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Comparative analysis of hydrodynamic flowrate sources as drivers of water quality models for nitrogenous compounds in complex ungauged South African rivers

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ABSTRACT

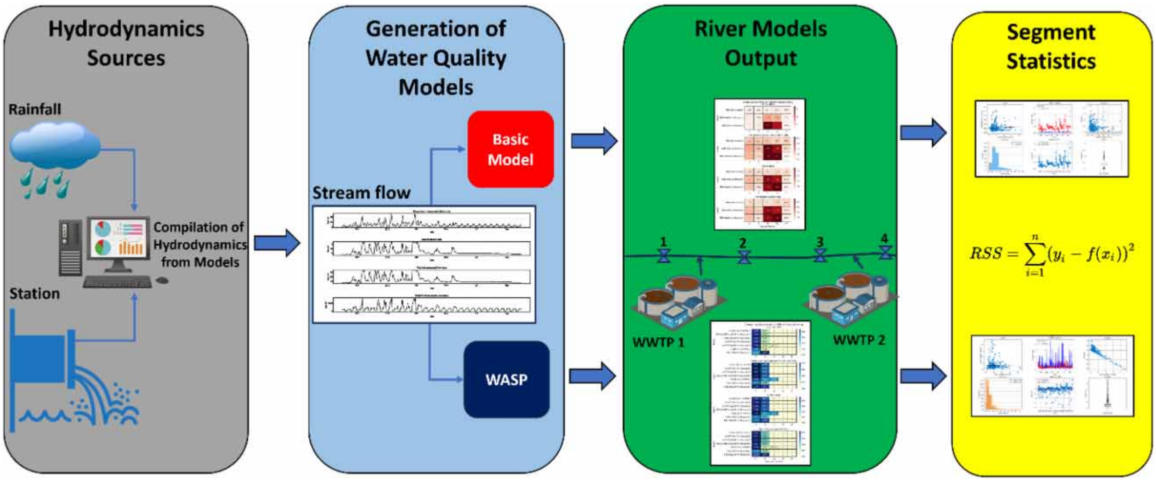
Water quality modelling is a critical tool for managing the health of river ecosystems, particularly in regions impacted by point source pollution activities. This study investigates the influence of different hydrodynamic data sources on the performance of two river water quality models, the Basic Model (BM) and the Water Quality Analysis Simulation Programme (WASP) for modelling nitrogenous compounds in a complex river system including wastewater treatment plant effluent discharges. Four diverse hydrodynamic data input types were considered. These included measured station data, altered station data, rainfall-generated flow, and the WRSM/Pitman model estimate. Findings revealed trends, analysis of variance (ANOVA), and *t*-test analyses consistently demonstrated significant disparities between model predictions and measured data in specific river segments, indicating a need for segment-specific modelling approaches. An increase in Root Mean Square Error (RMSE) and Mean Square Error (MSE) values in certain segments pointed to a decline in model accuracy when confronted with distinct hydrodynamic conditions. Additionally, application of four diverse hydrodynamic data input sources yielded similar performance for BM and WASP against measured data. The research findings indicated a complex interplay between river hydrodynamics and water quality modelling, resulting in a recommendation for tailored modelling strategies that account for unique characteristics of river segments.

Key words: model input data, nitrogenous compounds, river hydrodynamics, water quality modelling

HIGHLIGHTS

- Hydrodynamic data input sources yielded similar performance for the Basic Model and WASP against measured data for nitrogenous compounds.
- Reduced performance of models farther from boundary was detected.
- Altered station hydrology showed comparable impact on WASP and Basic Model.
- Examination of segment-specific model accuracy disparities across varied inputs and models.

GRAPHICAL ABSTRACT



INTRODUCTION

Assessing and predicting water quality are crucial for preserving the ecological health of river systems. The disposal of nitrogenous compounds, which encompass nitrates, nitrites, ammonia, nitrogen oxides, and organic nitrogen compounds, is linked to nutrient enrichment and eutrophication processes in aquatic ecosystems (Chapra 1997). These compounds serve as essential nutrients for plant growth, but excessive inputs can lead to nutrient overload, promoting algal blooms and subsequent oxygen depletion in water bodies – a phenomenon known as eutrophication (Harding 2015). Water quality models, in conjunction with extensive monitoring networks, have been essential tools for simulating and understating water quality dynamics in various scenarios (Sharma & Kansal 2013; Wang *et al.* 2013; Darji *et al.* 2022).

The success of water quality modelling largely depends on the availability of accurate and comprehensive hydrodynamic data, which forms the basis for simulating the transport and dispersion of pollutants within river systems (Radwan *et al.* 2005; Milledge *et al.* 2012; Kim *et al.* 2021). However, obtaining reliable hydrodynamic data is challenging in practice, leading to a significant decrease in data collection efforts across South African river systems (Horn *et al.* 2018). This lack of empirical data has led to the use of hydrodynamic models (Havenga *et al.* 2007) as a practical alternative; compensating for the data scarcity and accelerating the modelling process. For example, models like the Water Quality Analysis Simulation Programme (WASP) (Wool *et al.* 2020) rely on sets of limited hydrodynamics data for integration to simulate complex river systems. The crucial importance of rigorously testing model input data is underscored by the fact that the performance of water quality models hinges on both the accuracy of external inputs and the intricate dynamics within a water body. In the realm of modelling, particularly in expansive environments, errors in water quality predictions frequently stem from the limitations of available field data (Kim *et al.* 2021).

Despite these advancements, inconsistencies in the availability of hydrodynamic data remain a concern across South Africa's extensive river networks (Deventer *et al.* 2018). To address this, researchers have turned to surrogate data sources, such as rainfall models and proxy basin hydrodynamics gauge station data (Donmez *et al.* 2021) to supplement the lack of comprehensive data and leading to a variety of modelling approaches. However, this diversity in modelling strategies introduces discrepancies in simulation results, further complicating the field of water quality modelling (Hughes 2013; Daggupati *et al.* 2015).

The focus of this study is, specifically, on simulating nitrogenous compounds in South African river systems given the critical role these play in aquatic ecosystems and their potential impact on environmental and human health (Harding 2015; Rezagama *et al.* 2017). In this regard, a comparative investigation assessing the performance of two distinct water quality models, viz. the sophisticated WASP (Wool *et al.* 2020) and a Basic Model (BM) consisting of a series of Continuously Stirred Reactors (CSTRs) (Mahlathi *et al.* 2022), was conducted.

Furthermore, this study aims to enhance understanding water quality modelling in data-limited situations. It seeks to provide fundamental knowledge towards standardising the modelling process by addressing inconsistencies arising from using varied hydrodynamic data sources and improve model reliability. The research included a comparative analysis of two water quality models and explored alternative data sources, aiming to provide insights and innovative data usage approaches. Focusing on simulating nitrogenous compounds in South African river systems, the study is intended to improve predictive capabilities of models, refine modelling practices, and contribute to effective water resource management strategies.

METHODS

Data were obtained from the Natal Spruit River (Figure 1), a significant tributary that feeds into the Riet Spruit River, ultimately connecting to the Vaal River located at the Upper Vaal catchment in South Africa. The comparative analysis was centred on two distinct observation zones: the upstream and downstream sections of three wastewater treatment plants effluent discharge locations. Notably, this river system is a poignant example of a nutrient- and waste-affected river within the country, primarily attributed to intensive industrial operations that supports major economic activities for a population of more than 12 million people (du Plessis 2021).

