Response to Reviewers' Comments

This document contains copies of all comments of the reviewers (*in italicized, blue* text) and our planned effort to address them (in normal, black text). Our proposed manuscript revisions are <u>underlined</u>.

Reviewer 1

Overall I was not impressed by the methodological advancements or the scientific implications of this project. The authors built a standard ML algorithm, random forests, and applied it to a global nitrogen dataset. The portrayal of it as a spatiotemporal model is misleading: It is a standard random forest that uses month and lat/lon as additional predictors, which is perfectly fine but not a novel type of random forest model.

We are thankful to the reviewer for the time and effort spent on reviewing our paper. We believe that these comments help us reduce the possible confusion in the text with respect to paper's novelty and rigor that appear to have arisen due to lack of sufficient clarity in the original version.

We regret that the novelties and motivations of this study were not clearly stated in the original paper. To address this comment, we will revise the Introduction section. More importantly, to improve the linkage between study objectives and results, we propose to present additional results to highlight several model capabilities. These include model validation using a new validation strategy, adding partial dependence plots, presenting the distribution of R2 values, adding new predictor variables (i.e., forest fraction, urban fraction, and hydrography data) and further discussions on limitations of our approach along with recommendations for future studies (more details can be found in our response to the reviewer's comments throughout this document).

Regarding the use of lat/lon, as we extensively discussed in Section 3.1.1, two strategies have been proposed in the literature to account for spatial information: (1) using a hybrid modelling framework by embedding Kriging and Gaussian process modelling into the standard random forest method (Saha et al., 2021; Canion et al., 2019); and (2) using geographic information as the auxiliary inputs, for example, adding geographic coordinates (Behrens et al., 2018; Meng et al., 2018) or other spatial distances (Li et al., 2011; Wei et al., 2019) into the list of predictors. Since adding lat/lon as predictor variables to represent spatial relationship is common in data-driven modelling of Earth and environmental systems, we followed this strategy and incorporated lat/lon into our random forest model. <u>During the revision, we will highlight the weakness of the second strategy in not fully capturing the spatial relationships between observations and predictors</u>.

Overall, we believe that the reviewer has under-estimated the contribution in the paper. As outlined in this rebuttal document, the application of the random forest model can be considered to be state-of-the-art in a rapidly evolving field. The use of these techniques in the very challenging field of global water quality modelling is novel and has yielded predictive results that exceed other approaches in important respects.

The model appears to perform well on held out data, so the authors take that as evidence to then apply it globally and make maps. From those maps and the model itself, the authors pull out generally banal conclusions that have been recorded elsewhere. The 'so what' of the paper from the discussion section is that it could conceivably be used by other stakeholders in applications, but this link felt very light, so I am left skeptical of any pathway to impact.

We regret that the reviewer regards the conclusions as being banal. We admit that in trying to summarize a complex global picture we did not manage to fully highlight the originality and significance of the results.

The purpose of the model is to enable water quality assessment and quantification of future scenarios (e.g., of livestock pasture extent) at a global scale. Though some instances of analysis of these questions exist (e.g., Mayorga et al., 2010; He et al., 2011; Beusen et al., 2016; etc.) they all have inevitable limitations, and none have used our proposed approach which we believe yields worthwhile results, so it is important that the methodology is peer reviewed in the hydrological literature.

We further examine model validation by implementing another validation strategy known as Leave-Location-and-Time-Out Cross-Validation (LLTOCV) during the revision. For more details, please see our response to your comment regarding extrapolation issue. In addition, to address the comment on the innovations that this study brings, we will revise the Introduction and relevant sections in the Discussion to include a more substantive 'so what' from the paper.

Specific feedback:

The literature review of ML methods in water quality (Section 1.2) does not powerfully motivate the present study. Why are the "three critical observations" listed interesting and relevant? This section overall feels disconnected from the rest of the paper.

