

# Large-scale groundwater monitoring in Brazil assisted with satellite-based artificial intelligence techniques

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## Abstract

Here, we develop and test an artificial intelligence (AI)-based approach to monitor major Brazilian aquifers. The approach combines Gravity Recovery and Climate Experiment (GRACE) data and ground-based hydrogeological measurements from Brazil's Integrated Groundwater Monitoring Network at hundreds of wells distributed in twelve aquifers across the country. We use a model ensemble composed of four different AI models: Extreme Gradient Boost, Light Gradient Boosting Model, CatBoost and Multilayer Perceptron. The approach is further boosted with wavelet and seasonal decomposition processes applied to GRACE data. To determine the sensitivity of the AI approach to data availability, we propose four experiments combining hydrogeological measurements from different aquifers. Groundwater storage estimates from the Global Land Data Assimilation System (GLDAS) are used as the benchmark. The AI approach successfully reproduces groundwater storage estimates at all Brazilian aquifers. Results show that the proposed approach outperforms GLDAS in all experiments, with an average Nash-Sutcliffe efficiency of 0.91 and an average RMSE of 0.43cm for the experiment that covers all monitored wells in Brazil. GLDAS resulted in -1.311 and 5.84cm, respectively. This study demonstrates that combining satellite data and AI can be a cost-effective alternative to monitor poorly equipped aquifers at the continental scale.

# Large-scale groundwater monitoring in Brazil assisted with satellite-based artificial intelligence techniques

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**Abstract** – Here, we develop and test an artificial intelligence (AI)-based approach to monitor major Brazilian aquifers. The approach combines Gravity Recovery and Climate Experiment (GRACE) data and ground-based hydrogeological measurements from Brazil's Integrated Groundwater Monitoring Network at hundreds of wells distributed in twelve aquifers across the country. We use a model ensemble composed of four different AI models: Extreme Gradient Boost, Light Gradient Boosting Model, CatBoost and Multilayer Perceptron. The approach is further boosted with wavelet and seasonal decomposition processes applied to GRACE data. To determine the sensitivity of the AI approach to data availability, we propose four experiments combining hydrogeological measurements from different aquifers. Groundwater storage estimates from the Global Land Data Assimilation System (GLDAS) are used as the benchmark. The AI approach successfully reproduces groundwater storage estimates at all Brazilian aquifers. Results show that the proposed approach outperforms GLDAS in all experiments, with an average Nash-Sutcliffe efficiency of 0.91 and an average RMSE of 0.43cm for the experiment that covers all monitored wells in Brazil. GLDAS resulted in -1.311 and 5.84cm, respectively. This study demonstrates that combining satellite data and AI can be a cost-effective alternative to monitor poorly equipped aquifers at the continental scale.

27    **Key Points**

- 28        •    An Artificial Intelligence (AI)-based model was built to monitor groundwater in  
29                Brazilian aquifers using satellite gravimetry data
- 30        •    AI-based groundwater changes outperformed Global Land Data Assimilation  
31                System (GLDAS) estimates in all proposed experiments
- 32        •    Results show that satellite-based AI techniques can be an effective solution for  
33                groundwater monitoring in poorly equipped regions

## 1 - Introduction

Proper aquifer monitoring at local, regional and large scale faces enormous difficulties to be achieved due the complexity and diversity of geological formations and the corresponding lithologic and facial structures, hydraulic properties, recharge zones and groundwater exploitation accentuated by land use and land cover changes coupled to meteorological and climatic variability. There is definitely a demand for global and operational hydrogeological monitoring, once groundwater is the largest unfrozen freshwater stock on the planet and tightly connected to surface water, reservoir and lakes (Condon et al., 2021). In 2002, over 1.5 billion people were estimated to be directly supplied by groundwater (Alley *et al.*, 2002). This number has risen to 2 billion people in 2020 (UNESCO, 2020). It is estimated that 43% of the total water used in irrigation has underground origin (Siebert et al., 2010). Countries such as the United States and India use approximately 25% and 40% of groundwater resources to supply their respective needs (Getirana et al., 2021), resulting in significant aquifer depletions (e.g., Rodell *et al.* 2018; Nie *et al.* 2019). In Brazil, about 57% of its municipalities have groundwater supply to some extent (IBGE, 2020). The intensification of groundwater use, combined with the impacts of climate change, has been causing the depletion of aquifers worldwide (Richey et al., 2015). Therefore, it is essential to understand groundwater spatiotemporal dynamics to ensure its sustainable use.

Groundwater monitoring networks have been based on observation wells associated with the creation of conceptual and mathematical models (Condon et al., 2021). Large-scale hydrological model outputs, such as those produced by the Global Land Data Assimilation System (GLDAS; Rodell et al., 2003), can be used as an alternative to the absence of hydrogeological monitoring systems. Such modeling systems can explicitly represent, in a simplified way, groundwater dynamics (Getirana et al., 2020; Li et al., 2019). Such models are robust in their structure and have the ability to provide the behavior of surface water and groundwater at continental and global scales. However, these models still need to be adjusted for optimal regional use (Getirana et al., 2020).

A new frontier has been opened for the study of groundwater by gravitational data provided by the Gravity Recovery and Climate Experiment (GRACE) (Tapley et al., 2004) and GRACE Follow On (GRACE-FO) missions, which measure changes on global gravitational forces. Among those changes, there are those promoted by the water cycle. They can be mapped by satellites and later converted into terrestrial water storage (TWS)

variability. Several studies have used data from GRACE missions to capture regional groundwater behavior and to assess measurements related to groundwater levels (Andrew et al., 2017; Frappart and Ramillien, 2018; Getirana et al., 2020; Scanlon et al., 2012, 2018). In Brazil, the use of GRACE data to understand the water behavior can be found in recent studies (Getirana, 2016; Hu et al., 2017; Gonçalves et al., 2020; Getirana et al., 2021). Li et al. (2019) assimilated GRACE data into a hydrological model globally and analyzed groundwater variations, comparing model results to *in situ* observations.

There is a clear contribution of GRACE data assimilation (DA) into hydrological models in the representation and prediction of hydrological processes (Getirana et al., 2020; Getirana et al., 2020; Giroto et al., 2017; Jung et al., 2019; Kumar et al., 2016). Nevertheless, new tools based on the so-called artificial intelligence (AI) algorithms have also proved to be very efficient for the pattern recognition of groundwater behavior worldwide (Afzaal et al., 2020; Huang et al., 2019; Iqbal et al., 2021; Lähivaara et al., 2019; Ren et al., 2021; Tao et al., 2022; Zhang et al., 2020).

AI algorithms, associated with GRACE-based TWS variations can be of great value in the survey of aquifers. Groundwater studies using AI and GRACE data have been carried out for some years (Gemitzi and Lakshmi, 2017; Sun, 2013; Sun et al., 2019). Wave decomposition methods are also very useful in hydrological studies for flow prediction, seasonal analysis or even hydrogeological studies (Ashraf et al., 2022; Basu et al., 2022; Erkyihun et al., 2016; Qi and Neupauer, 2008). Hybrid use of AI and wavelet decomposition techniques turned out to be an important and active research area, resulting in more accurate models in water resources applications, due to its great ability to discriminate non-stationary and nonlinear trends that occur at different scales in groundwater time series (e.g., Tao et al., 2022). For example, Andrew et al. (2017) presented the possibility of disaggregating GRACE data using wavelets as a viable path to study groundwater under different observational spatiotemporal scales.

