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Special Edition

Analysis of the calibration and validation of hydrodynamic simulations with TELEMAC-3D model of the Patos Lagoon

Análise da calibração e da validação de simulações hidrodinâmicas da Lagoa dos Patos com o modelo TELEMAC-3D

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ABSTRACT

This work presents the analysis of the calibration and validation of the computational model for two configurations of the Jetties of the Rio Grande Barra for hydrodynamic studies of the Patos Lagoon and the continental shelf of southern Brazil. The model used was TELEMAC-3D, which solves the three-dimensional Navier-Stokes equations, considering the hydrostatic hypothesis, to describe the dynamics of free surface geophysical fluids. We developed two finite element triangular meshes, with about 75.000 elements and seven sigma levels. The numerical domain reaches depths up to 2.427 m, with fluvial and oceanic liquid boundaries. The horizontal turbulence model adopted was Smagorinsky and the vertical model of mixing length. Current velocity data obtained from December 2005 were used for calibration, varying the coefficient of wind friction, horizontal and vertical velocity diffusion, and the salinity tracer. The coefficient of wind influence was the factor that most influenced the model results. The calculated Relative Mean Absolute Error was 0.383 dn. for surface and 0.167 dn. for depth, rated good and excellent, respectively. For validation, we evaluated the model's performance in reproducing salinity behavior related to the depth of the environment, in January 2017. The calculated Root Mean Square Error was 7.37 dn. and the Relative Mean Absolute Error was 0.228 dn., rating the model performance as good. These variances between metrics are uniformly acceptable for real models. Salt transport is a complex phenomenon and depends on both advective and diffusive transport. Thus, it is possible to conclude that the proposed computational model is able to reproduce a complex phenomenon reliably.

Keywords: Three-dimensional Navier-Stokes equations; Hydrostatic hypothesis; Relative mean absolute error; Root mean square error

RESUMO

O objetivo deste trabalho é apresentar e analisar a calibração e a validação da modelagem hidrodinâmica de duas configurações dos molhes da Barra de Rio Grande, para estudos da Lagoa dos Patos e da plataforma continental do sul do Brasil. O modelo utilizado foi o TELEMAC-3D, que descreve a dinâmica dos fluidos geofísicos de superfície livre a partir das equações hidrostáticas e tridimensionais de Navier-Stokes. As malhas de elementos finitos e triangulares possuem cerca de 75.000 elementos, sete níveis verticais em coordenadas sigma e profundidade de até 2.427 m, com contornos abertos (continentais, oceânicos e superficiais) e fechados. O modelo de turbulência horizontal adotado foi Smagorinsky, e o vertical, de comprimento de mistura. Dados de velocidade de corrente obtidos na Praticagem de dezembro de 2005 foram usados para a calibração, variando o coeficiente de atrito do vento, de difusão horizontal e vertical de velocidade, além do traçador de salinidade. O coeficiente de influência do vento foi o fator que mais influenciou os resultados do modelo. O RMAE calculado foi de 0.383 para superfície e 0.167 para profundidade, classificados como excelente e boa, respectivamente. Para a validação, foi avaliada o comportamento de reprodução de salinidade para profundidade no ambiente no período de janeiro de 2017. O RMSE calculado foi de 7.37 e o RMAE foi de 0.228, classificando a reprodução como boa e excelente. Essa variância entre as métricas é uniformemente aceitável para modelos reais. O transporte de sal é um fenômeno complexo e depende de transporte advectivo e difusivo. Dessa forma, foi reproduzido um fenômeno complexo com confiabilidade para utilização do modelo.

