments), where biological activity is more intense and under the influence of river discharges, OM concentrations are expected to be higher. Model results for PON (Figure 9 and Figure 12) illustrate this relation, with higher values, peaking at 0.2 mg l^{-1}, observed in inner areas of the estuary where biological activity is intense and the influence of rivers is maximal. This is also true for the São Vicente channel area when compared with Santos channel. A small seasonal variation is observed in the results. The link to resuspension of PON is not so obvious because places under strong erosion do not necessarily lead to an increase of resuspension of PON. The rationale is that in some areas, PON may be absent from the sediments.

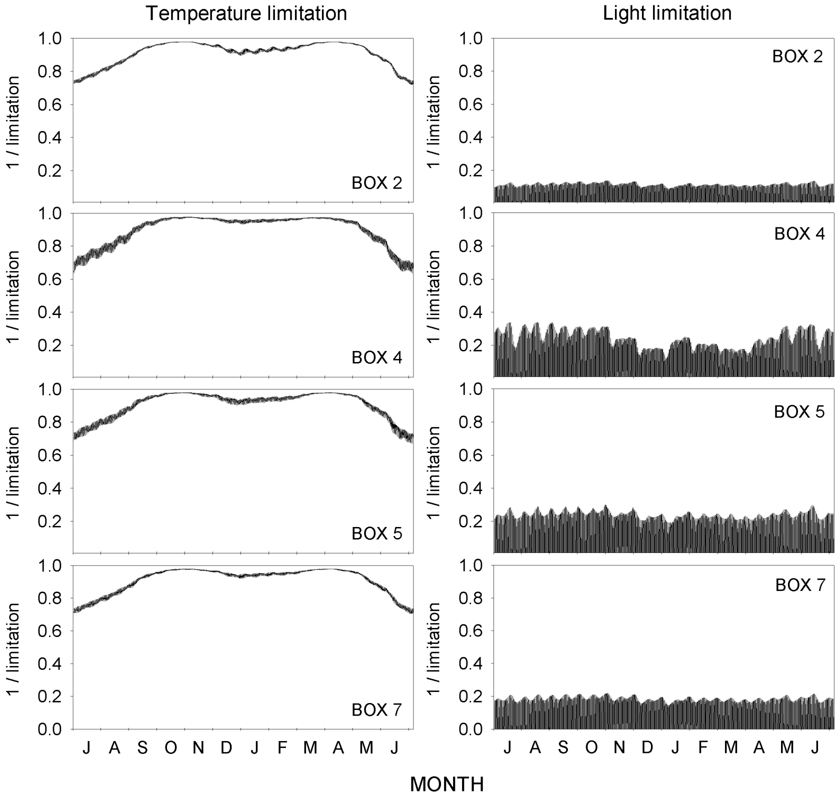

FIGURE 10: *Limitation factors calculate by the model for some integration boxes. Note that values in the Y axis stand for the inverse of limitation, i.e., the higher the value, the lower the limitation (total limitation = 0; no limitation = 1).*

3.7 Dissolved oxygen

Dissolved oxygen in the water is linked with biological activity and also dependent on water temperature. Areas with high phytoplankton biomass are expected to have higher saturations of oxygen (at least during daytime) as a result of photosynthesis. This oxygen production is balanced by the mineralization of organic matter which requires oxygen and produces carbon dioxide. So it is expected that oxygen concentrations and saturation values in the water track the dynamics of phytoplankton and organic matter closely. The interplay of these processes is seen in the horizontal fields of dissolved oxygen saturation (Figure 9). As an example, it is possible to see that saturation values vary considerably inside the estuary, especially near the influence area of the rivers Botoroca, Cubatão, Pereque, and the direct sewage discharges. In this particular case, oxygen consumption may exceed production and the high loads of organic matter at this time of year linked with decreased light availability may be the cause for under-saturation values.