Brazil's Integrated Groundwater Monitoring Network (RIMAS), conceived and built by the Geological Service of Brazil, initiated in 2010 and is currently composed of 409 wells, monitoring 24 aquifers across the country. The distribution of wells across the monitoring network is not homogeneous, leading to constraints in monitoring the spatiotemporal variability of the nation's aquifers. Also, only porous, free or semi-confined aquifers have been monitored by RIMAS. Such a sparse network is substantially less dense than those found in other large countries, such as the U.S. and India, which

have more than 16,000 and 22,000 wells, respectively (Getirana et al., 2021). That leads to limited groundwater monitoring in Brazil. The limited knowledge on Brazil's groundwater dynamics limits management and optimized use of its aquifers. The absence of data also limits the development and parameterization of hydrological and hydrogeological models to monitor Brazil's water resources, resulting in inaccurate water flow and storage calculations, affecting various sectors of society such as agriculture, energy generation and domestic supply (Getirana et al., 2021).

Considering the limitations described above, this work presents a methodology that combines point-based *in situ* groundwater measurements and spatially-distributed satellite-based TWS, in addition to wavelet decomposition techniques and artificial intelligence (AI) as tools to understand the behavior of large aquifers in Brazil. The main advantage of the proposed methodology is the use of a hybrid model (wave decomposition + ensemble model) with the application of four different AI techniques. GLDAS-based groundwater simulations are used as the benchmark to determine the potential of the proposed methodology. GLDAS simulations are those derived from the Catchment Land Surface Model (CLSM) (Koster et al., 2000) with GRACE-DA (Li et al., 2019). We considered such simulations as our benchmark because they have been comprehensively evaluated globally and are widely used. Also, it is currently the only temporally continuous and spatially distributed groundwater product available in Brazil. We expect that the proposed methodology can be used for the management of large Brazilian aquifers, in addition to enabling the monitoring of groundwater in places where monitoring networks are precarious, inexistent, or with heterogeneous hydrogeological and climatic conditions.

## **2 – Case study and Datasets**

### **2.1 – *In situ* data from aquifers**

Aquifers monitored by RIMAS total 2,839,558km<sup>2</sup>, or 34% of the Brazilian territory. Their sizes vary from 884km<sup>2</sup> (Missão Velha) to 774,385km<sup>2</sup> (Içá), with monitoring coverage varying from 3 (Ronuro) to 71 (Urucuia) wells. Their spatial distribution and RIMAS network are shown in Figure 1. The monitoring network density varies significantly, with Missão Velha being the aquifer with the highest density of wells (0.018 wells/km<sup>2</sup>) and Içá with the lowest density (0.000013 wells/km<sup>2</sup>). Such a heterogeneous density is mostly explained by the way the network is installed, which as initial criteria: sedimentary aquifers, socioeconomic importance of the water, water use

for public supply, natural vulnerability and risk aspects, spatial representativeness of the aquifer and existence of wells for monitoring (Mourão, 2009). Effective porosity ( $S_y$ ) values for each aquifer were estimated based on available data found in the literature (please refer to Table 1 for a full list), varying from 0.03 in Cabeças Aquifer to 0.18 in Alter do Chão Aquifer.

RIMAS is designed based on wells equipped with automatic level meters collecting data at the hourly step, which are subsequently subjected to consistency, treatment, and availability processes (<http://rimasweb.cprm.gov.br/layout/>). The estimated error of the measurements is the minimum resolution of the equipment, which varies between 0.01 and 1.5 cm. More specifically, porous, free, semi-confined and wells in areas of crystalline rocks are addressed in this study, focusing on the responses that different lithologies might produce and how that information could be translated into the building AI model approach we are developing in-here. Geological and hydrogeological description of the aquifers monitored by RIMAS can be found at <http://rimasweb.cprm.gov.br/layout/apresentacao.php>.

The RIMAS dataset is available at the hourly time step. Monthly groundwater level change ( $dh_i$ ) at each well was computed by first converting the time series to monthly means, then subtracting the value in the previous month ( $\eta_{i-1}$ ) from the subsequent one ( $\eta_i$ ), as follows:

$$dh_i = \eta_i - \eta_{i-1} \quad (1)$$

Where  $i$  stands for months of the time series. Each  $dh_i$  value was then subtracted by their respective long-term mean, and multiplied by their corresponding aquifer  $S_y$  value, resulting in the time series used as input in our approach, named hereafter as  $GWS_{OBS}(cm)$ .  $S_y$  was used in order to normalize time series at all wells, from groundwater level to storage equivalent. Equation 2 shows the calculation of  $GWS_{OBS}$  (cm) for each month  $i$ :

$$GWS_{OBS}(i) = [dh_i - \text{mean}(dh)] \cdot S_y \quad (2)$$

## 2.2 - Terrestrial water storage

GRACE RL06 Mascon data, processed by the Center of Space Research (CSR; Save et al., 2016), is retrieved at 0.25-degree spatial resolution and monthly time step from

April, 2002 to present with gaps throughout the period. Initially, monthly GRACE-based TWS values had uncertainties estimated at 1cm for areas equal to or greater than 400,000km<sup>2</sup> (Swenson et al., 2003). However, such estimates had a significant improvement, as described in Ditmar (2018), obtaining more refined results for TWS approximations at 0.25-degree spatial resolution. Such Mascon-based products have lower errors compared to spherical harmonics (Rowlands et al., 2010). Even maintaining a resolution limited by the nature of the GRACE data and uncertainties in the TWS of 1cm, these estimates allow a more detailed study of hydrological and hydrogeological basins with dimensions smaller than those indicated by Save (2020) as demonstrated in Melati et al. (2019) and Gonçalves et al. (2020), both carried out in Brazil.

### 2.3 – GLDAS-based groundwater

The CLSM with GRACE-DA was chosen among the different GLDAS products for presenting an explicit and more accurate representation groundwater storage (GWS). CLSM is a state-of-the-art energy and water balance model of the Earth's surface, designed for use in models of global earth systems. The model simulates a dynamic water table with a spatial distribution related to the topography of the basin (Bechtold et al., 2019). Details about the model configuration and global evaluation can be found in Li et al. (2019).

## 3 – Methodology

Briefly, the methodology follows four steps. First, wave decomposition (wavelet and seasonal) on the TWS values for Brazil. Second, interpolation of the values obtained by the wavelets for the original time scale. Third, the decomposition results are associated with the RIMAS measurements, according to latitude, longitude and time. Hydrogeological data of the Hydrogeological Map of Brazil (HMB) is also associated with RIMAS wells according to latitude and longitude. Finally, the dataset is inserted into an AI model to approximate the groundwater storage (GWS<sub>OBS</sub>) values obtained by the RIMAS wells. The input values in the model are: TWS values, decompositions (wavelet and seasonal), hydrogeological description of the HMB in addition to the latitude and longitude values of wells. Groundwater storage estimates from the CLSM GRACE-DA (GWS<sub>CLSM</sub>) are used as the benchmark.

Wavelet transform is a technique that has proven to be effective for capturing nonlinear relationships in time series (Tao et al., 2022). It removes noise in the data and



allows a better performance in AI models. Several hydrogeological studies have combined these techniques and demonstrated the ability to approximate variations in groundwater levels from different data sources (Barzegar et al., 2017; Ebrahimi and Rajaei, 2017; Khalil et al., 2015; Moosavi et al., 2014, 2013; Yosefvand and Shabanlou, 2020; Zare and Koch, 2018). Here, GRACE-based TWS was decomposed using two techniques: the wavelet transform and the seasonal decomposition.