Palavras-chave: Equações tridimensionais Navier-Stokes; Hipótese hidrostática; Erro médio relativo absoluto; Erro médio quadrado raiz

1 INTRODUCTION

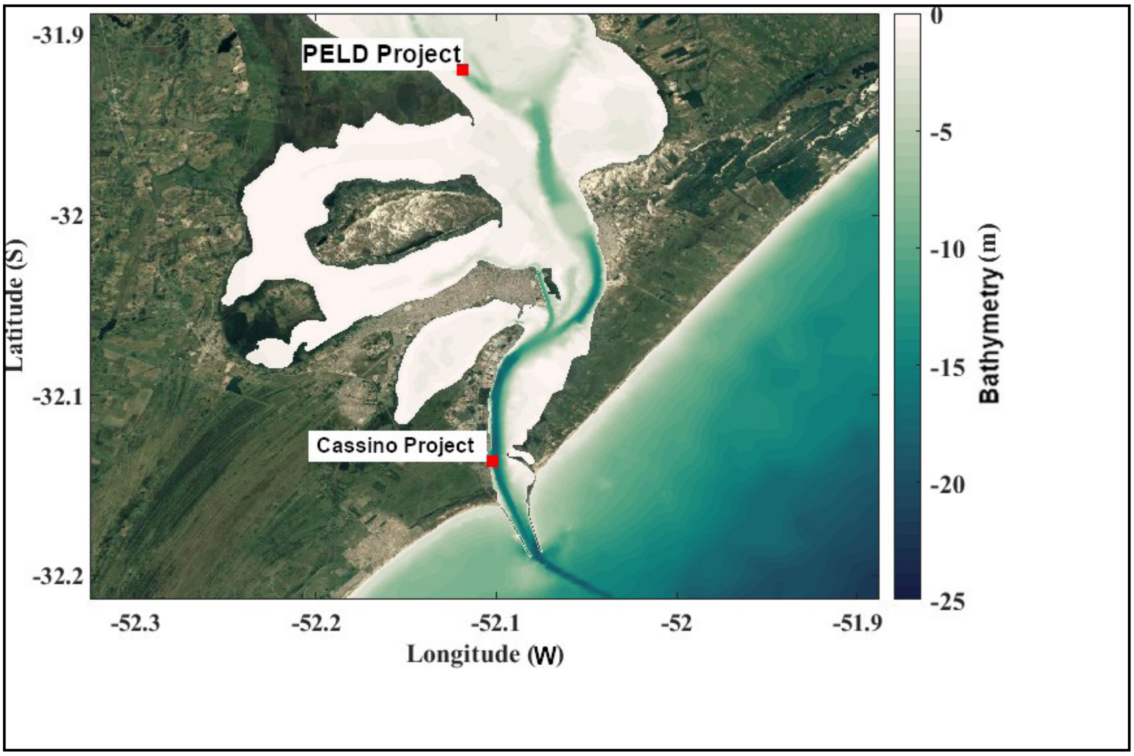
Numerical models developed in recent decades are able to simulate dynamic environments with variables such as currents, waves, and the transport of conservative and non-conservative constituents in estuaries and continental shelf areas. Among so many relevant models, the following stand out: The POM model by authores Blumberg and Mellor (1987); the FVCOM for estuaries circulation, based on finite volume schemes, proposed by Ou et al. (2007); the SWAN by Holthuijsen et al. (2003) for studying wave propagation in shallow waters. It is also possible to mention ROMS used by Shchepetkin and McWilliams (2005); SAM-3D, for plume modeling in the Siene River used by Cugier e Le Hir (2002); MIKE developed by the DHI Water and Environment Institute; MOHID, developed by the Center for Environment and Marine Technology in Lisbon; and Delft-3D, developed by the Deltares Research Institute in the Netherlands.

The use of in situ observations for hydrological and coastal management have high cost, making it difficult to cover large areas in a short time interval. Numerical models allow investigation on larger scales of space and time, with the necessary detail integrated (Martins et al., 1989). In this context, the objective of this paper is to present and analyze the calibration and validation of the computational modeling of the two configurations of the Jetties of the Rio Grande Barra for hydrodynamic studies of the Patos Lagoon and the continental shelf of southern Brazil. Computational modeling has been gaining space in practical applications for the management and monitoring of the Port of the Rio Grande and the region.

1.1 Study area

The study area is located 32°, 34.9° south, 48° and 54° west, encompassing the Patos Lagoon and the continental shelf of southern Brazil (Fig. 1. With an extension of 180 km to the south, in the Arroyo Chuy, going about 100 km north, at Cabo de Santa Marta.