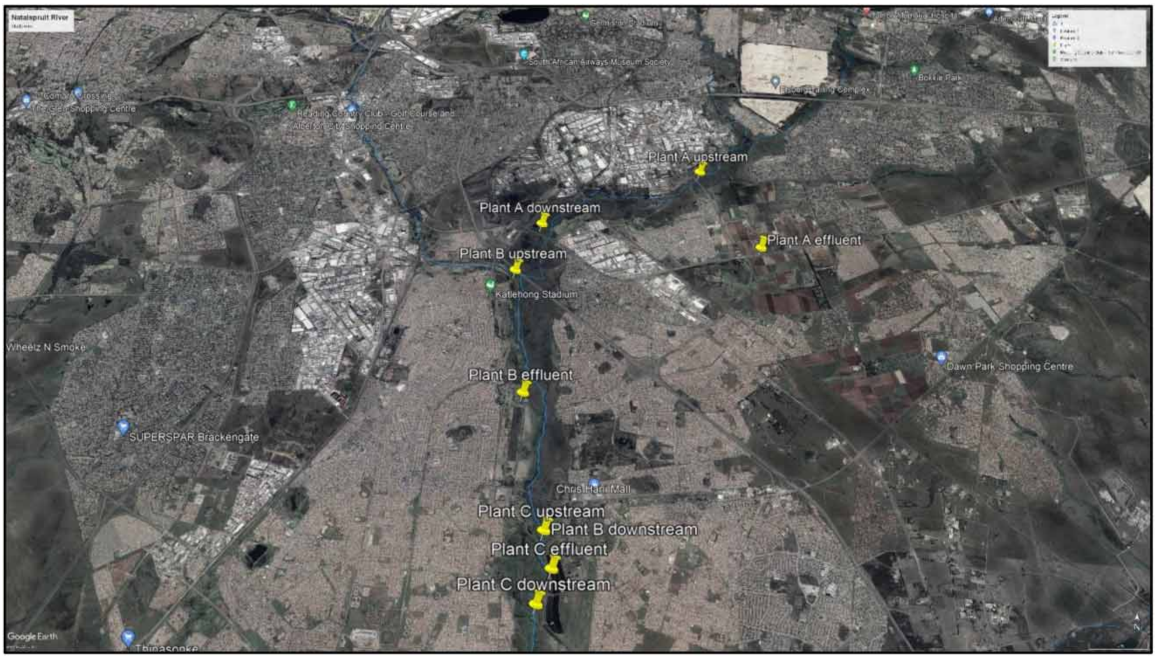


Figure 1 | Study area with multiple study locations upstream and downstream of three WWTPs (Google Earth Pro 7.3.4, Natal Spruit, 26°15′55′′S, 25°11′30′′E, Maxar Technologies, August 2023).

River flowrates

Four distinct hydrodynamics data sources were used for comparison. Each source represents the best closest estimate of hydrodynamic at this ungauged river system with no direct hydrodynamics data:

1. Proxy basin station data: This data category encompasses hydrodynamics data sourced from a dedicated monitoring station situated near the study area. The concept of using proxy basin station data for modelling studies is adapted from Daggupati *et al.* (2015) where proxy basin station data can be used for model calibration and validation strategy. To emphasise the impact of conducting a modelling study under scarce data conditions, these stations provide real-time measurements of flow velocities, water depths, and associated hydraulic parameters, offering direct insights into the river system's hydrodynamic behaviour.
2. Altered station data: This dataset comprises modified measurements obtained from the proxy basin stations hydrodynamics. Utilising a multiplier function, these altered station data points represent the effects of applying a multiplier (double flow) to the station flow data. This approach aids in evaluating the sensitivity of modelling outcomes to different flow scenarios and allows for an assessment of the potential range of variations.

3. Rainfall-generated flow data: In this category, flow data are generated based on observed rainfall patterns. The intricate relationship between precipitation and resulting river flow is harnessed to simulate hydrodynamics. This approach is particularly relevant in regions where reliable hydrodynamics measurements might be limited but where rainfall data are more accessible.
4. WRSM/Pitman model estimates: Simulated River flow data are obtained from the calibrated and validated Water Resources System Model (WRSM/Pitman) (Bailey & Pitman 2016) of the WR12 study conducted in the Upper Vaal covered by this study, which provides predictive insights into hydrodynamics behaviour based on established models. This source offers an opportunity to assess the accuracy and applicability of model-derived hydrodynamics data when compared to direct measurements.

These diverse hydrodynamics data sources provide a comprehensive framework for evaluating the Natal Spruit River dynamics within the Vaal River watershed context. Figure 2 shows the four hydrodynamic input data time series for the selected study period. The hydrodynamic station data were sourced from the National Integrated Water Information System (NIWIS) (Department of Water & Sanitation 2019), a comprehensive database for water monitoring networks in South Africa. Rainfall station data were obtained from the Water Research Commission (WRC) database (Lynch 2004). Additionally, the WRSM Model estimation data were extracted from the WR2012 Water Resource Information System website, which houses model configurations for a multitude of rivers across South Africa.

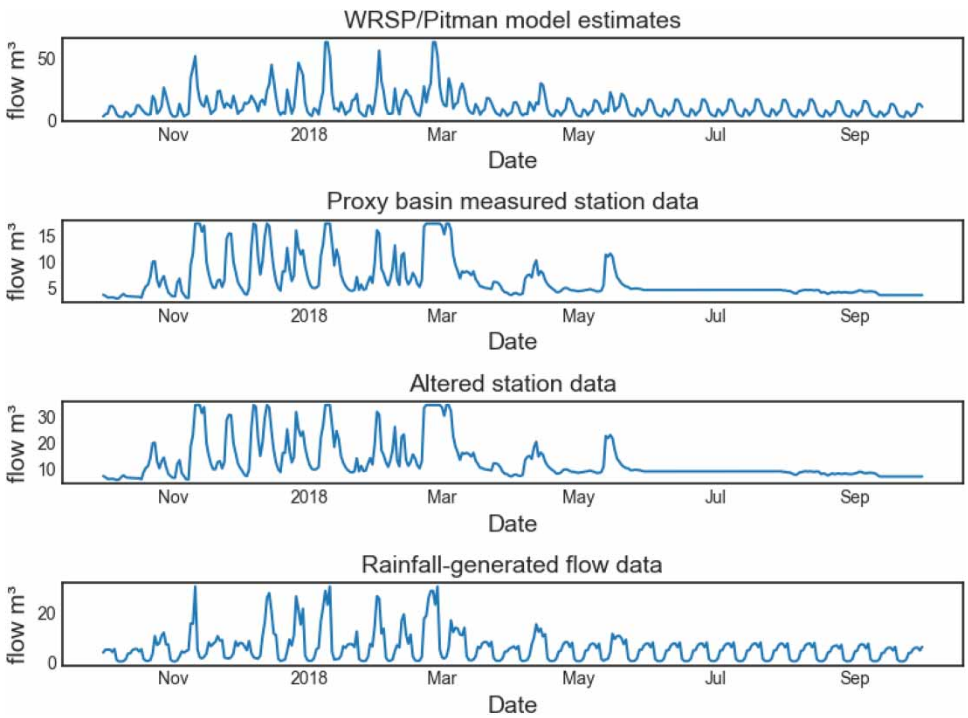


Figure 2 | Flow input data from the WRSM/Pitman model, proxy basin station, altered proxy basin station data, and rainfall data sources.