Wavelet transform (WT) is a mathematical tool to decompose functions hierarchically, and can be considered as a technique for transforming a signal, sampled in the time domain, into a frequency-scaled domain, defining different components of the signal frequency spectrum (Stollnitz et al., 1995). WT consists of approximating a function by a linear combination of basic functions (also called wavelets), obtaining a representation of the original function. The application of wavelets does not necessarily require the stationarity of the time series as a prerequisite, being appropriate for the analysis of irregularly distributed and extreme events (Torrence and Compo, 1998). For non-continuous functions, the use of the discrete wavelet decomposition (DWT) is recommended (Daubechies, 1992), as in the case of this study.

To apply the wavelet transform, the highest possible decomposition level of the TWS signal was tested, resulting in five levels. The wavelet family chosen for the decomposition was db3 (Daubechies, 1992). The signal extension model was observed, seeking the best possible application of DWT. The data normalization mode adopted for the WT was the *antireflect*, signal is extended by reflecting anti-symmetrically about the edge sample (PyWavelets, 2022). After decomposing the TWS with DWT, the results are a sequence compressed in one of the dimensions. As the TWS is being treated in three dimensions (i.e., latitude, longitude and time), and decomposed into the time dimension, the transform results reduce the time dimension. The time scale reduction occurs because DWT employs a grid where the mother wavelet is scaled by power two, expressing the results of each decomposition level as half of the previous level (Rhif et al., 2019). As the TWS input data has 194 data points per time series, DWT returns the approximation values A5 (194 values) and details, namely D1 (96 values), D2 (48 values), D3 (24 values), D4 (12 values) and D5 (6 values). To return the time dimension to the original scale of the decomposition, an interpolation model in *Spline* was applied. This method adapts a smooth variation of values for locations without data. This procedure requires the application of a mathematical function that minimizes the curvature of the surface,

obtaining a result where the response is smooth and the surface passes exactly through the given entry points (Marcuzzo et al., 2012).

TWS time series has also passed through the seasonal decomposition method, which returns a moving average around an established window value. The chosen window size was 12 months, seeking to observe the annual variations in the data. The model is additive and suggests that the components are added together as follows (Perktold et al., 2022):

$$TWS_{[t]} = T_{[t]} + S_{[t]} + e_{[t]} \quad (3)$$

The results are represented in three outputs at each time step  $[t]$ , seasonality ( $S$ ), trend ( $T$ ) and residual ( $e$ ).  $T$  is an increasing or decreasing value in the series,  $S$  is the short-term repetitive cycle in the series, and  $e$  is the random variation of the series.

Hydrogeological characteristics of aquifers obtained from the Hydrogeological Map of Brazil (Diniz et al., 2014) were inserted into the model. The characteristics observed in each well were as follows: geological group, lithological description of the group, the type of aquifer, the degree of fracturing and the productivity of the aquifer. These non-numerical data were converted into zero and one values (0, 1) by the *one-hot* function (Scikit-learn, 2021) to be better used in the model.

### 3.1 - Ensemble model

The ensemble model is composed of four different AI models, three of which use the Decision Tree (DT technique); the Extreme Gradient Boost (XGB; Chen and Guestrin, 2016), the Light Gradient Boosting Model (LGBM; Ke et al., 2017) and the CatBoost (CtB; Prokhorenkova et al., 2017), followed by an Artificial Neural Network, Multilayer Perceptron (MLP; Manaswi, 2018). Figure 2 shows the data processing flow and the architecture of the ensemble model. The input data in the model are the TWS, decompositions (wavelet and seasonal), the hydrogeological characteristics depicted by the hydrogeological map and the position of the well in space (latitude and longitude). The extreme values are removed from the input dataset by quantile threshold evaluation, respecting the criteria of being greater than 99% and less than 1% of the  $GWS_{OBS}$ . Finally, the data are normalized. It should be noted that the  $GWS_{OBS}$  values are not normalized. After the initial processes, the data are inserted into the DT models for the first approximations of the  $GWS_{OBS}$  values from the input data. The results obtained after

processing in the DT models are then inserted into the MLP that finalizes the approximations of the  $GWS_{OBS}$  observed in the wells. The ensemble model application uses the AI premise that weak models joined together can build a stronger model (Géron, 2019).

The architecture of the AI models used was:

XGB: estimators 3000; learning rate 0.001; sampling set 1; maximum depth 7; *XGBRegressor – gbtree*; early stop 150 steps.

LGBM: regression *boosting\_type gbdt*; 11 and 12 metrics; learning rate of 0.001; layer fraction of 0.9; *bagging\_fraction* 0.7; *bagging\_freq* 20; maximum depth 8; number of sheets 128; *max\_bin* 512; number of interactions 3000; early stop 150 steps.

CtB: number of iterations 3000, learning rate 0.01, depth 7, RMSE rating metric, *bagging\_temperature* 0.01, *od\_type*: Iter and *od\_wait*: 20.

MLP: *Selu* activation functions in the input layer with 128 neurons and *Swish*; in the others, with 256/256/128 neurons; 10000 epochs; between the hidden layers the functions *Dropout* (0.2) and *GaussianNoise* (0.5); *LazyAdam* optimizer; with a reduction in the learning rate over time; 150 steps early stop.

For MLP, the *Swish* activation function (Ramachandran et al., 2017) was used because it presents great empirical performance. The *Selu* function or Scaled Exponential Linear Unit (Klambauer et al., 2017) was selected for inducing properties of self-normalization in the data; this function allows training deep networks with many layers, employing strong regularization schemes and making the learning highly robust. Finally, the optimizer chosen was *LazyAdam*, which is a stochastic gradient descent method. This optimizer is adapted from the *Adam* method (Kingma and Ba, 2015), which in turn combines the advantages of two methods, *AdaGrad* (Duchi and Singer, 2011) and *RMSProp* (Hinton et al., 2012). *AdaGrad* works well with sparse gradients, and *RMSProp* shows good results for non-stationary configurations.

The data entered in the models are divided into two sets. The first with 80% of the data for training/testing the model and the second with 20% of the data for blind testing the model, noting that the second batch was selected from the initial data set at random. In the first batch of data, for separating training from testing, 80% of the data is for training and 20% for testing the models during processing. After training and testing with

the first batch, the model is retested with the blind test wells. This procedure was performed to observe the real capacity of the model to adapt to different data sets.

The hyperparameters of the models had their initial adjustment by the Hyperactive algorithm (Blanke, 2021). However the final adjustment was done manually. We chose to use cross-validation (*K-Fold*) with ten ( $k=10$ ) non-random subsets. Cross-validation is used to measure the accuracy of a model. The method consists of dividing the dataset into  $k$  mutually exclusive subsets of the same size and, from there, one subset is used for testing and the remaining  $k-1$  are used for error estimation (Sklearn, 2022).

### 3.2 Evaluation of the ensemble model

The RIMAS network monitors the largest porous aquifers in Brazil, as illustrated in Figure 1. To assess the ability of the model proposed in this work to approximate the values of  $GWS_{OBS}$  observed *in situ*, the error analysis statistical metrics described in this section were used. However, in seeking a realistic comparison for the study areas with results obtained from a robust and widely tested model, the GWS results obtained from the CLSM model with GRACE-DA ( $GWS_{CLSM}$ ), were used as baseline. For a comparison of the results obtained by the proposed ensemble model with  $GWS_{CLSM}$  and *in situ* data, four experiments were carried out, all using the same model described in the previous section. The experiments were designed to observe the model's ability to adjust to different datasets, training and test batch sizes, and different hydrological and hydrogeological conditions.