We remain convinced that our 'three critical observations' from review of the literature were strong enough to motivate this study because: first, despite a plethora of powerful machine learning methods, ANN is the most popular method for water quality modelling. To fill this gap, we applied random forest algorithm to examine its predictive performance when applied to large spatial scales. Second, our thorough search of the relevant literature indicated that machine learning methods, particularly random forests, have not been implemented at global scale to identify hotspots of nitrogen concentrations nor to systematically determine high importance factors influencing nitrogen variability. Third, despite being successful in simulating and predicting surface water quality at catchment-scale, machine learning methods have not been utilized to provide spatially explicit (gridded) estimates of nitrogen levels. Based on our observation, almost all machine learning models are lumped in space (see Table 1). This gap further motivated our development of the spatiotemporal random forest-based global model in the present study. In the revised manuscript, we will improve the writing to reduce the reviewer's confusion that appear to have arisen due to lack of sufficient clarity in the original versions.

The authors also fail to discuss why so few papers attempt to apply their models at a global scale (extrapolation risks) and make it seem that the community just never tried before, which is not the case. Broadly, the motivation for this work is not clear and compelling.

Thanks for pointing this out. In the revised manuscript, we will explain these major challenges associate with building data-driven models at global scale, particularly extrapolation risks and sampling bias. It is worth noting that we believe that by addressing these obstacles we have made a significant methodological contribution.

"The primary goal of this study is to introduce a global WQ model that is based on ML approach. (Section 1.3)". There are hundreds of water quality models that are based on ML, as they mention in their previous section.

As mentioned in Section 1.2 of the paper, we agree with the reviewer that there are many MLbased water quality models at catchment scale, but there are only a few models at 'global scale'. In the revised manuscript, we will further clarify our research goal, which is the use of an appropriately refined ML method to predict spatial and temporal variations in WQ at a global scale.

This paper is not really about providing a new dataset then, but a new model. **But their model is relatively** off the shelf and does not tell us anything about the systems we do not already know. Overall building a ML model, because we can, is not a compelling motivation in 2022.

We disagree with this remark at several levels. There is a long tradition of publishing the application of mathematical and statistical methods to hydrological problems. Because of the complexity of hydrology (and water quality in particular) this is far from trivial. The application

was definitely not "off the shelf", involving careful and rigorous selection, testing and adaptation of the ML method, alongside a vast exercise in data preparation.

Regarding the lack of new information, we politely disagree. We'd like to highlight that our model was validated with data from river basins outside the training dataset and was used to predict nitrogen concentrations in large river basins globally, providing new information about dynamics of nitrogen concentrations in location with scarce/no observations. Furthermore, we provide NOx-N concentrations (mg/l) worldwide (180°E-180°W; 90°S-90°N) at a spatial grain of 0.5degree. The NOx-N concentrations, mapped across the globe for 1992-2010, are available in a compressed GeoTiff file format in the WGS84 coordinate reference system (EPSG:4326 code). The developed stream nitrogen concentration maps have a wide array of potential applications in stream ecology, biodiversity research, conservation science, and stream and lake restoration ecology. For instance, the produced maps can be used to quantify the overall mass of nitrogen discharged into a specific lake or ocean body, enabling a deeper understanding of global-scale eutrophication. Furthermore, our estimates of nitrogen concentration can be used to verify new process-based models that predict nitrogen concentrations and transformations in inland waters worldwide. We encourage potential users of the described geo-dataset to contact the authors for future product updates. We will add this to the revised manuscript to better highlight the usefulness of our findings.

Observational data:

Why is the data collection period ceased in 2010? Data continues to be collected, so this seems an arbitrary cutoff removing potentially more data.

Data collection was not an arbitrary process in this study. We agree that new water quality data is collected on a continuous basis. As mentioned in the paper (Section 2.1), the observational data used for this study was obtained from the GEMStat repository which provides an online, globally harmonized, open-access database for approximately 250 water quality indicators. Based on our analysis, we found that the spatial coverage of the monitoring stations for the 1992-2010 period was sufficiently high to train our model, whilst for other time periods the number of monitoring stations were smaller.