Including direct measurements and modelled estimates along with the exploration of altered and rainfall-generated data enriches the study's ability to capture the multifaceted hydrodynamics intricacies present in the study area. This source of data is listed as one of the limited sources of hydrodynamic data outlined in the recent work of Mahlathi *et al.* (2024).

Simulation models

Two types of water quality models were applied to simulate water quality. The primary focus on the nitrification process is described in Chapra (1997).

CSTR in a series model

The investigation employed a basic CSTR model to replicate the dynamics of a thoroughly mixed natural water body. The approach involved arranging multiple CSTRs in a series configuration to simulate discrete river sections. This technique, extensively outlined by Chapra (1997) and recently applied by Mahlathi *et al.* (2022), revolves around solving the mass balance equation, represented by Equation (1) below, with a focus on a feed-forward system.

$$V\frac{dc}{dt} = W(t) - kV_c - vA_sc \tag{1}$$

In Equation (1), V denotes the reactor volume, c is parameter concentration in the reactor, $W(t)$ represents the lumped loading, t is time, k is the reaction rate constant, As is the cross-sectional area and v is the flow velocity.

The mass balance equation's reaction term encapsulates the nitrification process within the river system. This process unfolds through two sequential reaction steps. Step 1 (Equation (2)) illustrates the conversion of ammonium ion into nitrite by nitrifying organisms (Chapra 1997).

$$\mathrm{NH_4^+} + 1.5\mathrm{O_2} \rightarrow 2\mathrm{H^+} + \mathrm{H_2O} + \mathrm{NO_2^-} \tag{2}$$

Step 2 (Equation (3)) entails the conversion of nitrite to nitrate:

$$\mathrm{NO_2^-} + 0.5\mathrm{O_2} \rightarrow \mathrm{NO_3^-} \tag{3}$$

The oxygen requirements for both steps are ascertainable through Equation (4) (Chapra 1997):

$$r_{on} = r_{oa} + r_{oi} = 4.57\ \mathrm{gO\ gN^{-1}} \tag{4}$$

where r_{on} is the amount of oxygen consumed per a unit mass of nitrogen in the total nitrification reaction. r_{oa} and r_{oi} is the total oxygen consumed due to nitrification of ammonia and nitrite, respectively. Usually, first-order kinetics are assumed for modelling the nitrification process and the following Equations (5)–(8) as described in Chapra (1997) were included:

$$\frac{dN_o}{dt} = -k_{oa}N_o \tag{5}$$

$$\frac{dN_a}{dt} = k_{oa}N_o - k_{ai}N_a \tag{6}$$

$$\frac{dN_i}{dt} = k_{ai}N_a - k_{in}N_i \tag{7}$$

$$\frac{dN_n}{dt} = k_{in}N_i \tag{8}$$

In Equations (5)–(8), N is the parameter concentration and the subscripts o, a, i and n denote organic, ammonium, nitrite, and nitrate, respectively. The oxygen deficit (D) balance can be computed with Equation (9).

$$\frac{dD}{dt} = r_{oa}k_{ai}N_a + r_{oi}k_{in}N_i - k_aD \tag{9}$$

These differential equations were solved with fourth order Runge-Kutta method and the ammonia concentrations were computed on the selected checkpoints in the river reach.

Water Quality Analysis Simulation Programme

WASP is a versatile modelling tool used to simulate and predict water quality dynamics in various aquatic environments. It integrates hydrodynamics with water quality processes, offering insights into the behaviour of pollutants and nutrients within rivers, lakes, estuaries, and coastal areas. WASP divides the aquatic system into compartments to model complex interactions among water quality constituents, considering processes such as diffusion, advection, decay, and biological interactions. It accommodates biological processes such as nutrient cycling, algal growth, and bacterial activities, which are crucial to understanding aquatic ecosystem health. The programme accounts for point and non-point pollution sources, enables scenario analysis, and assists in model calibration and validation against real-world data.

Modelling approach

The simulation framework was devised to emulate the behaviour of nitrogenous compounds within the river system, encompassing the influences of wastewater treatment plants. This approach involved configuring both the BM and the WASP model to incorporate hydrodynamics data obtained from the four distinct sources. The BM and WASP model we calibrated using the proxy basin data input, the best-fit model was then used with the different hydrodynamic data sets. The objective was to comprehensively capture the effects of these approaches on the output water quality dynamics. The model output was subsequently juxtaposed against observed data at upstream and downstream points of each wastewater treatment plant location within the study area.

To effectively gauge the disparities between model outputs, the following comparison methods were employed:

1. **BM vs. WASP model:** This assessment leveraged statistical techniques, *t*-test and ANOVA, to discern significant differences between the BM and WASP respective outputs.
2. **BM vs. measured data and WASP model vs. measured data:** The accuracy of the models was evaluated against real-world measurements at each output location. Root Mean Square Error (RMSE) plots were employed to visualise and quantify the deviations between model predictions and observed data.
3. **Models vs. location plots:** Plots were generated to illustrate how well the models aligned with actual data across different locations. Mean Squared Error (MSE) plots and accompanying statistical tables offered insights into the model fits at various points.
4. **Overall model vs. model vs. location visualisation:** A comprehensive visualisation strategy involved the use of heat maps, which facilitated a holistic assessment of the model's performances across multiple locations.

By adopting this comprehensive approach to model comparison, the study aimed to discern nuanced patterns, strengths, and limitations of the BM and the WASP model in predicting the behaviour of nitrogenous compounds in the presence of wastewater treatment plants using multiple hydrodynamics sources to drive the water quality models.

Considering the limitations posed by the number of available data points and data scarcity, the comparative study was constrained to the timeframe from 2017 to 2018. This specific period was chosen due to its alignment with the availability of pertinent measurements and wastewater treatment plant effluent discharge data. This temporal focus was instrumental to ensuring that the study's analyses and comparisons were grounded in reliable and relevant information. This was pursued in the context of varying hydrodynamics input data, recognising the pivotal role of these inputs in shaping the behaviour of pollutants.

Limitations

The study operated under the assumption that the hydrodynamic flowrates derived from the four selected sources, sufficiently represented the conditions prevailing within the river system under the circumstances. Additionally, the models presuppose a scenario where the river is thoroughly mixed, disregarding any potential heterogeneity in flow patterns. Furthermore, the models exclusively consider the pollution sources explicitly incorporated into their formulations, potentially overlooking other significant sources of pollution that could influence the water quality dynamics within the river. It is important to acknowledge these limitations, as they may impact the models' ability to precisely replicate real-world conditions and underscore the need for cautious interpretation of the study's findings.

Investigation design

The investigation was carefully structured to comprehensively explore the dynamics of nitrogenous compounds within the river system, focusing on the impact of wastewater treatment plants and the influence of variable hydrodynamics input data. A series of interconnected steps guided the design to derive meaningful insights and robust conclusions.