Experiment E1 – RIMAS and GRACE data used in Li et al. (2019), plus data obtained from the HMB. For this experiment, 60 wells with 4504 monthly *in situ* measurements were used.

Experiment E2 – In this experiment, all wells contained in the RIMAS database with more than 24 months of measurements were analyzed, as well as GRACE-based TWS and HMB data referring to the wells. In this experiment, 373 wells were used, resulting in 16,487 monthly *in situ* measurements.

Experiment E3 - RIMAS and GRACE data used in the work by Li et al. (2019), plus the data obtained from the MHB and separating the wells by monitored aquifer. Eight aquifers were selected, as follows: Alter do Chão, Parecis, Urucuia, Bauru-Caiuá, Guarani, Cabeças, Poti and Serra Grande. The Cabeças, Poti and Serra Grande aquifers were included in the same model as Poti and Serra Grande present similar effective

porosity ( $S_y$ ) and close spatial distribution, renamed Cabeças/Serra Grande. Experiment 3 was not performed in the Içá, Missão Velha, and Mauruti aquifers, as there are only two wells in this aquifer in the dataset used by Li et al. (2019), which made it not possible to execute the model.

Experiment E4 - In this experiment, all wells contained in the RIMAS database with more than 24 months of measurements were analyzed, in addition to the GRACE and HMB data referring to the wells. Data were separated by monitored aquifer. Eleven aquifers were selected, as follows: Alter do Chão, Parecis, Urucuia, Bauru-Caiuá, Guarani, Cabeças, Poti, Serra Grande, Içá, Missão Velha and Mauruti. As in experiment E3, the Cabeças, Poti and Serra Grande aquifers were included in the same model as Poti and Serra Grande present similar effective porosity and close spatial distribution. The same procedure was performed for the Missão Velha and Mauruti aquifers, included in the same model, as they have a very close spatial distribution, wells in the same GRACE pixel, renamed as Araripe.

In experiments E3 and E4, not all monitored aquifers were addressed, as the number of wells used in the work by Li et al. (2019) is very small or non-existent in several of them. However, aquifers were selected in all regions of Brazil. It is important to emphasize that the input data in the model is related to the RIMAS data in spatial (*pixel*) and temporal scales, since each input data in the model has as reference the location of a well on a given date.

Cross-validation (*K-Fold*) was applied only in E1 and E2, due to the limited amount of data for training in E3 and E4.

As statistical metrics adopted for error evaluation across all experiments, the mean absolute error (MAE) (Equation 4), the root mean square error (RMSE) (Equation 5) and the Nash-Sutcliffe Efficiency (NSE) (Equation 6), were selected. For MAE and RMSE, the ideal values are zero. For the NSE, values closer to one indicate a better adjusted model.

$$MAE = \sum_{i=1}^n |x_i - y_i| \quad (4)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (x_i - y_i)^2}{n}} \quad (5)$$

$$NSE = 1 - \frac{\sum_{i=1}^n (x_i - y_i)^2}{\sum_{i=1}^n (x_i - \bar{y})^2} \quad (6)$$

where  $x_i$  stands for the *in situ* measurements,  $y_i$  the estimated values by the model,  $\bar{y}$  the average of the model estimates, and  $n$  is the number of observations.

## 4 - Results and Discussion

### 4.1 Experiments E1 and E2

In experiments E1 and E2, the small errors were concentrated in the central and northeastern region of Brazil (Figure 3a, 3b), areas with a greater number of wells, while the largest errors were concentrated in the northern portion of the country, where there are fewer RIMAS wells inserted into the models. In general, the model built for experiments E1 and E2 presented  $MAE < 2$  cm and  $RMSE < 3$  cm (Figure 3a, 3b).

An interesting aspect that draws special attention in examining such results is the ability of the model to simulate the values of  $GWS_{OBS}$  in wells inserted in an environment of crystalline rocks, presented in the results of E2 (Figure 3b), southeastern region of Brazil. Despite the great variability of the GRACE signal in both experiments E1 and E2, which used data from all regions of Brazil, the average results show the great approximation of the simulated values  $GWS_{SIM}$  and  $GWS_{OBS}$  (Figures 3c to 3f), demonstrating the low variance of the presented results achieved by the constructed model. NSE values for E1 and E2 were 0.80 and 0.65, respectively (Figures 3a, 3b), indicating a good fit of the models to the datasets. However, those results make clear that not all the dependent variables were explained with precision. On the other hand, the low RMSE and MAE values show that the prediction errors presented for large areas are much lower than those derived from  $GWS_{CLSM}$  (see Table 2).

The cross-validation result (*K-Fold*) shows values very close to the complete model. For E1,  $NSE = 0.78$ ,  $RMSE = 2.01$  and  $MAE = 1.30$ . For E2, results are  $NSE = 0.64$ ,  $RMSE = 2.67$  and  $MAE = 1.68$ . Artificial intelligence models tend to perform better with larger batches of training and testing (Lecun et al., 2015). Due to the large

concentration of data in the central and northeast regions of Brazil, the model may have presented a biased result (Figure 3a, 3b), that is, with a tendency to present better results in areas with greater amount of data. In addition, there is a greater variability of GRACE signals in the north of the country.

As for the variability of the GRACE signal, it is expected that groundwater will present a different participation in each region of Brazil and in each aquifer studied. Signal variability is related to the hydrological processes of each region, as well as types, cover and land use. The northern region of Brazil has large bodies of surface water such as the Tocantins, Solimões, Negro and Amazon rivers, in addition to extensive floodable areas in the Amazon region, indicating a large contribution of surface water to the region's TWS signal (Getirana et al. 2017; Melo and Getirana 2019). Unlike the northern region and the swamps of the Brazilian Pantanal, the other regions of the country have a smaller amount of large surface water bodies. Even with the water filled up reservoirs built for the hydroelectric plants in these regions, a smaller component of surface water in the TWS signal is expected. Complementarily, these areas other than the northern regions have a higher groundwater extraction rate compared to the northern region of Brazil (IBGE, 2020). These factors may help to explain greater errors in the northern region of Brazil.

#### 4.2 Experiments E3 and E4

Experiment E4 denotes that the highest values for RMSE are in Alter do Chão (Figure 4b), Parecis (Figure 4h) and Guaraní (Figure 4f) aquifers. Although featuring RMSE values of 3.11 cm and MAE of 2.36 cm, Alter do Chão aquifer has an NSE value of 0.89. This result may occur due to the proximity of the wells to the Amazon River, which would affect the static water level fluctuations according to the water level variation of the river. In addition, many of these wells are inserted in an urban context, where land use and land cover jointly with underground water exploitation water can interfere in the results achieved by the models.

In the case of the Parecis aquifer, RMSE, MAE and NSE are 2.4cm, 1.36cm and 0.90, respectively. Uncertainties might be related once more to groundwater pumping, as the region has witnessed an increasing agricultural expansion in the past several years (IBGE, 2020).

For the Guarani aquifer, the variability of the GRACE signal associated with extraction processes might have hindered the best convergence of the models. The aquifer extends over thousands of kilometers and has experienced increasing groundwater pumping in its recharge areas for many years, as described by Takahashi (2012).

Areas with a higher concentration of monitoring wells return lower error values for each aquifer. Such a relationship is more visible in the results for the Cabeças/Serra Grande aquifers (Figure 4c) and Urucuia (Figure 4e). Errors of the test wells present lower values in these areas. Içá and Alter do Chão aquifers do not have as much data for training, resulting in model errors. However, results of all the aquifer models still return  $GWS_{SIM}$  values better than  $GWS_{CLSM}$ .