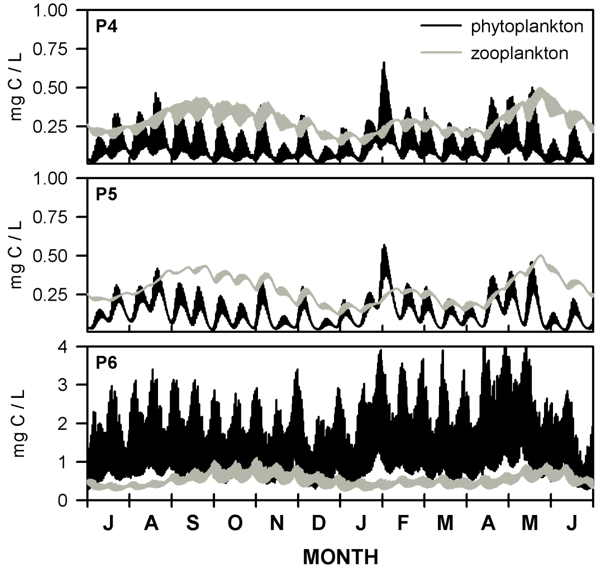

FIGURE 11: *Model results phytoplankton and zooplankton concentration at three monitoring points. Sampling points were selected to consider the inner areas (P4 and P5) and a channel (P6).*

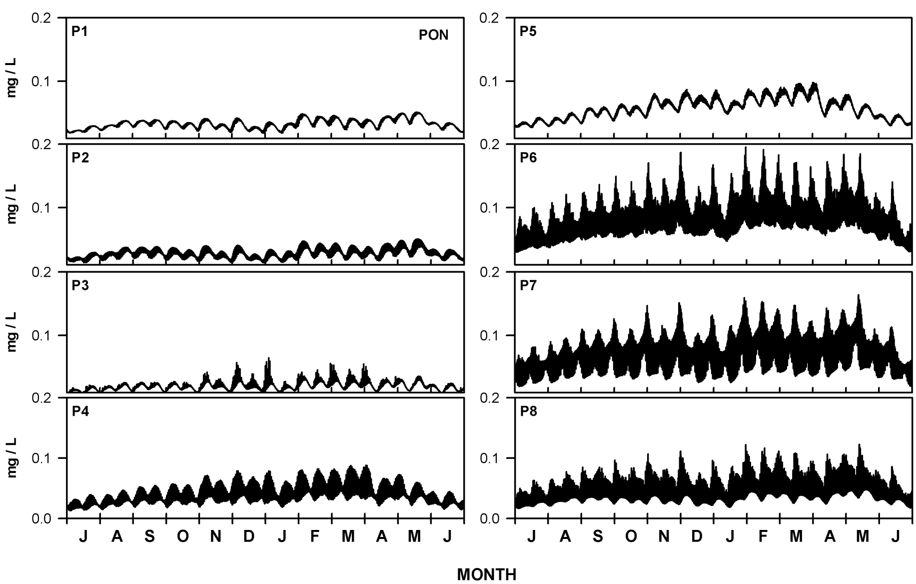

FIGURE 12: *Model results for particulate organic nitrogen (PON) at the monitoring points.*

Supersaturation values are observed in the bay and outer oceanic area, but also in some areas inside the estuary where local conditions cause production to exceed consumption. This pattern has also been observed in the nearby system of Cananéia which shares many physical and biological features with the Santos estuary (Berrera-Alba et al. 2007). This occurrence means that despite the eutrophic state of these systems, oxygen production in the water column can still compensate for the consumption caused by organic matter degradation. The results show that the system can be highly heterotrophic at some places (saturation values below 50%), due to the high loads of allochthonous organic matter, as seen in Figure 9. There is a slight decrease in oxygen concentrations in summer months observed at all stations.