Figure 1 – Map of study area. The red dots represent the location of the equipment whose data were used for the TELEMAC-3D model calibration and validation exercises



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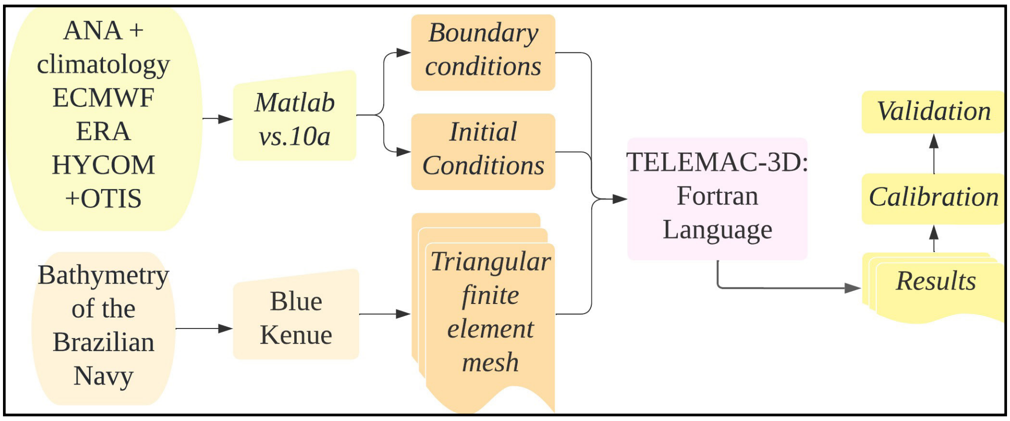
The inner platform, encompasses a mixture of different waters, coming from the platform and the freshwater outflow. The discharge of the La Plata River and the Patos Lagoon are determinants for the continental shelf (Ciotti et al., 1995). In this region farther from the mouth, the mixing processes depend on the prior advection of waters of continental origin and are mainly controlled by the direct action of the coastal circulation along the coast and the Ekman transport induced by the remote action of the wind (Marques et al., 2010b).

Figure 2 – Flowchart showing the sequence of simulation processes carried out with TELEMAC-3D



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2 MATERIAL AND METHODS

The TELEMAC-3D model solves the three-dimensional Navier-Stokes equations, considering Boussinesq and hydrostatic approximations. The model applies the finite element technique to solve the hydrodynamic equations using the sigma coordinate system in the vertical discretization to follow the surface and bottom boundaries (Pham et al., 2013). Different force terms are included, such as the Coriolis term, the free surface and density gradients. After the advection and diffusion steps, the treatment of the set of equations to solve is based on the fact that the hydrostatic approximation is equivalent to the long time (associated with shallow water waves) (Marques et al., 2010a).

Applied to hydrodynamic motion and assumption of hydrostatic pressure and mass conservation laws. It can also calculate vertical density effects resulting from temperature and/or salinization. Fully applied for simulations of saline and/or maximum turbidity regions, such as in an estuary, can be solved with TELEMAC-3D (Pham et al., 2013). The process of using the data, and methods followed, are described in Fig. 2. As described, the external data input, organized with software Matlab. The construction of the finite element triangular meshes was developed in software BlueKenue. The simulations were performed on the computers of the Laboratory of Coastal and Estuaries Oceanography - LOCOSTE/FURG.

2.1 Initial and boundary conditions of the hydrodynamic modules

Initial fields of salinity (Fig. 3) and temperature were prescribed in the entire three-dimensional domain based on the results of the HYCOM + NCODA Global Project (HYbrid Coordinate Ocean Model), which have a temporal resolution of 1 day and spatial resolution of 0.083° x 0.083°. Initial suspended sediment concentrations were assumed to be zero. The computational meshes have open boundaries, which can be divided into continental, oceanic and surface boundaries, where the different boundary conditions are prescribed for performing the simulations. The other boundaries are considered closed boundaries.