As noted by Brookfield et al. (2018), linear correlation analyses do not have the ability to extract from the TWS data relationships of water level variations of *in situ* measurements in areas with large vadose zones, areas that present greater depth of the static level. Different from the non-linear model presented in-here. This is highlighted in the responses of the ensemble model proposed and used in this work, mainly for the Urucuia aquifer (Figure 4e), an area of significant groundwater extraction and deep static water levels. Our model also has the ability to provide accurate estimates over areas with low thickness of the vadose zone and with great influence of surface waters, as observed in the wells present in the Içá (Figure 4a) and Alter do Chão (Figure 4b) aquifers.

The difference in scale between satellite data and *in situ* measurement data is addressed in many works, which may use statistical, dynamic methods (Gaur and Simonovic, 2019; Sehgal et al., 2021; Yin et al., 2018) and more recently artificial intelligence (Ali et al., 2021; Liu et al., 2020; Miro and Famiglietti, 2018). This issue was well solved by our model, as demonstrated in the results. Results are above expectations in the Araripe aquifer (Figure 4d), with RMSE, MAE and NSE of 0.24cm, 0.88cm and 0.88, respectively. This shows that aquifers inserted in a small area and wells in the same GRACE pixel were not a problem for the approximations made by the model.

Experiment E4 (Figure 5) indicate that, when the input data is concentrated in the same aquifer (e.g., Guarani, Urucuia and Bauru aquifers), estimated groundwater storage change less, which is expected due to the lower variability of the TWS signal, as well as constant geological characteristics of the aquifer under study. However, there were small gains, which can be explained by the amount of training data for the models.



Figure 5 shows the average observed and simulated (CLSM and our approach) GWS in the Guarani, Bauru-Caiuá and Urucuia aquifers. For the Guarani aquifer, experiment E4 shows that the model can predict with good accuracy the average behavior of the wells. It is worth noting that the test wells show a better result than  $GWS_{CLSM}$  (Figure 5). However, these wells depict a deviation from the expected response obtained for the wells included in the blind group for testing, which could indicate that the number of values for training the series might have directly interfered in the result. In the Bauru-Caiuá aquifer, the model presents results very close to RIMAS measurements (Figure 5).

The model's response could be associated with the spatial distribution of the RIMAS monitoring wells within the aquifer (Figure 4g), which covers almost the entire aquifer with a relatively constant spacing between the wells. In this aquifer, it is possible to notice that the model can approximate with great precision the RIMAS values for E4.

For experiment E3, the response is superior to that derived from  $GWS_{CLSM}$ , even with a high RMSE. This may have occurred because the wells included in this experiment are concentrated in an area of intense underground water extraction.

For the Urucuia aquifer, the behavior of adherence between AI model and measurements is superior to that of Bauru-Caiuá, however the great variability of the GRACE-based TWS estimates at each studied point, associated with different responses in each monitoring well to the groundwater extraction processes in the region, might contribute to a small departure of the predicted data with respect to the data measured by RIMAS in the blind test, even though this area presented the best results in the study (Figure 5). The small variation of the GWS observed and the one estimated by the model could indicate a constant loss of water along the column in the aquifer, as reported by the work of Gonçalves et al. (2020).

## **5 – Conclusions and recommendations**

Here, we demonstrate the viability of satellite-based monitoring of Brazilian aquifers. A novel artificial intelligence model was conceived and built by employing GRACE-based TWS data and its decomposition using wavelet and seasonal techniques, jointly with point-based *in situ* hydrogeological data. As a benchmark for our results, we used GLDAS outputs, specifically, groundwater simulations derived from the CLSM model with GRACE data assimilation ( $GWS_{CLSM}$ ). Results of the proposed methodology

over all selected aquifers showed accurate groundwater estimates, overperforming GLDAS estimates.

The TWS signal decomposition process proved to be very useful for the model, which adequately approximates the variations in groundwater storage in the different experiments. The proposed methodology can be applied in areas with a short history of groundwater monitoring and discontinuous time series, since aquifers such as Parecis, Iça and Cabeças/Serra Grande have less than ten years of static water level measurements and all wells in the RIMAS have gaps in their time series.

It is important to emphasize that the proposed models are representing the sample space inserted in the dataset. The big difference between the scales of the GRACE data with a resolution of  $0.25^\circ$  and *in situ* RIMAS measurements collected at an approximate point scale, were overcome by the models. Furthermore, more than one well per pixel was also not a problem, demonstrated by the results for the aquifers Iça, Parecis, Araripe and Urucuia. It is expected that the proposed model can be applied in areas with physical and geological characteristics similar to the training region, since the response of GRACE-based TWS signals tend to be similar. This feature can help to spatialize the storage of groundwater to unmonitored areas, being very useful for large aquifers.

As a model constraint, aquifers without a history of groundwater monitoring are difficult to approximate. Regions with great variation in physical characteristics, such as soil type, geology, land use and occupation, precipitation rates or groundwater extraction, can create situations in which the proposed model does not respond as expected. Another limitation of the model is the spatial resolution for unmonitored areas, which initially depends on the resolution of the GRACE data. In experiment E2, some wells are inserted in an environment of crystalline rocks. Despite the good results, the model has not yet been properly adjusted for this geological environment, as well as for karstic aquifers, being the subject of future investigation.

Groundwater monitoring using satellite data and artificial intelligence can be a solution to spatialize groundwater storage values with good accuracy. Additionally, it is possible to make predictions for storage in different scenarios and with low computational costs, modifying only TWS values. This approach can also help in understanding aquifer dynamics, since, after the initial adjustments, the model can evaluate the past groundwater behavior using the GRACE data that started in 2002.

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810 **Tables and Figures**

811 **Table 1** – Effective porosity in Brazilian aquifers.