4 MASS FLUXES IN THE ESTUARY

The model results for mass fluxes between different regions in the estuary (integration boxes in Figure 3) of some selected properties are listed in Table 4 and presented in Figure 13. The values were integrated for a period of one year and account for net fluxes across the boundary between adjacent boxes. Considering the boundary of the bay area (box 7) to the open ocean as a hypothetical limit of the estuary, it is possible to look at the model results as an estimate of the export-import of mass from the estuary to the coastal area. The net balance between these two areas is seen in Table 4 in the column 7 to 0. The results show that all described state-variables except oxygen are exported from the estuary to the coastal area. Under these conditions, the model shows that the estuary is exporting nutrients and organic matter (both living and non-living) and importing oxygen. These results suggest that the nutrients that enter in the system via rivers fuel local production but exceed the local needs, thus enriching the system and coastal areas. The oxygen dynamics need further attention because the estuary exports oxygen to the bay via São Vicente channel ($\sim$27 ton yr^{-1}) and much of this production enters the estuary again via Santos channel ($\sim$20 ton yr^{-1}). Because oxygen can be introduced in the system from the atmosphere, no simple inference can be made from the results about the dynamics of the system. However, it can be speculated that the production in some areas can be surpassed by respiration (mineralization of autochthonous and allochthonous organic matter that enters via rivers).

There are other interesting patterns that can be found by looking at some distinct areas of the systems. A striking feature of the system is the net balance between the bay area and both channels (box 7 to box 5 and to box 1). Apparently, the channels have distinct flux dynamics. There is a net positive balance from São Vicente channel (box 5) to the bay (box 7) for all the monitored state-variables. The opposite situation is observed for the fluxes between Santos channel and the bay, where the net fluxes are negative towards the bay, meaning that Santos channel is an entrance route for matter in the estuary. Curiously, a fraction of what is being exported by the São Vicente channel enters the estuary again by Santos channel.

According to model results, Santos channel is a sink for phytoplankton, because only 106 ton yr^{-1} transit from box 2 to 6, whereas 965 ton yr^{-1} transit from box 7 to 2. This sink of phytoplankton explains why the fluxes from Santos channel to Bagres island area (box 2 to 6) of all other variables increase (detrital matter, mineralized nutrients, oxygen consumption). In contrast, Pombeba large area (box 3) is a source of phytoplankton, where the amount that is exported to São Vicente channel (box 1) is more than double the imported quantity from the Cubatão area (box 4). Model results for the fluxes point to an eutrophication of the system.

5 CALIBRATION AND VALIDATION

The calibration and validation exercise was carried out with the aim of qualitatively assessing the model performance. The main purpose was to test the ability of the model to reproduce the overall dynamics of the system and its adequacy as a tool for the prediction of the consequences of different (reduction) scenarios for effluent flow, nutrient loads, etc. To assess the performance of the model, i.e., whether it is able to reproduce the observed spatial and temporal patterns and their variability, model results were compared with observational data. Much of the available data for calibration (Braga et al. 2000, Bosquilha 2002, Moser et al. 2002, Lima 2003) provided significant information on the patterns and variability in nutrient concentrations and organic matter components. After calibration, the model was able to reproduce some of the patterns in the dynamics of the system as presented in these studies.

Validation was made by matching simulated values with field data for the respective properties, as shown in Figure 14. Simulated dynamics correspond well with data from the eight monitoring sites in the estuary. In general, the model produced realistic estimates for temperature, oxygen and nutrients. The magnitude and timing of the phytoplankton peak in in the model reproduced field measurements satisfactorily. A match in values has been regularly achieved, but sometimes not at the same station, as seen in the Chla values for August 2005. The largest mismatches are found regularly at stations 3 and 7. Despite these divergences between model results and data, the model matched validation data with a fair degree of accuracy. The noted discrepancies between modelled and measured values may be due at least partially to our simplification of the dynamics of system components such as the mangroves and inaccurate estimates of the nutrient loads to the system.