1. **Objective formulation:** The primary objectives of the investigation were established and included the need to assess the behaviour of nitrogenous compounds in a complex river system, evaluate the efficacy of different modelling approaches, and understand the interplay between hydrodynamics input and water quality model output.
2. **Data acquisition and preprocessing:** Pertinent data sources were identified and collected, encompassing hydrodynamics measurements, pollutant concentrations, and effluent discharge data from wastewater treatment plants. This data formed the foundation for subsequent analyses.
3. **Hydrodynamics model setup:** Simulation models, including the Basic WASP, were configured to incorporate the hydrodynamics input data from multiple sources from point 2.
4. **Temporal scope definition:** The study's temporal scope was delineated to encompass the period between 2017 and 2018. This time frame was selected to align with available measurements and wastewater treatment plant effluent data.
5. **Comparative analysis:** Model outputs were compared against observed data at upstream and downstream points of wastewater treatment plant discharge locations. Various techniques, including statistical tests (*t*-test, ANOVA), goodness-of-fit metrics (RMSE, MAE), and visualisation tools (residual curves, time series plots), were employed to assess model performance.
6. **Visualisation and pattern recognition:** Frequency distribution histograms, boxplots, and heat maps were used to visualise discrepancies and variations in model predictions across different scenarios and locations.
7. **Interpretation and conclusion:** The findings were systematically interpreted considering the limitations of the study design and the implications of the results. Conclusions were drawn regarding the accuracy of the models and the significance of hydrodynamics input variability.

By structuring the investigation in this manner, this research aimed to provide a comprehensive and rigorous analysis of nitrogenous compound dynamics within a river system while accounting for the complexities introduced by wastewater treatment plant effluents and hydrodynamics variability under scarce data conditions. The computational structure of the river system was divided into 17 distinct reaches, as detailed in Table 1. Seven observation points were designated to assess the models' performance under different hydrodynamic inputs. These observation points were key locations for comparing and evaluating the model outputs based on the varying hydrodynamic inputs.

Table 1 | Study segment names and locations of significance

Segment numbers	Segment name	Measured data location
1	Upstream WWTP A	Boundary water quality data
2	Stream 1	-
3	Effluent at WWTP A	Effluent composition data
4	Stream 2	-
5	Downstream WWTP A	Measured data point 1
6	Stream 3	
7	Upstream WWTP B	Measured data point 2
8	Stream 4	
9	Effluent at WWTP B	Measured data point 3
10	Stream 5	
11	Downstream WWTP B	Measured data point 4
12	Stream 6	
13	Upstream WWTP C	Measured data point 5
14	Stream 7	
15	Effluent WWTP C	Measured data point 6
16	Stream 8	
17	Downstream WWTP C	Measured data point 7

Interpretation of results

The interpretation of results encompassed a multifaceted approach; leveraging diverse analytical techniques to assess the outcomes comprehensively. The investigation embraced several key methods:

1. **Residual curves:** Residual curves visualise the differences between observed and model-predicted values over time. These curves provide insights into the magnitude and patterns of deviations, aiding in identifying trends and potential discrepancies (Martin *et al.* 2017).
2. **Time series curves:** Time series curves offer a dynamic visualisation of modelled and observed data over the study period. This approach has demonstrated precise assessment of temporal patterns, trends, and variations in water quality dynamics studies (Hobson *et al.* 2015; Monteiro & Costa 2018).
3. **Frequency distribution histograms:** Frequency distribution histograms enable the examination of the distribution of model residuals or observed data values. These provide a glimpse into the spread and frequency of discrepancies, facilitating the identification of potential biases (Wilks 2011).
4. **Goodness-of-fit metrics:** Goodness-of-fit metrics, such as RMSE and Mean Absolute Error (MAE), quantify the overall agreement between model predictions and observed data. These metrics offer quantitative insights into the accuracy of the models (Legates & McCabe 1999).
5. **Boxplots and residual curves:** Boxplots illustrate using diagrams the distribution of model residuals of statistical data across different subsets. These aid in identifying potential trends, outliers, and variations in model performance (Jandu *et al.* 2021)

RESULTS AND DISCUSSION

Statistics and trends

Proxy basin station and altered proxy basin station data hydrodynamics

The model output comparison statistics, which include *p*-values for the *t*-test and ANOVA, as well as RMSE and MSE for proxy basin station and altered proxy basin station data input, are presented in Table 2. Trendlines were included to illustrate the variations between the models and the measured data downstream of the simulated river system.

Results for the proxy basin station data hydrodynamic input show that in Segment 5, both ANOVA and *t*-test comparisons for this segment show high *p*-values indicating no significant differences between the BM and WASP or between these models and measured data. RMSE and MSE values are relatively low, indicating good agreement between model outputs and measured data. Similarly, ANOVA and *t*-test comparisons show no significant differences between models and measured data, with *p*-values above 0.05. RMSE and MSE values also remained relatively low, suggesting favourable model performance. In Segment 11, ANOVA tests showed *p*-values lower than 0.05, indicating that there are significant differences between model outputs and measured data. *t*-Test comparisons revealed mixed results, with a *p*-value of 0.15 suggesting some agreement between BM and WASP, but not with measured data. RMSE and MSE values are notably higher, indicating larger errors between the models and measured data. Segment 15 and Segment 17 ANOVA tests indicate a significant difference between model outputs and measured data (*p*-value less than 0.05). *t*-Test comparisons also show no agreement between the models and measured data. RMSE and MSE values are considerably higher, indicating substantial errors between models and measured data. Similar statistical significance results can be observed from the altered proxy basin station hydrodynamic input results.

The analysis of proxy basin station and altered proxy station data input demonstrate varying degrees of agreement between model outputs (BM and WASP) and measured data across different segments. Segments 5 and 9 exhibit good model performance with low RMSE and MSE values and no significant differences in statistical tests. In contrast, Segments 11, 15, and 17 show significant differences between models and measured data, along with higher RMSE and MSE values, indicating poorer model performance.

These trends highlight the importance of segment-specific assessments and suggest that model performance can vary significantly depending on the conditions and inputs. Further investigation into the factors contributing to the discrepancies in Segments 11, 15, and 17 is warranted to improve the accuracy of water quality modelling in these areas.

Rainfall hydrodynamic input

The model output comparison statistics, which include *p*-values for the *t*-test and ANOVA, as well as RMSE and MSE for rainfall and WRSM/Pitman data input, are presented in Table 3.

Table 2 | Statistics of WASP and BM output for simulations with proxy basin station and altered station data hydrodynamics