2.2 Ocean, surface and continental boundaries

Current velocities, sea level, salinity, and temperature were prescribed in the oceanic boundary of the domain. The data was obtained from the Hycom global reanalysis project. Tidal elevation and current velocity were included using the OSU Tidal Inversion System Zu et al. (2008), Dawson and Riedlinger (2009)), providing the surface elevation and regional tidal current velocity. The surface of the computational mesh is dynamically forced with results from the global model European Center for Medium- Range Weather

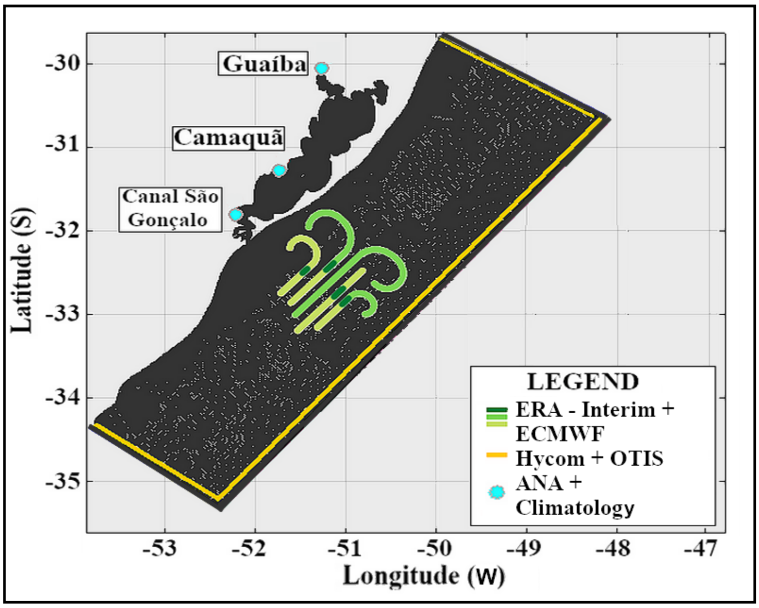
Forecast with contribution of wind speed, air temperature and atmospheric pressure from the reanalysis ensemble (at the surface) with interval with a temporal resolution of 6 h and spatial resolution of 0. 75°, European Centre for Medium-Range

Weather Forecasts interim reanalysis used in works such as those of (Marques, 2010); (Fernandes et al., 2021).

For the continental open boundaries of the simulations mesh, daily flow data from the Guaíba River and Camaquã River were used, obtained from the National Water Agency. For the São Gonçalo Channel flow, level data obtained from the Lagoa Mirim Agency were used and transformed into daily flow data from the key curve Oliveira et al. (2015), and subsequently calculated its climatology for the time interval of (1991 - 2012) (Cyan points in Fig. 3).

For calibration and validation of TELEMAC-3D, the data measured during the years 2005 and 2017 were used. Obtained through the Cassino Project, and data from the Long Term Ecological Research Project - PELD.

Figure 3 – Location of open boundaries in the meshes and boundary conditions inserted in the model: wind, salinity, current, tide, discharge and suspended material concentration



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The response of the TELEMAC- 3D Model to the variation of the main physical parameters that control the hydrodynamics of the environment, and its ability to reproduce the environmental conditions observed in the study area, were evaluated during the calibration and validation stages, respectively.

For calibration of the hydrodynamics, we considered current velocity and direction data for the month of December 2005 in Patos Lagoon. These data were obtained by an Acoustic Doppler Profiler - ADP Sontek, of 1000 Hz with temporal resolution of 1h, anchored in the Docking Station at 12 m depth and located at 32° 08′ 12″ S and 52° 06′ 09″ W (Fig. 3). For the validation of the hydrodynamic modeling, salinity data for the period January 2017, obtained by sample collection, located at 31° 55′ 06″ S and 52° 07′ 07″ W (Fig. 3), anchored at 4 m depth, were used as part of the PELD Project, with hourly acquisition rate.

2.3 Physical parameters considered in the simulations

A summary of the main physical parameters used in the simulations is shown in the following Table 1.

2.4 Finite and triangular mesh elements

The mesh domain extends between 30° and 36° to the south, 48° and 54° to the west, including the Patos Lagoon, a large part of the South Brazilian Continental Shelf and abyssal region. After being tested and adjusted, the final meshes have about 75,000 elements and 52,000 points, both with seven sigma levels and their depth extends to 2,427 m depth (Fig. 4).