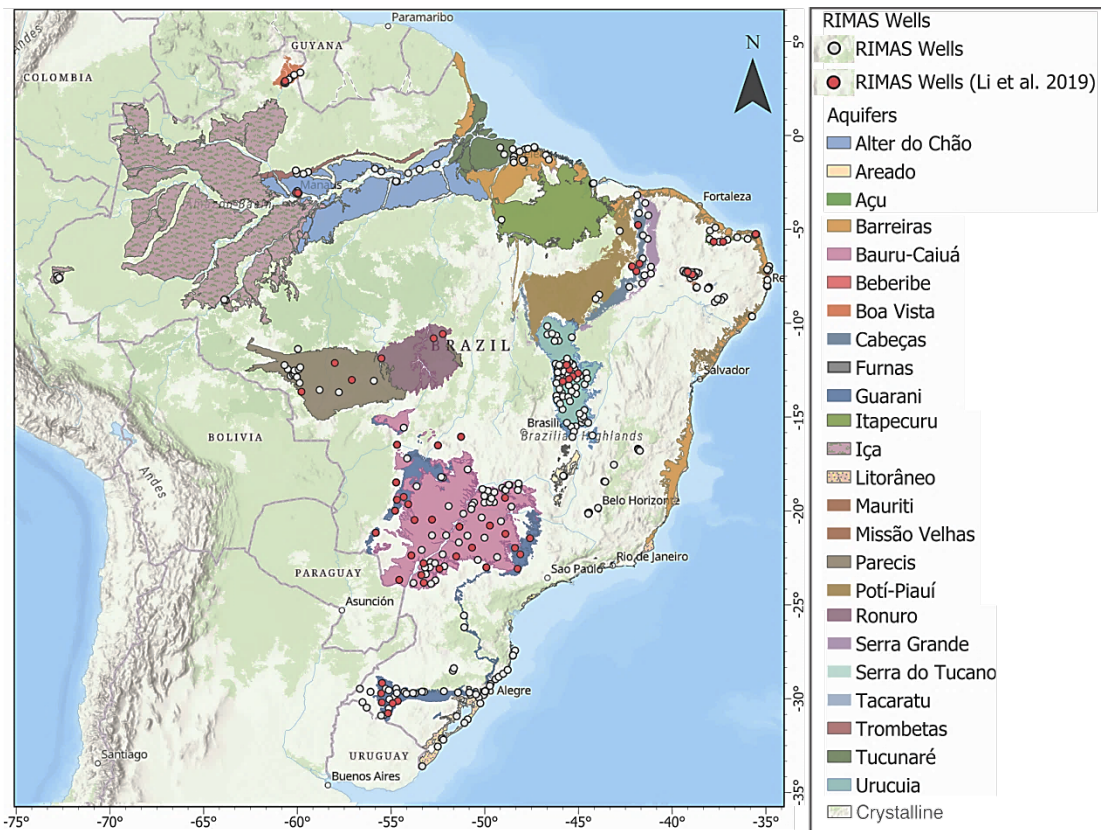
<b>Aquifer</b>	<b>Effective porosity (<math>S_y</math>)</b>	<b>Reference</b>
<b>Açu</b>	0.10	(Diniz et al., 2012)
<b>Alter do Chão</b>	0.18	(Aguiar & Mourão, 2012)
<b>Areado</b>	0.05	Estimated
<b>Barreiras (Pirabas e Grajau)</b>	0.10	(Silva et al., 2008)
<b>Caiuá</b>	0.17	(Franzini, 2012)
<b>Beberibe</b>	0.10	(Silva et al., 2008)
<b>Boa Vista</b>	0.18	Estimated
<b>Cabeças</b>	0.03	(Correia Filho et al., 2010)
<b>Cenozoic Covers Aquifer</b>	0.10	Estimated
<b>Furnas</b>	0.13	(Peixoto et al., 2012a)
<b>Guarani</b>	0.18	(Takahashi, 2012)
<b>Iça</b>	0.10	(Galvão et al., 2012)
<b>Itapicurú</b>	0.13	(Santos, 2005)
<b>Coastal</b>	0.14	Estimated
<b>Missão/Velha-Mauriti</b>	0.10	(Souza and Castro, 2013)
<b>Parecis</b>	0.15	(Silva, 2013)
<b>Poti Piauí</b>	0.15	(Correia Filho et al., 2010)
<b>Prosperança</b>	0.15	(Peixoto et al., 2012b)
<b>Ronuro</b>	0.12	(Peixoto et al., 2012b)
<b>Salto das Nuvens</b>	0.13	(Peixoto et al., 2012b)
<b>Serra do Tucano</b>	0.17	Estimated
<b>Serra Grande</b>	0.03	(Aguiar, 2017)
<b>Tacaratu</b>	0.03	(Diniz et al., 2012)
<b>Trombetas</b>	0.15	Estimated
<b>Tucunare</b>	0.10	Estimated
<b>Urucuia</b>	0.13	(Gaspar and Campos, 2007)

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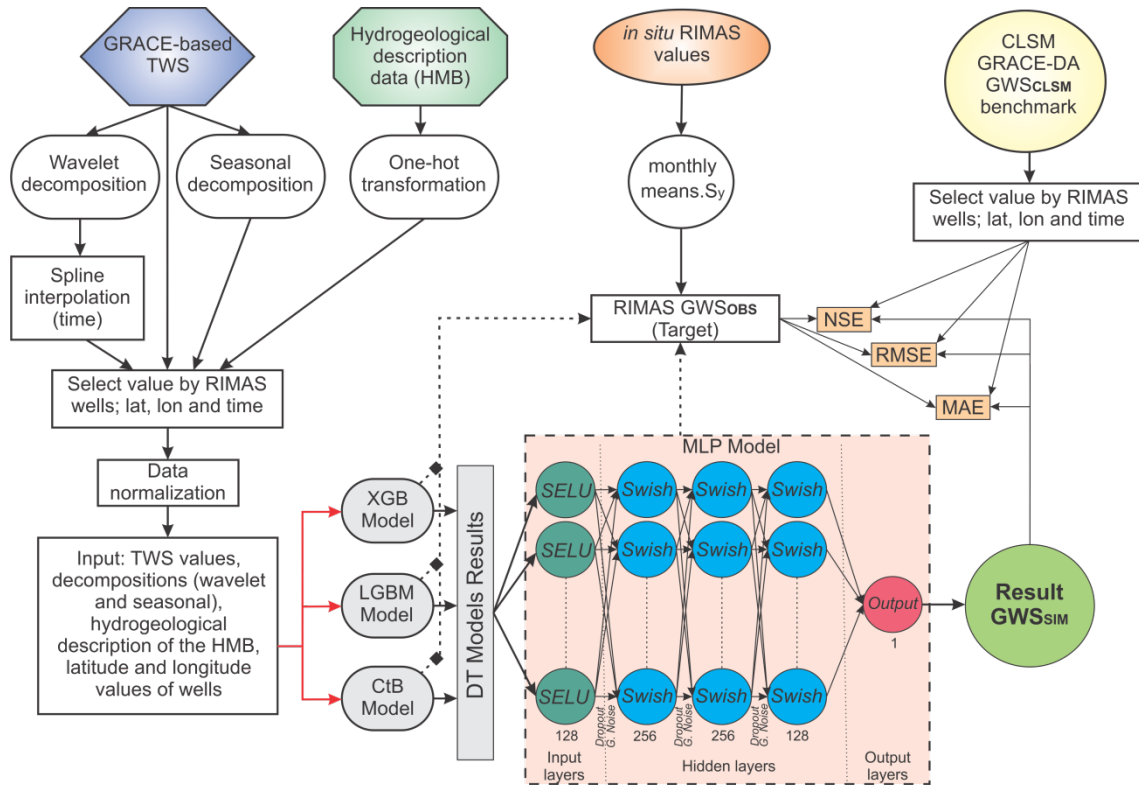
813 **Table 2** - Results of the E3 and E4 experiments for Brazilian aquifers.