6 MODEL PERFORMANCE EVALUATION

The model was able to reproduce the major features of a typical tropical estuarine ecosystem such as Santos Estuary: large temperature variation along the salinity gradient, high mean water temperatures, low light penetration, and variability in the flushing times and sediment and nutrient discharges caused by marked temporal variability in fresh water discharges (Eyre and Balls 1999). The model results reveal a complex interaction of these factors. The seasonal cycle is evident in the results, mostly governed by river discharge associated with the rainy season, and by the light regime (with both temporal and spatial variation). Also, the results show a marked (fortnightly) spring-neap cycle, evident in the time series plots for all properties.

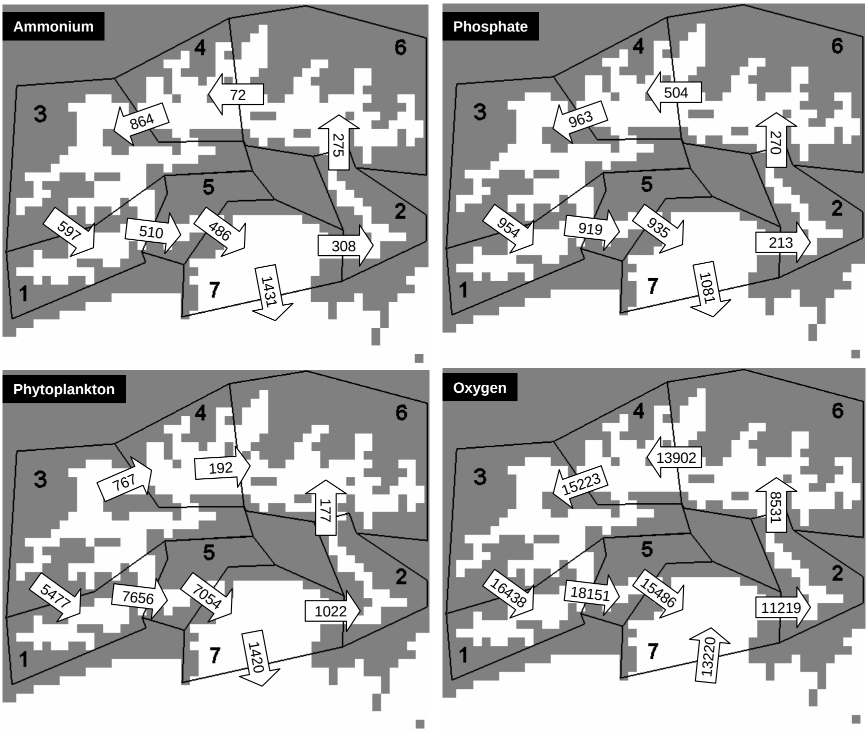

FIGURE 13: *Model estimates for the fluxes of nutrients, phytoplankton biomass and oxygen between different areas of the estuary. All values in metric tones per year.*

TABLE 4: *Mass fluxes between adjacent boxes integrated for one year at the boundary of each box. Positive values mean a net positive balance from one box to the other, while negative values express a negative balance. Column 7 to 0 is relative to fluxes at the boundary of box 7 with the coastal area.*

	mass fluxes between boxes (ton yr-1)							
	1 to 5	**2 to 6**	**3 to 1**	**3 to 4**	**4 to 6**	**5 to 7**	**7 to 0**	**7 to 2**
Ammonium	510	275	597	-864	-72	486	1431	308
Nitrate	2067	742	2332	-2907	-1673	2115	2482	464
Phosphate	919	270	954	-963	-504	935	1081	213
Oxygen	18151	8531	16438	-15223	-13902	15486	-13220	11219
Phytoplankton	7656	177	5477	767	192	7054	1427	1022
PON	407	81	324	-88	16	467	287	92

The organic matter and nutrient concentrations calculated in this study generally fall in the same range as the field data. However, the modelled phosphorus values appear to be higher than the corresponding field data. This suggests that P loads can be overestimated or that the boundary conditions may be too high. From this, we can conclude that a correct characterization of inputs to the system is a prerequisite for a successful calibration effort. The model reproduces the spatial pattern for the properties, where higher values occur in inner estuarine areas, with a limited circulation, and lower values in the main channels with shorter residence times.