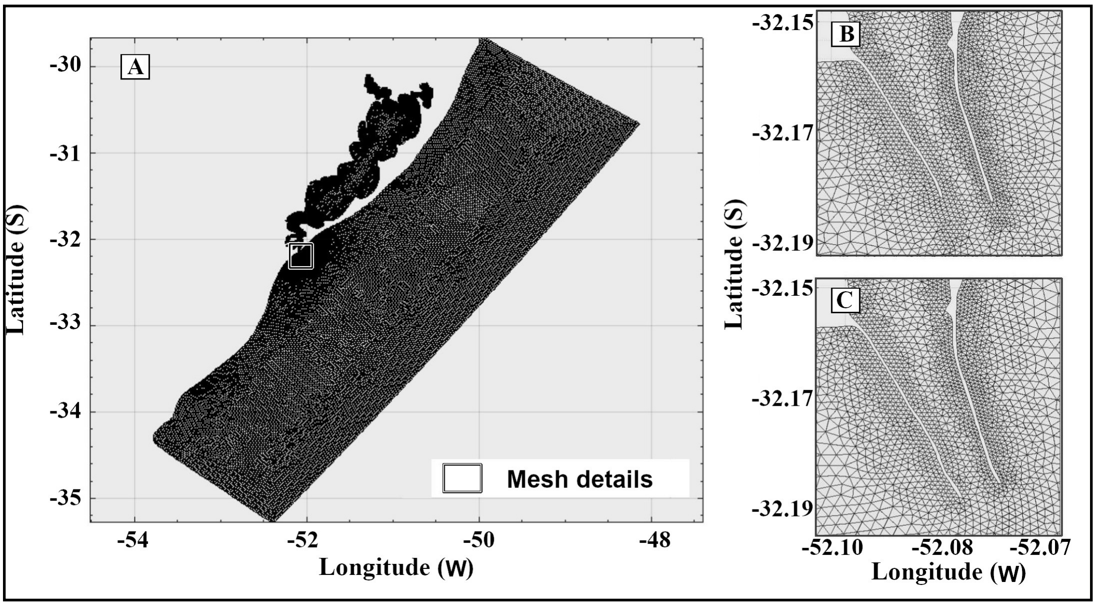
The adopted mesh dimensions went through several attempts to find the best configuration to be adopted; this ensures better performance of the simulations, with the edges kept far enough from the Patos Lagoon plume region, thus avoiding problems with numerical inconsistencies originating at the edge (due to the imposition of boundary conditions) that affect the area of interest.

Table 1– Parameters adopted in the TELEMAC - 3D model

Parameters	Values
Coriolis Coefficient	$-7.70x10^{-5}$
Horizontal Turbulence Model	Smagorinski
Vertical Turbulence Model	Length and Blending
Tidal Flats	Yes
Time Step	60 s
Law of Bottom Friction	Nikuradse
Friction Coefficient for the Bottom	$1x10^{-5}$
Mean Diameter of the Sediment	$1x10^{-5}$ m
Critical Shear Stress for Erosion	1.5 N/m^2
Critical Shear Stress for Deposition	0.15 N/m^2
Gibson Consolidation Model	Yes
Maximum Concentration of the Consolidated Mud	1500.0 km/m^3
Flocculation Coefficient	0.3
Coefficient of Wind Influence	$3x10^{-6}$

Source: authors

Figure 4 – **A)** General mesh of the study area; the differences between the meshes, being: **B)** Scenario I: pre-enlargement of the jetties in 2010; **C)** Scenario II: post-extension of the jetties



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3 RESULTS AND DISCUSSIONS

3.1 Model calibration

The ability of the numerical model to reproduce the environmental conditions was evaluated by comparing the model results and current time series described above. The quality of the model results was evaluated by calculating the correlation between simulated and measured current velocity, and by applying the indices Relative Mean Absolute Error (RMAE) and the Root Mean Square Error (RMSE) (Helena Fernandes and Hax Niencheski, 2001).

The RMAE allows one to rate the quality of the results on a scale from poor to excellent (Table 2), while the RMSE reports the magnitude of the error with dimensional values. Thus, both measures express the average error of the predictive model, relative to the original and test data. They are in the 0-infinite range and return the magnitude of the errors, not their direction. Finally, the smaller, the better in both cases.