Furthermore, unlike other temporal ranges, the quality of dataset within the 1992–2010 period was higher, in terms of temporal consistency and number of missing values. The selected period was also compatible with most of our predictor variable datasets (see Section 2.2). In addition, as mentioned in Section 4.1 (lines 351-354), the rest of the observations (sample size = 28,802) which does not belong to the 1992-2010 period was used for out-of-sample testing. <u>To address</u>

this comment and improve the clarification of data collection, we will add explanations in Section 2.1 on why this time span was selected in our study.

Second, the stations used to build the model have large geographic disparities the authors do not discuss at length (e.g. abundance of sites in Brazil and Europe). **Sampling bias by location is a huge consideration** when applying the map globally.

Thank you, this is a very good point. The sampling bias is a common challenge in machine learning-based water quality studies. To address this comment, we will introduce new results that map R2 values spatially. We will add a new 'Discussion' section to better describe caveats/limitations of our approach and will reflect on this issue (i.e., sampling bias), how it was corrected for and how it might, nonetheless, impact our results.

I think this manuscript is an unsupported (by the data validation presented) extrapolation of a model to locations far different that those used to train the model. The authors gloss over this critical consideration when making the main global maps (Figs. 6-8).

The performance of the model in spatial extrapolation has been extensively tested. Our results in Fig. 5 clearly shows that the proposed model reproduced the *new* NOx—N values at sites outside the training dataset with a reasonable accuracy. This fair agreement between random forest predictions and independent NOx—N observations provides confidence to the overall approach.

In the revised manuscript, we further investigate the extrapolation issue to address this very important comment. We will implement another validation strategy known as Leave-Locationand-Time-Out Cross-Validation (LLTOCV). In this method, like standard cross validation (CV), the dataset is split into folds again, but this time each fold left the data of complete locations or time steps or locations as well as time steps out. Over-fitting of the model in space and time can be then quantified by comparing the random 10-fold CV results with this 'target-oriented' validation results. Consequently, the high difference between 10-fold CV implemented in this study (lower error estimates) and LLTOCV (higher error estimates) can be an indication of spatial over-fitting as the models can very well predict on subsets of the time series of the locations used for training but fail in the prediction of unknown locations. We will also expand the relevant discussions in Sections 3.2 & 4.1.

Predictors data:

The authors say they started with a list of 27 candidate variables but then reduced it by more than half, to around 13 variables, to "reduce…redundant information" but one of the key advantages of random forests is that they work well with highly correlated variables. What were the other variables considered that were ultimately not included?

We politely disagree the comment that 'one of the key advantages of random forests is that they work well with highly correlated variables.' In fact, the effect of correlations on random forest algorithm has been studied by many researchers, particularly how it might impact variable importance measured by random forest (see, e.g., Archer and Kimes, 2008; Strobl et al., 2008; Nicodemus and Malley, 2009; Nicodemus, 2011; Auret and Aldrich, 2011; Toloşi and Lengauer, 2011; etc.). For example, Archer and Kimes (2008) observed that the Gini measure of random forest is less able to detect the most relevant variables when the correlation increases, and they mentioned that the same is true for the permutation-based importance measure. Auret and Aldrich (2011) also confirmed these observations, and Toloşi and Lengauer (2011) called it "correlation bias". In summary, most of these studies reported two key impacts of the correlation on permutation importance measures: (1) the importance values of the most discriminant correlated variables are not necessarily higher than a less discriminant one, and (2) the permutation importance measure depends on the size of the correlated groups. In an important study, Gregorutti et al. (2017) provided theoretical validations for these assertations, in a particular statistical framework.

Since one of the main objectives of our study was identifying key drivers of nitrogen variability at global scale, we tried to reduce the number of correlated predictors to minimize the negative impact of correlations. To address this comment, we will provide the list of 27 potential explanatory variables in Appendix of the revised manuscript. We will also add relevant discussions on the correlation and variable importance in random forests in Section 3.1.2 and provide more appropriate references.

Were the datasets aggregated over the watershed boundaries corresponding to each sampling location (for variables like precipitation and runoff they need to be)?