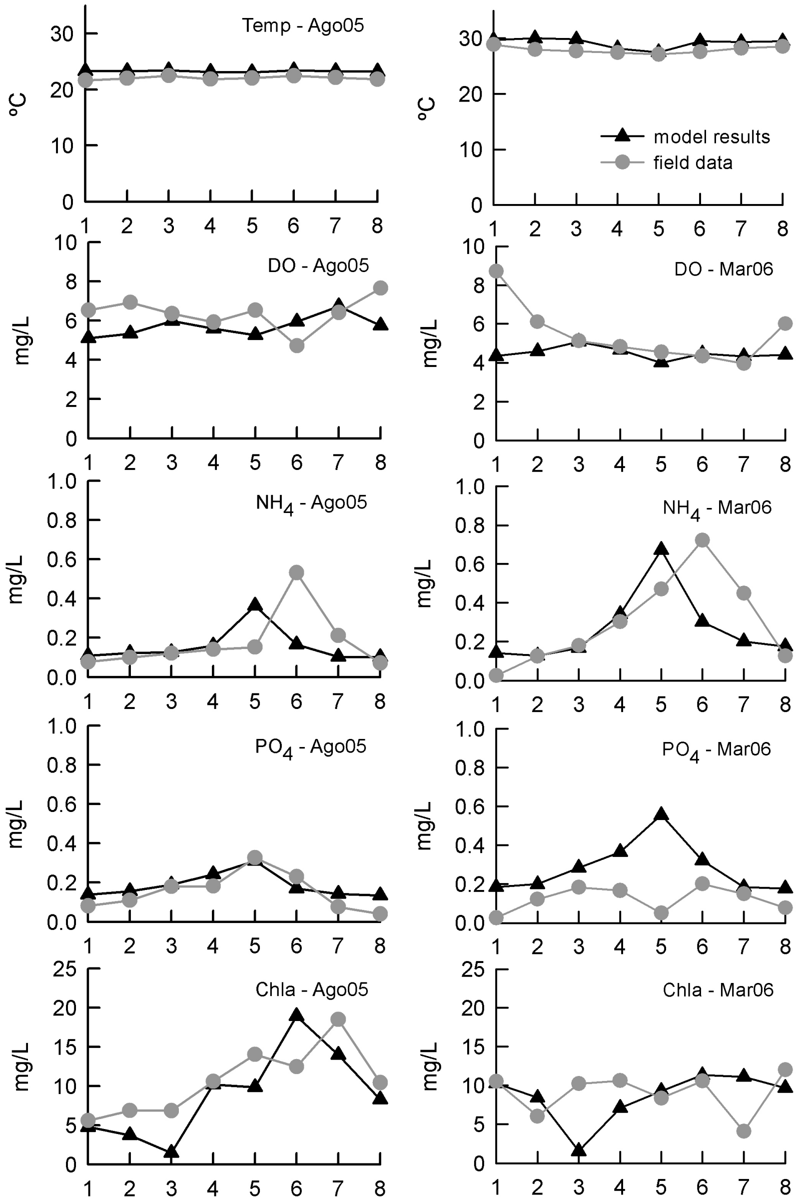

FIGURE 14: *Model output at the monitored stations for several simulated properties (▲) compared with validation data (●). Validation data from the ECOMANAGE monitoring campaigns.*

The model results suggest that São Vicente channel is the main exit route of materials from the estuary, a part of which enters the estuary again via the Santos channel. The model shows a distinct dynamic between these two channels, controlled mainly by the residence time (controlled by physical factors) and the presence of nutrient sources. The residence time in São Vicente channel is higher than in Santos channel, a difference that controls much of the dynamics of material between the channel and the bay. The fast renewal time of water in Santos estuary means that much of the water comes from the bay, which explains the import of material exported from the São Vicente channel.