The calibration exercise of the hydrodynamic model (TELEMAC-3D) was performed for the period December 2005, for which current velocity data obtained from the Wharf age were available. The model was run using the same initial and boundary condition categories. Forty-five calibration tests were performed by varying the wind friction coefficient and values for horizontal and vertical velocity diffusion coefficients, and the salinity tracer.

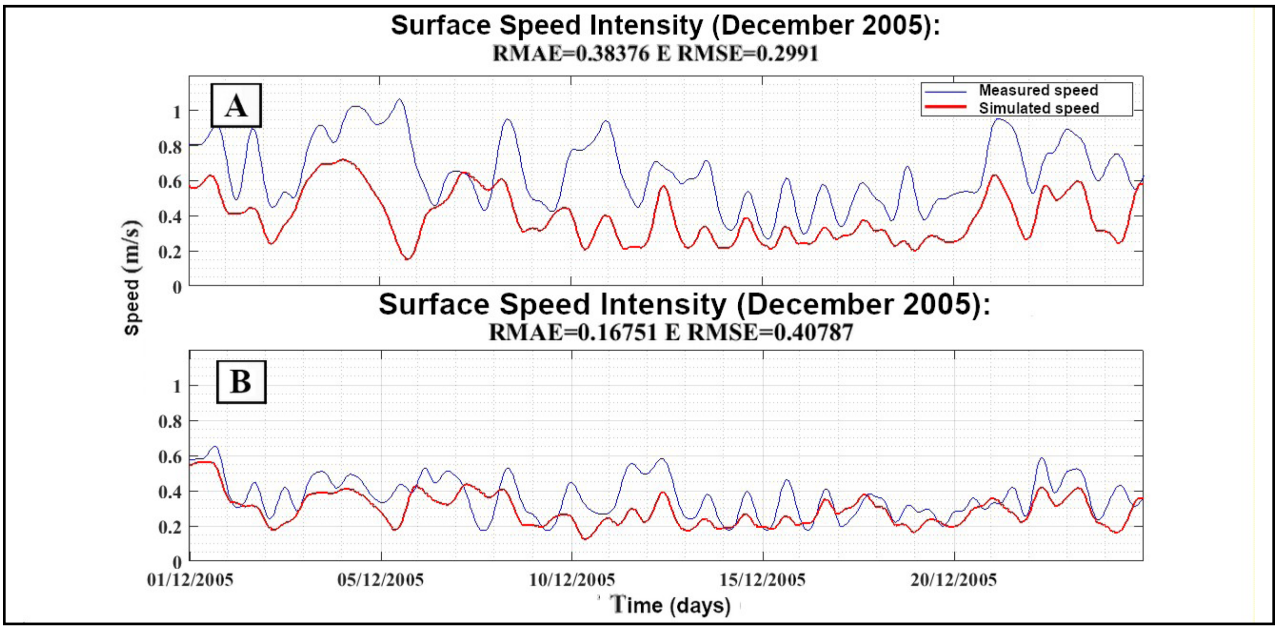
Table 2 – Qualification Relative Mean Absolute Error (RMAE)

Qualification	RMAE
Excellent	<0.2
Good	0.2 — 0.4
Fair	0.4 — 0.7
Poor	0.7 — 1.0
Bad	>1.0

Source: authors

The value that showed the best results in wind calibration was $3x10^{-6}$. The best reproduction of the environmental data was achieved by the model in Test 40, shows the parameters tested in the model calibration. Fig. 5 presents the comparison between the current velocity intensity data calculated by the model and those measured by ADP, at the depth of 12 m (Fig. 5 A) and 0 m (Fig. 5 B). The solid line in red indicates the model results, while the ADP data are represented by the dashed blue line. It can be seen that the model represents well the trends of increasing and decreasing current velocity intensities, however at some points it underestimates the values.

Figure 5 – Time evolution of the current intensity measured by ADP (dashed blue line) at the Wharf in December 2005 and calculated by the model (solid red line). Depth 12 m (**A**) and depth 0 m(**B**)



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The calculated RMAE was 0.383 for surface (12 m) and 0.167 for depth (0 m), rating the model reproduction as excellent and good respectively (Sadiku, 2004). The calculated RMSE was 0.299 m/s for 12 m and 0.407 m/s for 0 m depth. A feature of RMSE is that the errors (actual - predictions) are squared before averaging. Therefore, different weights will be assigned to the sum and as the error values of the instances increase the index of the RMSE increases considerably, as presented with the background result. That is, if there is an outlier in the dataset, its weight will be greater for the calculation of the RMSE consequently hurting its metric by making it larger.