Segment number Models compare	Proxy basin station data 5	9	11	15	17	Trend
	***p*-value**					
ANOVA (BM vs. WASP)	0.79	0.24	0.0012	0.00012	0.0003	
ANOVA (BM vs. Measured)	0.79	0.24	0.0012	0.00012	0.0001	
ANOVA (WASP vs. Measured)	0.78	0.24	0.0012	0.0007	0.00047	
ANOVA (BM vs. WASP vs. Measured)	0.79	0.24	0.0012	0.0006	0.00145	
t-Test (BM vs. WASP)	0.79	0.16	0.15	0.0024	0.00136	
t-Test (BM vs. Measured)	0.65	0.16	0.00047	0.00032	0.00014	
t-Test (WASP vs. Measured)	0.53	0.89	0.00023	0.0005	0.00032	
Errors	**Statistic**					
RMSE (BM vs. WASP)	0.8	0.87	0.86	0.97	0.97	
MSE (BM vs. WASP)	0.89	0.75	0.74	0.94	0.94	
RMSE (BM vs. Measured)	1.03	0.96	2.6	2.41	0.8	
MSE (BM vs. Measured)	1.06	0.91	6.74	5.83	0.64	
RMSE (WASP vs. Measured)	1.07	0.77	2.61	2.78	0.52	
MSE (WASP vs. Measured)	1.13	0.59	6.82	7.74	0.27	
Segment number	**Altered proxy basin station data** **5**	**9**	**11**	**15**	**17**	**Trend**
Models compare	***p*-value**					
ANOVA (BM vs. WASP)	0.8	0.59	0.0032	0.00013	0.00027	
ANOVA (BM vs. Measured)	0.8	0.59	0.0032	0.00013	0.0001	
ANOVA (WASP vs. Measured)	0.8	0.59	0.0012	0.0007	0.00037	
ANOVA (BM vs. WASP vs. Measured)	0.8	0.59	0.0012	0.0006	0.00185	
t-Test (BM vs. WASP)	0.69	0.52	0.51	0.0064	0.00166	
t-Test (BM vs. Measured)	0.52	0.32	0.00037	0.00032	0.00014	
t-Test (WASP vs. Measured)	0.76	0.7	0.00013	0.0007	0.00022	
Errors	**Error**					
RMSE (BM vs. WASP)	0.93	0.91	0.91	0.85	0.85	
MSE (BM vs. WASP)	0.87		0.82	0.72	0.72	
RMSE (BM vs. Measured)	1.11	0.96	2.61	2.4	0.77	
MSE (BM vs. Measured)	1.23	0.92	6.8	5.74	0.6	
RMSE (WASP vs. Measured)	1.05	0.84	2.62	2.62	0.43	
MSE (WASP vs. Measured)	1.1	0.7	6.86	6.87	0.18	

For the rainfall hydrodynamic input, overall ANOVA tests indicate significant differences between models and measured data in Segments 11, 15, and 17, while Segments 5 and 9 show no significant differences. *t*-Test results also reveal a lack of agreement between models and measured data in Segments 11, 15, and 17. RMSE and MSE values increase in Segments 11, 15, and 17, indicating deteriorating model performance and larger errors compared to Segments 5 and 9.

In a broad overview, ANOVA tests highlight substantial disparities between model predictions and observed data in Segments 11, 15, and 17, whereas Segments 5 and 9 exhibit consistent patterns with no statistically notable distinctions. Furthermore, *t*-test findings underscore the absence of alignment between model outputs

Table 3 | Statistics of WASP and BM output for simulations with rainfall and WRSM/pitman data hydrodynamics

	Rainfall					
Segment Number	**5**	**9**	**11**	**15**	**17**	**Trend**
Models compare	***p*-value**					
ANOVA (BM vs. WASP)	0.86	0.7	0.00145	0.00134	0.00124	
ANOVA (BM vs. Measured)	0.86	0.7	0.00145	0.00134	0.00124	
ANOVA (WASP vs. Measured)	0.86	0.7	0.00145	0.00134	0.00124	
ANOVA (BM vs. WASP vs. Measured)	0.86	0.7	0.00144	0.00134	0.00124	
t-Test (BM vs. WASP)	0.94	0.57	0.58	0.0144	0.0014	
t-Test (BM vs. Measured)	0.64	0.44	0.0002	0.0018	0.00315	
t-Test (WASP vs. Measured)	0.67	0.78	0.0114	0.0056	0.00014	
Errors	**Error**					
RMSE (BM vs. WASP)	0.89	0.85	0.84	0.9	0.9	
MSE (BM vs. WASP)	0.8	0.72	0.71	0.8	0.8	
RMSE (BM vs. Measured)	1.11	0.95	2.63	2.46	0.76	
MSE (BM vs. Measured)	1.23	0.91	6.9	6.03	0.57	
RMSE (WASP vs. Measured)	1.02	0.78	2.61	2.78	0.52	
MSE (WASP vs. Measured)	1.05	0.61	6.83	7.71	0.27	
	WRSM/Pitman					
Segment Number	**5**	**9**	**11**	**15**	**17**	**Trend**
Models compare	***p*-value**					
ANOVA (BM vs. WASP)	0.81	0.34	0.00001	0.00134	0.00034	
ANOVA (BM vs. Measured)	0.81	0.34	0.00003	0.00134	0.00224	
ANOVA (WASP vs. Measured)	0.81	0.34	0.00004	0.00134	0.0003124	
ANOVA (BM vs. WASP vs. Measured)	0.81	0.34	0.00001	0.00134	0.0004	
t-Test (BM vs. WASP)	0.79	0.17	0.16	0.02314	0.0014	
t-Test (BM vs. Measured)	0.56	0.28	0.0006	0.0018	0.00015	
t-Test (WASP vs. Measured)	0.69	0.85	0.0003	0.0056	0.00014	
Errors	**Error**					
RMSE (BM vs. WASP)	0.89	0.84	0.83	0.96	0.97	
MSE (BM vs. WASP)	0.79	0.7	0.69	0.93	0.93	
RMSE (BM vs. Measured)	1.12	0.97	2.61	2.44	0.79	
MSE (BM vs. Measured)	1.26	0.95	6.83	5.94	0.63	
RMSE (WASP vs. Measured)	1.03	0.77	2.62	2.8	0.53	
MSE (WASP vs. Measured)	1.05	0.59	6.84	7.84	0.28	

and empirical measurements in Segments 11, 15, and 17. It is noteworthy that RMSE and MSE values escalate in Segments 11, 15, and 17, signalling a decline in model performance and larger discrepancies when compared to Segments 5 and 9.

The analysis of WRSM/Pitman estimated hydrodynamic data reveals varying levels of accord between model outputs (BM and WASP) and measured data across different segments within the context of WRSM/Pitman hydrodynamic data input. Segments 5 and 9 demonstrate commendable model performance characterised by minimal RMSE and MSE values and a lack of statistically significant differences in the conducted statistical tests for the WRSM/Pitman estimated hydrodynamic input types. In contrast, Segments 11, 15, and 17 display substantial disparities between model predictions and observed data, along with elevated RMSE and MSE values, indicative of inferior model performance.

These trends emphasise the necessity of segment-specific assessments when employing WRSM/Pitman estimated hydrodynamic data as input, underscoring the potential for considerable variations in model performance contingent on prevailing conditions and input sources. Delving deeper into the factors contributing to the disparities in Segments 11, 15, and 17 is pivotal for refining the accuracy of water quality modelling in these specific regions.

Segment error compound analysis

The models, result with rainfall hydrodynamic input is selected as a representative example of WASP and BM performance near the boundary segment (Segment 5), selected because of proximity to model input boundary data. The models, performance results for Segment 17 also are discussed because it is located further downstream the river to demonstrate error compounding. Figures 3 and 4 illustrate scatter plot, residual curve, timeseries plot, goodness-of-fit, and box plot for the BM and WASP model, respectively.