Aquifer	Wells	Correlation RIMAS x GRACE	RMSE (cm) GWS <sub>SSIM</sub>	MAE(cm) GWS <sub>SSIM</sub>	NSE GWS <sub>SSIM</sub>	RMSE (cm) GWS <sub>CLSM</sub>	MAE(cm) GWS <sub>CLSM</sub>		
Guarani	Exp. 3	Train	-0.305	1.651	1.430	0.63	3.629	2.802	
		Test	-0.529	1.492	1.044	-	-	-	
	Exp. 4	Train	-0.312	2.351	1.535	0.63	5.958	4.562	
		Test	-0.134	3.168	2.309	-	-	-	
Bauru-Caiuá	Exp. 3	Train	-0.394	1.520	0.894	0.84	6.662	5.492	
		Test	-0.367	2.502	1.660	-	-	-	
	Exp. 4	Train	-0.408	1.911	1.120	0.85	6.854	5.375	
		Test	-0.411	1.100	1.934	-	-	-	
Parecis	Exp. 3	Train	-0.569	1.733	1.207	0.84	9.680	8.224	
		Test	-0.59	3.104	2.493	-	-	-	
	Exp. 4	Train	-0.445	2.412	1.361	0.90	9.118	6.984	
		Test	-0.417	2.979	2.368	-	-	-	
Urucuia	Exp. 3	Train	-0.153	0.705	0.37	0.88	2.812	2.124	
		Test	-0.411	1.593	0.95	-	-	-	
	Exp. 4	Train	-0.178	0.645	0.361	0.74	3.247	2.440	
		Test	-0.108	1.431	1.015	-	-	-	
Cabeças	Exp. 3	Train	-0.229	0.216	0.123	0.92	5.541	4.427	
		Test	-0.465	0.88	0.597	-	-	-	
	Exp.4	Train	-0.049	0.412	0.34	0.73	5.543	4.271	
		Test	-0.297	0.668	0.47	-	-	-	
Alter do Chão	Exp. 4	Train	-0.028	3.114	2.364	0.89	9.749	7.601	
		Test	0.187	7.265	5.940	-	-	-	
	Araripe	Exp. 4	Train	-0.205	0.240	0.880	0.88	2.161	1.519
			Test	-0.302	2.127	1.714	-	-	-
Iça	Exp. 4	Train	-0.043	1.112	0.685	0.91	4.237	3.131	
		Test	-0.01	4.936	3.733	-	-	-	

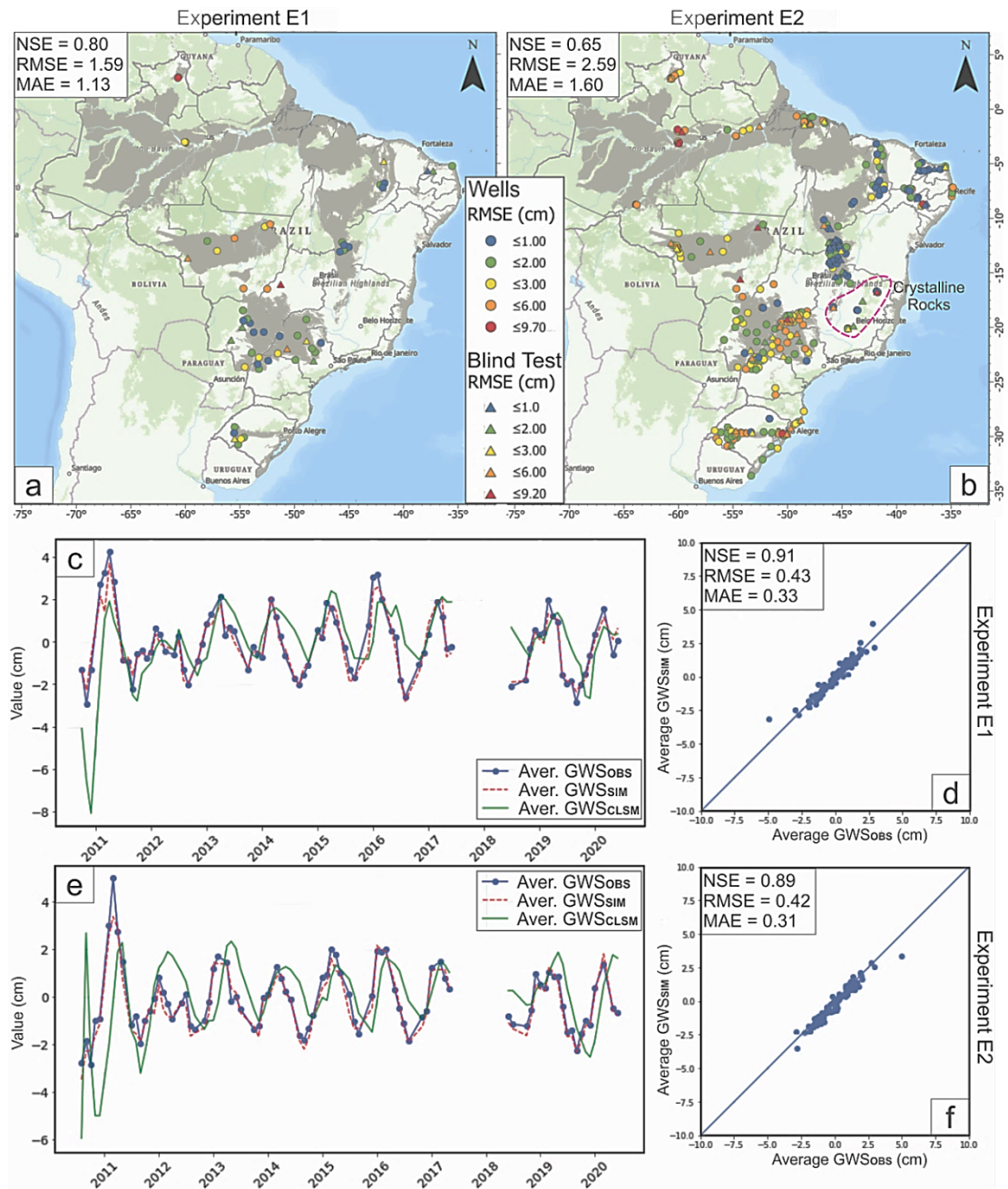
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**Figure 1** - Geographical location of Brazilian aquifers and spatial distribution of the RIMAS groundwater monitoring network. RIMAS wells colored in red are those used in Li et al. (2019).