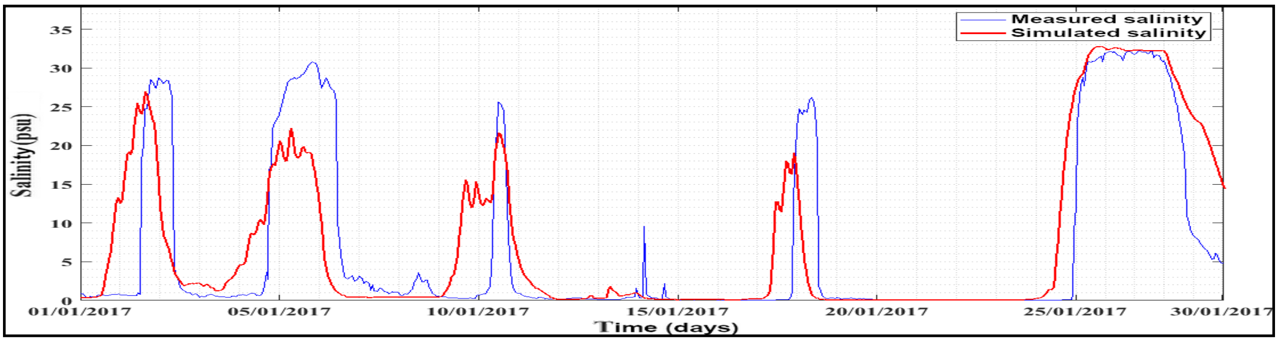
Very small errors favor the RMSE, while as the RMSE errors increase, the RMAE gets smaller. For errors between 0 and 1 (very high accuracy), the RMSE $\leqslant$ RMAE, so the RMSE tends to have increasing values and the RMAE grows as the test sample size increases. For the surface case, on the other hand, the RMAE $<$ RMSE, represents a small variance between the metrics, which presents a uniform variance, which is also acceptable when comparing real models.

3.2 Model Validation

The behavior of salinity in the environment by comparing the model prediction for the January 2017 period and the measured data in this same period were used for model validation (Fig. 6).

Fig. 6 presents the temporal evolution of salinity calculated by the model and measured in the field, PELD Project (Fig. 6), both at 4 m depth. The calculated RMSE was 7.37 psu (in a range from 0 to 35) and the RMAE was 0.228, classifying the model reproduction as, good (Sadiku, 2004). Salt transport is a complex phenomenon and depends on both advective and diffusive transport, thus, a RMAE of 0.228 indicates that the model was able to reproduce a complex phenomenon reliably.

Figure 6 – Temporal evolution of salinity calculated by the model (blue solid line) and measured by CT (red dashed line) at the PELD Project station



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The calibration and validation results found, had statistical results presented in Table 3 above. The calibration results, about standard deviation, show that the values are well distributed around the mean. The validation, on the other hand, indicates that they are condensed close to the mean. However, both results are homogeneous over the data set studied.

Table 3 – Sigma statistics on the surface

Modeled Std		Measured Std	Modeled MAE	Measured MAE
Calibration	11.54	10.08	0.06	0.25
Validation	10.54	11.05	1.08	0.20

Source: authors

4 CONCLUSIONS

The present work achieved the calibration and validation required for reproducing the TELEMAC model in the Patos Lagoon environment. The calculated Root Mean Square Error of salinity data was 7.37 and the Relative Mean Absolute Error was 0.228, rating the model performance as good. These variances between metrics is uniformly acceptable for real models. The calibration parameters can be used to applied studies, and to improve the model for the region.

Despite the limitations of the horizontal turbulent model used, the calibration and validation results, indicated that the model adequately reproduces the environmental conditions (current, level and salinity) observed in Patos Lagoon, its estuary and adjacent coastal zone.