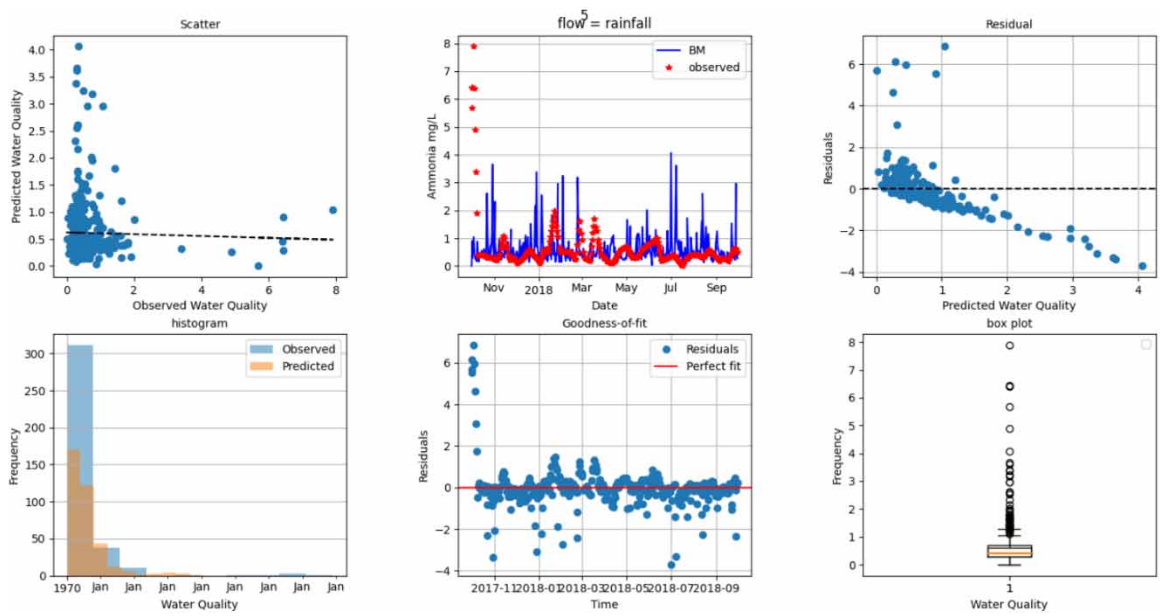


Figure 3 | BM output at Segment 5 for rainfall hydrodynamic input data.

Figures 3 and 4, which include scatter plots, residual curves, time series plots, goodness-of-fit, and box plots for the BM and WASP Model, collectively reflect the minor visual differences in model performance and agreement with statistical data as described for Segment 5. This indicates that the BM performed similarly to the WASP model for the same inputs, when data quantity and quality was sufficient to good predictions, indicating that the BM may be used with confidence by water quality modellers in lieu of the WASP model if preferred.

The model performance results for both BM and WASP model were studied to investigate the effect of the error compounding further from the model boundary input data. Figures 5 and 6 show model performance for BM and WASP model at Segment 17.

From the results relating to Segment 17, it is evident that both the WASP and BM s exhibit subpar performance when compared to the measured data, with the WASP model showing a slightly better fit than the BM. This improved performance of the WASP model may be attributed to its more complex structure, which includes a built-in parameter estimation capability. This capability allows the WASP model to fine-tune its parameters and adapt to the specific conditions of Segment 17, leading to a closer alignment with the observed data. Therefore, it can be concluded that both models performed poorly in the case of poor data availability, even when different hydrodynamic models are used, with the WASP model seeming to perform slightly less poorly.

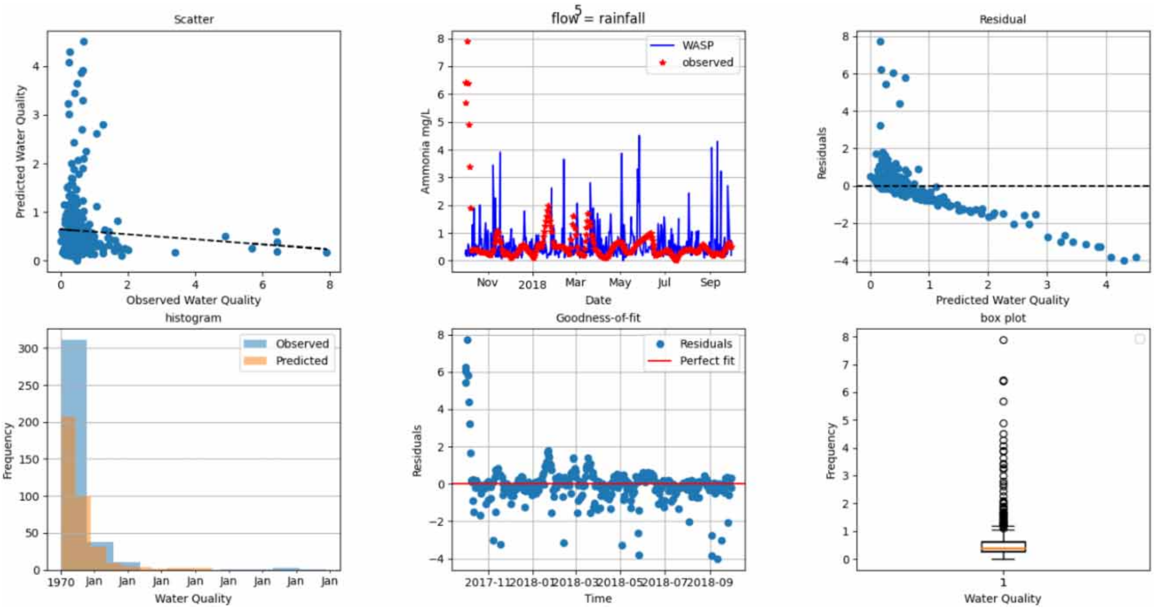


Figure 4 | WASP output at Segment 5 for rainfall hydrodynamic input data.

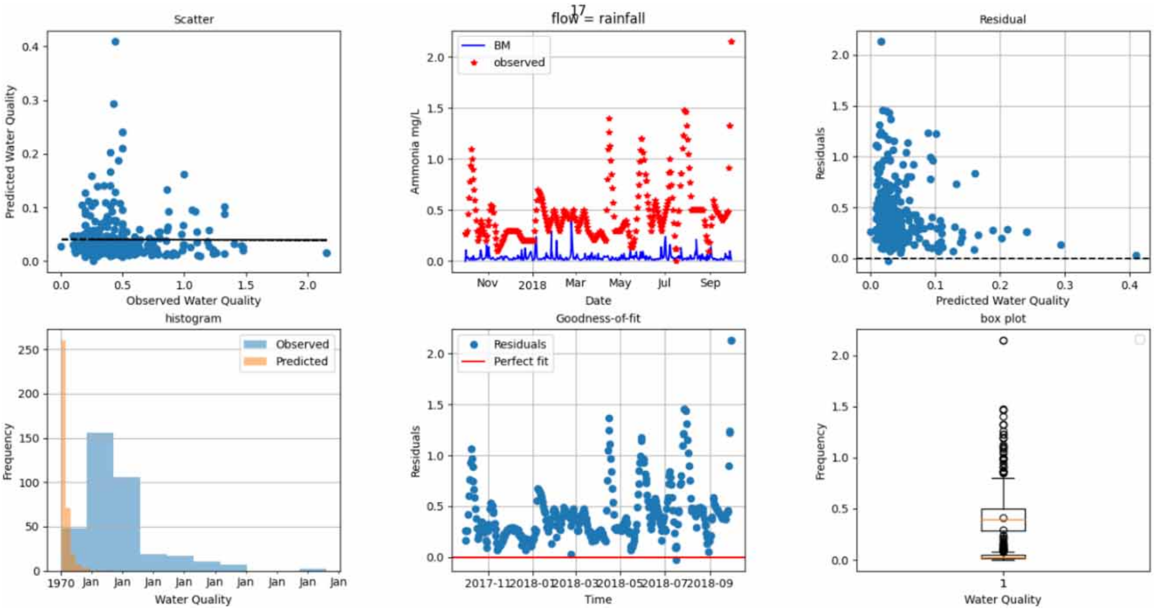


Figure 5 | BM output at Segment 17 for rainfall hydrodynamic input data.