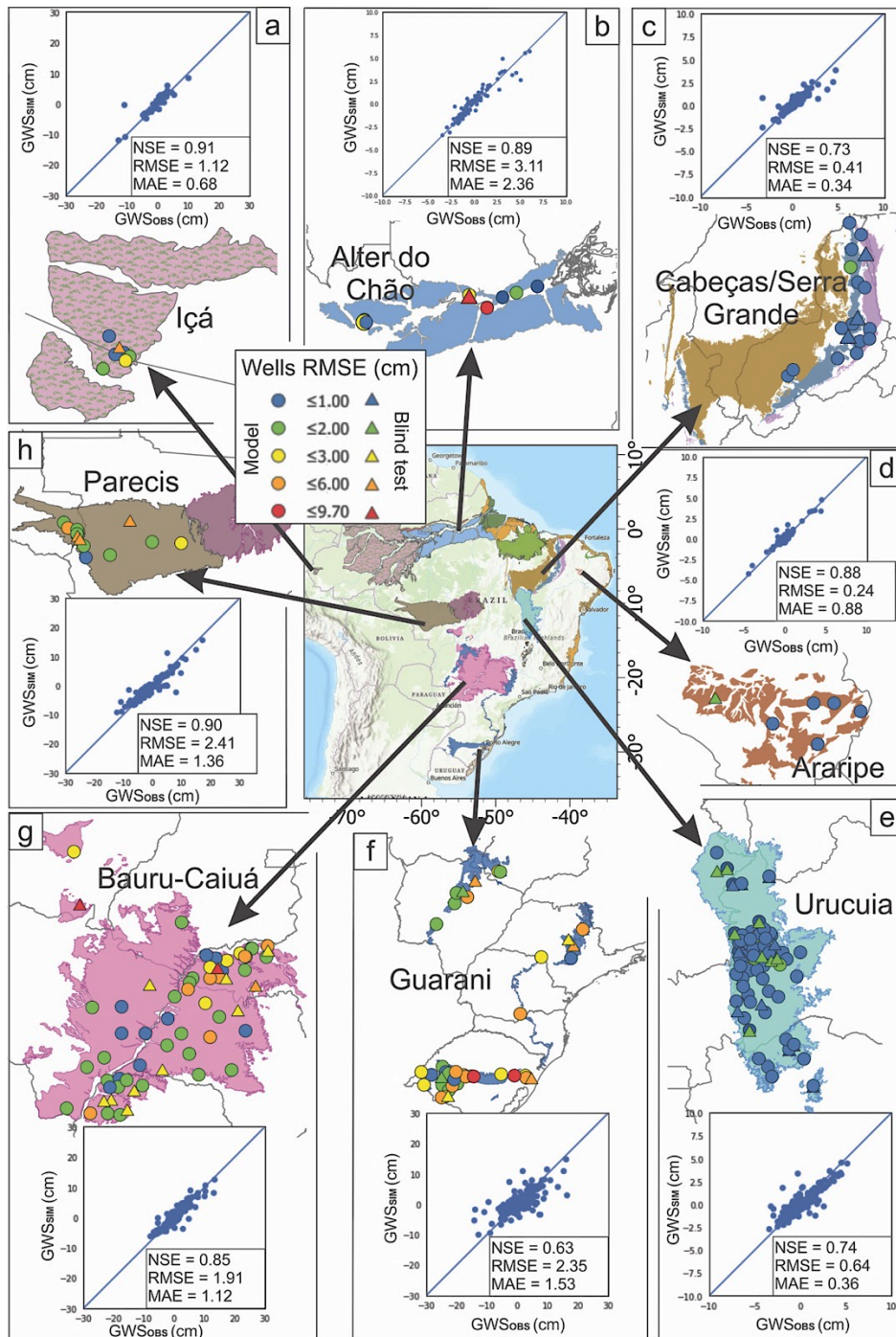


**Figure 2** - Processing flow diagram and ensemble model architecture. It should be emphasized that both the DT models and the MLP model target the  $GWS_{OBS}$ , values observed in the RIMAS wells.



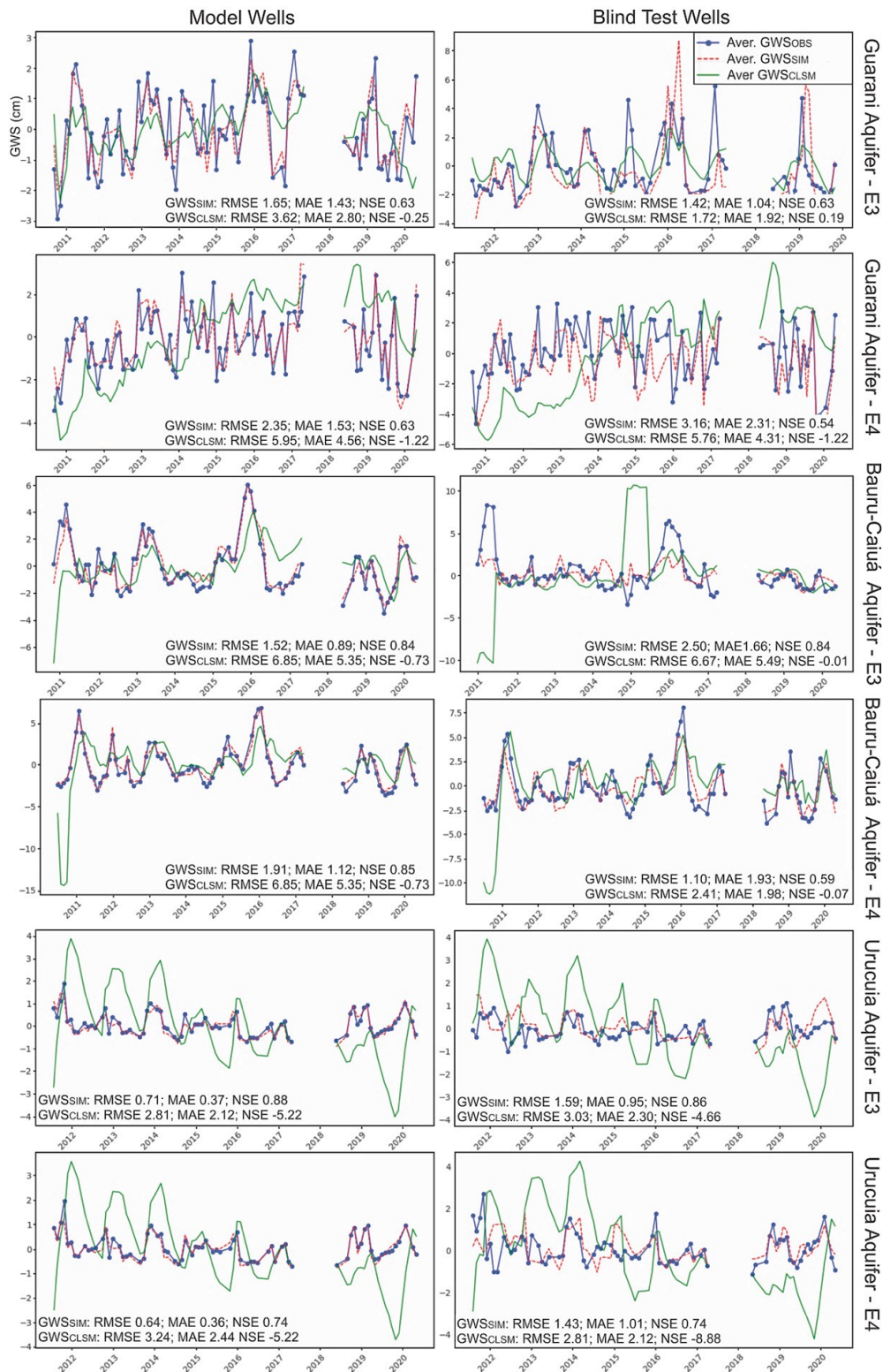
**Figure 3** – Experimental results for E1 and E2: (a) RMSE (cm) mapping of the forecast model set for the wells used in Li et al. (2019) and statistical metrics of the model for the data set used; (b) RMSE (cm) mapping of all RIMAS wells in Brazil and model metrics for the dataset used, highlighted area of crystalline rocks; (c), (e) graphs of the average results GWS, E1 and E2, for the observed values ( $GWS_{OBS}$ ), simulated ( $GWS_{SIM}$ ) and obtained from CLSM ( $GWS_{CLSM}$ ); and (d), (f) values of NSE, RMSE and MAE for the means of the results of E1 and E2.





**Figure 4** – Results for experiments E4: RMSE (cm) mapping for Içá, Alter do Chão and Parecis aquifers, featuring wells inserted in an Equatorial climate and with great contribution of surface water in the TWS response (a, b and h); RMSE (cm) mapping for Cabeças, Serra Grande, Poti aquifers (Cabeças/Serra Grande), Missão Velha and Mauriti (Araripe) and Urucuia, a region of great exploitation of groundwater, inserted in a semi-arid climate (c, d and e); RMSE (cm) mapping for Guarani and Bauru-Caiuá aquifers, region of intense exploitation of groundwater and tropical climate (f and g). The scatter plots represent the 20% simulated test values (GWS<sub>sim</sub>) and observed values (GWS<sub>obs</sub>), in each aquifer.





**Figure 5** - Average results of the GWS for the experiments E3 and E4, in the Guarani, Bauru-Caiuá and Urucua aquifers, considering *in situ* values (GWS<sub>OBS</sub>), forecasted values (GWS<sub>SIM</sub>) and CLSM results (GWS<sub>CLSM</sub>). RMSE [cm], MAE [cm] and NSE [-] values for both GWS<sub>SIM</sub> and GWS<sub>CLSM</sub> are also provided.