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REFERENCES

Blumberg, A. F., Mellor, G. L. (1987). Description Of A Three-Dimensional Coastal Ocean Circulation Model, In Three-Dimensional Coastal Ocean Models. *Coastal Estuarine Sci*, *4*.

Ciotti, Á. M., Odebrecht, C., Fillmann, G., Moller, O. O. (1995). Freshwater outflow and Subtropical Convergence influence on phytoplankton biomass on the southern Brazilian continental shelf. *Continental Shelf Research*, *15*(14), 1737–1756.

Cugier, P., Le Hir, P. (2002). Development of a 3D hydrodynamic model for coastal ecosystem modelling. Application to the plume of the Seine River (France). *Estuarine, Coastal and Shelf Science*, *55*(5), 673–695.

Dawson, G. M., Riedlinger, S. H. (2009). Use of the Oregon State University Tidal Inversion Software (OTIS) to Generate Improved Tidal Prediction in the East-Asian Seas. Relatório Técnico APRIL 2009, Oceanography Division.

Fernandes, E. H., da Silva, P. D., Gonçalves, G. A., Möller, O. O. (2021). Dispersion plumes in open ocean disposal sites of dredged sediment. *Water (Switzerland)*, *13*(6), 1–20.

Fernandes, K. H., Elisa; Dyer R., Niencheski, L. F. H. (2001). Calibration and Validation of the TELEMAC- 2D Model to the Patos Lagoon (Calibration and Validation of the TELEMAC-2D Model to the Patos Lagoon (Brazil). *Source: Journal of Coastal Research*, *1*(1991), 470–488.

Holthuijsen, L. H., Booij, N., Ris, R. C., Haagsma, I. G., Kieftenburg, A. T. M. M., Kriezi, E. E., Zijlema, M. (2003). SWAN Cycle III version 40.20 USERMANUAL.

Marques, E. H. M. O. O., Wiliam C. Fernandes (2010). Straining and advection contributions to the mixing process of the Patos Lagoon coastal plume, Brazil. Journal of Geophysical Research: Oceans, 115(6), URL http://www.agu.org/pubs/crossref/2010/2009JC005653.shtml.

Marques, W., Fernandes, E., Moraes, B., Möller, O., Malcherek, A. (2010a). The dynamics of Patos Lagoon coastal plume and their contribution for the deposition pattern of suspended sediments in the Southern Brazilian inner Shelf. *Journal of Geophysical Research*, *in press*.

Marques, W. C., Fernandes, E. H., Moraes, B. C., Möller, O. O., Malcherek, A. (2010b). Dynamics of the Patos Lagoon coastal plume and its contribution to the deposition pattern of the southern Brazilian inner shelf. *Journal of Geophysical Research: Oceans*, *115*(10), 1–22.

Martins, I. d. R., Villock, J. A., Martins, L. R., Bemvenuti, C. E. (1989). The Lagoa Dos Patos Estuarine Ecosystem (RS, Brazil). *Pesquisas em Geociências*, *22*(22), 5.

Oliveira, H., Fernandes, E., Junior, O., COLLARES, G. (2015). Processos Hidrológicos e Hidrodinâmicos da Lagoa Mirim. *Revista Brasileira de Recursos Hídricos*, *20*(1), 34–45.

Ou, S., Zhang, W., Hong, D. x., He, J. (2007). Horizontal Characteristics of Buoyant Plume off the Pearl River Estuary during Summer. *Journal of Coastal Research*, *50*(0749.0208), 652–657.

Pham, C. T., Bourban, S., Durand, N., Turnbull, M. (2013). Telemac Modelling System: Telemac-3D Software – Operating Manual. Relatório Técnico, EDF, Chateau, France.

Sadiku, M. N. O. (2004). *Elementos de eletromagnetismo*, bookman edn. Oxford University Press, New York. Shchepetkin, A. F., McWilliams, J. C. (2005). The regional oceanic modeling system (ROMS): A split-explicit, free-surface, topography-following-coordinate oceanic model. *Ocean Modelling*, *9*(4), 347–404.

Zu, T., Gan, J., Erofeeva, S. Y. (2008). Numerical study of the tide and tidal dynamics in the South China Sea. *Deep-Sea Research Part I: Oceanographic Research Papers, 55*(2), 137–154.

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