Furthermore, a noteworthy trend becomes apparent when considering the entire study area: as you move further away from the boundary input, both models tend to perform less accurately. This trend suggests that the models excel in capturing the dynamics and interactions in areas closer to the hydrodynamic input source, but their accuracy diminishes as you move downstream, likely due to the increasing complexity and variability of the river system.

These trends emphasise the importance of segment-specific assessments and data provision when using rainfall hydrodynamic input and suggest that model performance can vary significantly based on the conditions and inputs.

In the comprehensive analysis of water quality modelling using varying hydrodynamic data inputs, several key trends emerge. Across multiple segments, statistical tests consistently reveal significant differences between model predictions (both BM and WASP) and measured data, particularly in Segments 11, 15, and 17. Figures 7 and 8 illustrates deteriorating model performance the further the output location is to the boundary data input

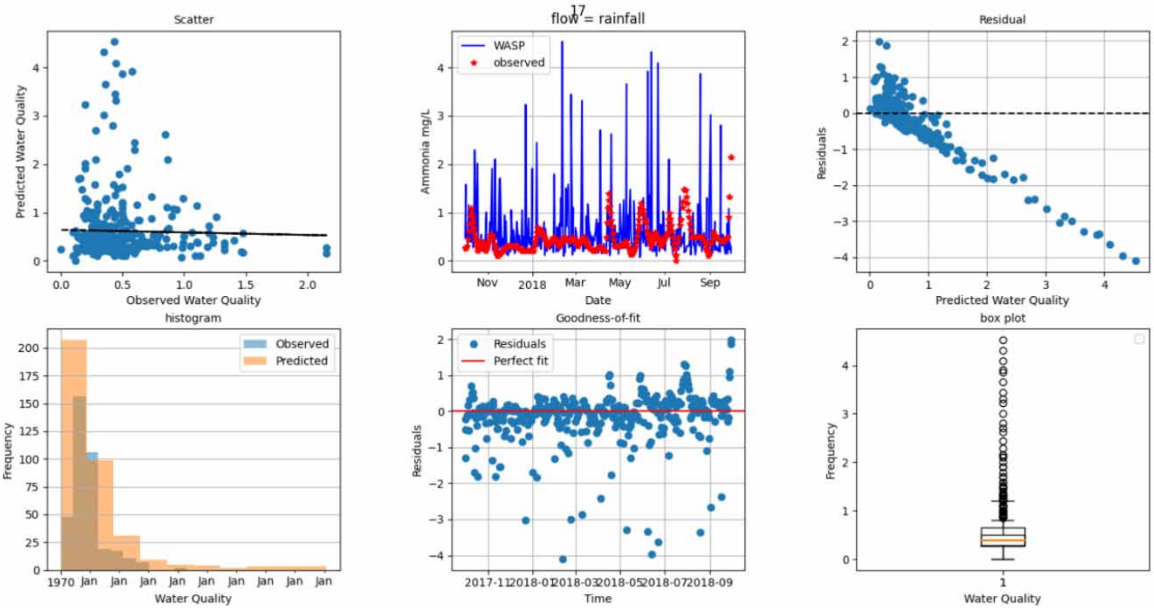


Figure 6 | WASP model output at Segment 17 for rainfall hydrodynamic input data.

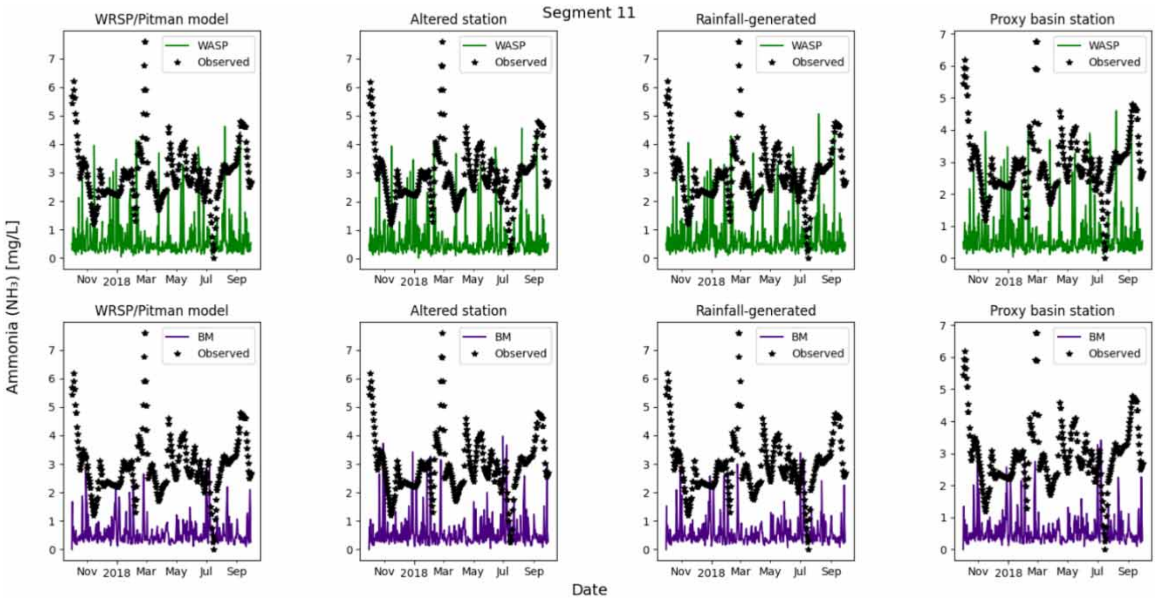


Figure 7 | Time series plots of BM and WASP model against measured data at Segment 11.

indicating compounding of errors with distance at Segment 11 and Segment 15. Results for Segment 17 were omitted since these results are discussed previously.

These segments consistently display a lack of agreement between model outputs and empirical measurements, as corroborated by *t*-test results. Furthermore, RMSE and MSE values consistently rise in Segments 11 and 15 signifying a decline in model performance and the presence of larger errors compared to Segments 5 (discussed previously) and Segment 9. To reiterate, Figure 9 illustrates that the BM and WASP model perform better against measured data compared at Segment 9 for all the hydrodynamics sources.

These results support the importance of conducting segment-specific data inputs and assessments when utilising model-generated hydrodynamic data, as model performance can vary significantly depending on the conditions and input sources. Addressing the factors contributing to disparities in these segments is crucial for enhancing the accuracy of water quality modelling in these specific regions.