Although the recycling of nutrients in the system appears to be important, there is a clear control by allochthonous nutrients. Much of the behavior of the system is determined by the large amounts of nutrients (mineral and organic) that are discharged via sewage and rivers. A striking pattern to notice is the oxygen demand in the system, most obvious in the importation of oxygen from the bay (Figure 13). This behavior of the system (as a large bioreactor) poses a challenging demand its management, considering the large anthropogenic pressure expressed in the marked eutrophication of the estuary. In contrast to oxygen, the estuary exports nutrients and organic matter to the coastal area. These results strongly suggest that the Santos estuary is in a highly eutrophic condition, compromising the water quality in the adjacent coastal areas.

Overall, the model is able to reproduce much of the features from the conceptual model derived from field data. The most significant features where the model agrees with data can be summarized in:

- A general pattern in dissolved nutrient concentrations with higher values in the direction of the estuary's head waters, especially in the areas of industrial effluents (e.g., Piaçaguera channel and Largo do Canéu), and with relatively low values in the outer areas close to the open sea. This pattern is shaped mostly by physical mixing processes. Some increases are found near densely populated urban areas where sewage is directly discharged into the estuary. A clear gradient of dilution from the estuary's interior to its mouth is seen along the natural channels (Braga et al. 2000).
- The relation between the spring-neap cycle and the nutrient and phytoplankton concentrations. Phytoplankton has marked variations during neap-tide when nutrient, light availability and residence time all reach maximal values (Moser et al. 2005). Light is usually the limiting factor for phytoplankton growth in estuaries (Cloern et al. 1995, Cloern 1999). The oscillations in light and nutrient conditions between spring and neap tides shape phytoplankton growth. Neap tide conditions enhance the stability in the water column, decreasing the suspended sediments that block the light, and create bloom conditions by increasing the residence time. This pattern has been observed in Bertioga channel, a channel connected to the upper Santos channel (Gianesella et al. 2000), suggesting that the Santos Estuary also shares this feature. Changes in light conditions and flushing ultimately control phytoplankton distribution in the estuary.

- Export of organic matter, inorganic nutrients and phytoplankton to the bay highlighting the contribution of the estuary to the eutrophication of Santos bay, especially during the rainy season when river flow is higher (Moser et al. 2005).
- The increase in particulate matter is mostly from allochthonous sources, not from local phytoplankton production.
- Nutrient limitation does not play a significant role in phytoplankton dynamics. While in the inner parts of the estuary this pattern is explained by the nutrient inputs from rivers and direct sewage discharges, in the bay area this can be explained by the inorganic nutrients contributed by the submarine outfall (Moser et al. 2002, Moser et al. 2004).

7 THE MODEL AS A MANAGEMENT TOOL

For a model to be useful as a management tool it must reproduce the main features of the system under study. This implies that the model must capture the significant processes and interactions between compartments. In short, the model must be able to reproduce the basic elements of the conceptual model of the system.

Under a DPSIR framework, the model establishes a clear relation between anthropogenic nutrient sources (Pressures), the cycling of carbon biomass in the system and oxygen-related problems (State). The outfall emission, river discharges, storm drains and sewage discharges all contribute to its enrichment with nutrients. At the same time, the emissions have a clear impact on oxygen dynamics by increasing the organic matter concentrations, enhancing heterotrophic activity, which in turn contributes still more nutrients to the system. The more complex the system is the more difficult is the task to model it. This is particularly true in cases where the anthropogenic influences are many-faceted, as they are in the Santos estuary. There is always a degree of uncertainty in the load estimates used in the model because of the impossibility to quantify the loads accurately, and this uncertainty negatively affects the modelling exercise. Despite all the uncertainty, the model has the capability to reproduce major features of the ecological conceptual model of Santos and the links between environmental State and human Drivers.

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