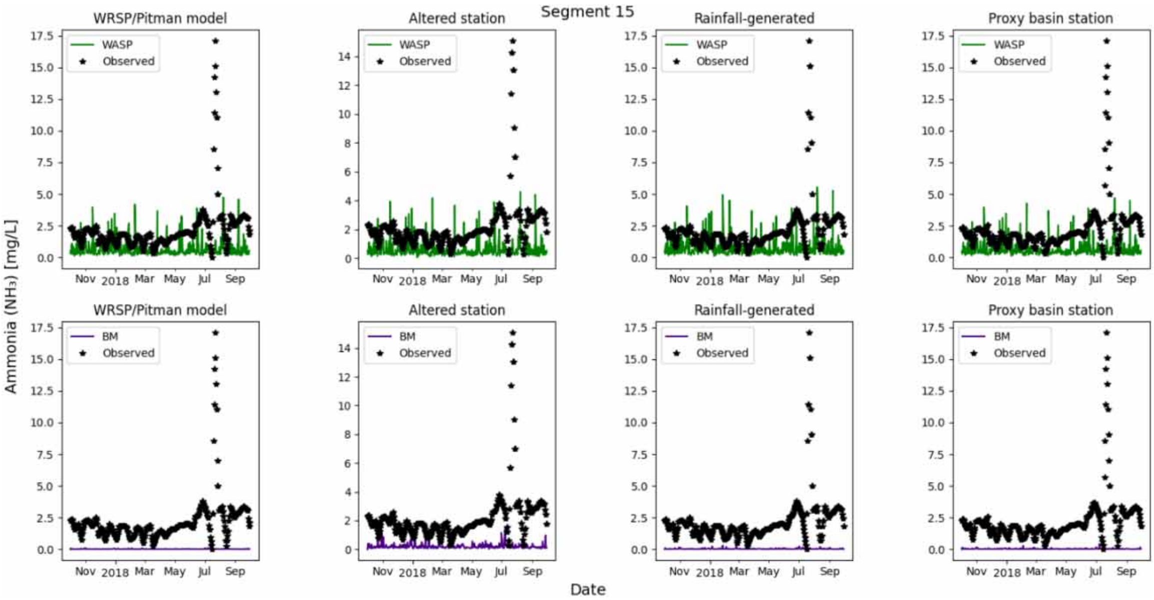


Figure 8 | Time series plots of BM and WASP model against measured data at Segment 15.

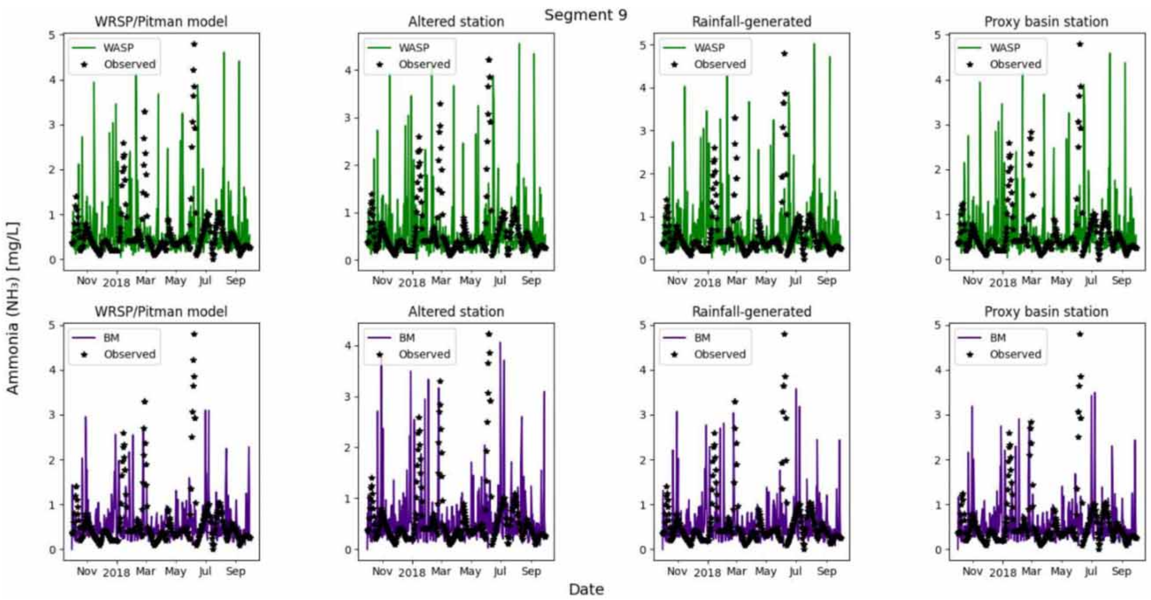


Figure 9 | Time series plots of BM and WASP model against measured data at Segment 9.

The models' poor performance in certain segments can be attributed to several possible factors. Firstly, the uncertainties arising from the transfer of hydrological data sources to ungauged basins may have introduced inaccuracies in the model predictions. Additionally, the hydro-geometry of ungauged river channels may not have been adequately accounted for, as the hydrodynamic data were transferred from neighbouring streams that may only be similar, but not identical, in their characteristics. Moreover, the study primarily focused on assessing the differences in model performance resulting from varying hydrodynamic data sources, rather than specifically evaluating the models' capabilities to match measured data. This emphasis may have led to less attention being paid to factors influencing model accuracy in specific segments. Ultimately, the study aimed to highlight the implications of transferring data sources to ungauged river systems using water quality models, serving to quantify the discrepancies. However, further research into these factors is warranted to better understand and address the sources of poor model performance in certain segments.

CONCLUSIONS

The outcomes of this study have shed crucial light on the intricacies of water quality modelling of nitrogenous compounds within river systems, particularly concerning the utilisation of various hydrodynamic data inputs. Two river water quality models were compared, viz. the BM (BM) and WASP across multiple segments of the Natal Spruit River in South Africa using different hydrodynamic data sources as inputs. These models notably both performed well for all the hydrodynamic data source inputs closer to the model boundary, with a significant drop in performance with distance downstream.

Statistical analysis showed that the ANOVA and *t*-test results consistently produced significant disparities between model predictions and measured data in Segments 11, 15, and 17. This finding highlights the intricate relationship between hydrodynamics and water quality modelling, emphasising that a one-size-fits-all approach may not be suitable for all river segments, especially in areas with data scarcity. Instead, it emphasises the importance of tailored modelling strategies, particularly in regions characterised by distinct hydrodynamic conditions.

A notable rise in RMSE and MSE values in Segments 11, 15, and 17 indicates the emergence of larger errors and declining model performance along the river reach when compared to the more harmonious results observed in Segments 5 and 9. This further accentuates the necessity of segment-specific assessments, as water quality modelling accuracy is inherently linked to the nature and accuracy of hydrodynamic data inputs.

In conclusion, this study underscores the dynamic nature of water quality modelling and emphasises the critical role played by hydrodynamic data sources in shaping model outcomes. It highlights the nuanced endeavour required to achieve precise water quality predictions, contingent upon the unique characteristics of each river segment. The findings compel a deeper understanding of the significant impact that compounding errors can have on model accuracy, particularly in relation to river length. As demonstrated by the research outcomes, there is a clear need for a more refined and localised approach to water quality modelling, acknowledging the diversity of hydrodynamic conditions within river systems.

Future research into lengths of river segments, for different water quality models and hydrodynamic inputs that result in acceptable modelling errors is warranted. This to inform future data acquisition plans for river water quality modellers.

DATA AVAILABILITY STATEMENT

Data cannot be made publicly available; readers should contact the corresponding author for details.

CONFLICT OF INTEREST

The authors declare there is no conflict.

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