Thanks for raising this point. Please note that we modeled nitrogen concentrations at 0.5-degree gird cell (not at watershed scale). Thus, the current predictors for in-stream nitrogen concentrations prediction only cover the properties within the grid cell of interest.

This can be resolved, for example, by considering hydrography data delineating global river networks, though it will presumably add more complexity to the model. In the revision, we will add more variables to the list of predictors, including upstream characteristics, stream proximity (e.g., distance up to the stream) or log-transformed flow accumulation for better capturing

<u>spatial characteristics of watersheds.</u> Previous studies have shown that these variables can be key drivers of water quality responses in rivers (see, e.g., Staponites et al., 2017; Lintern et al., 2017; Grabowski et al., 2016; Peterson et al., 2010). Particularly, they reported that accounting for the hydrological flow paths and flow accumulation through the landscape and coupling these processes with specific landscape features can improve model performance. <u>We will also elaborate more on this with the supporting literature.</u>

Land cover is also known to be relevant but only cropland area was included.

This is a valid concern. Note that, however, the predictor selection process used in this study were based on an extensive literature review and domain knowledge. In fact, the random forestbased model presented in this study were developed using those key controls previously identified, without any additional predictor selection processes. We found that, among various land related variables, the cropland area has been frequently reported as the factor that strongly influences nitrogen variability. Our numerical results also confirmed this fact as shown in Fig. 9. To address this comment, we will add more land-related variables (e.g., forest fraction and urban fraction) to the list of predictors and will investigate how it may impact model performance and results.

Model development:

The novelty of this random forest methodology is greatly overemphasized. There is research into spatiotemporal random forests, but those are far more advanced than what was applied here, making the title of the paper misleading. Here is an off-the-shelf random forest that anyone taking a Coursera data science course could apply successfully. To clarify, I am okay with the algorithm but troubled by the emphasis on its importance and novelty. Including latitude and longitude as predictors hardly makes this a spatial statistical model. Including month of the year hardly makes this a time series model.

Thanks for your opinion, please see our response to the first two comments of this document. We also did not want by any means to imply that the idea of using lat/lon or cumulative month or month of the year were the novelty of this paper. In fact, the term '**novel**' has not been used even once throughout the paper, and we have not suggested that the algorithm is novel. So, it is not clear to us why the reviewer concluded that '*The novelty of this random forest methodology is greatly overemphasized*'. Furthermore, we'd be more than happy if the reviewer helps us identify some of the studies '*into spatio-temporal random forests, but those are far more advanced than what was applied here*' in the context of water quality, so we can cite them in the revised manuscript to strengthen the literature review part.

Regarding the merit of the utilized methodology, we restate the points about our study that we have made above, which the reviewer does not seem to have recognized or has under-estimated. We simply do not think it is accurate to dismiss a comprehensive exercise in data processing, model selection, adaptation, and validation as something "that anyone taking a Coursera data science course could apply successfully".

<u>Testing set:</u> I would like to see sites completely held out as well to see how well the model predicts at new locations.

As mentioned in our response to the second comment regarding extrapolation issue, <u>we are</u> <u>currently running Leave-Time-and-Location-Out Cross-Validation (LLTOCV) strategy, and we will</u> <u>update the relevant results and discussions in the revised manuscript.</u> In this method, like standard cross validation, the dataset is split into folds again, but this time each fold left the data of complete locations or time steps or locations as well as time steps (LLTO) out.

Model evaluation:

What is the distribution of R2 values by location? Presumably some locations perform better than others.

Thank you for this recommendation. We agree with the reviewer that some locations certainly perform better than others in terms of prediction accuracy. This is mainly due to the lack of sufficient, well-distributed measurements. In the revised manuscript, we will add a figure to show how R2 values vary in space. This figure will further help us evaluate the performance of the model.

Also, the metrics are produced on a log-transformed scale. What is the mean absolute error or root-meansquared error in interpretable, mg/L units? A strong performing model in log-log space is quite easy to produce (across domains, not just water quality) so it is important to record performance metrics in the back-transformed data space relevant to decision makers.

We are rather surprised by this comment. The reviewer certainly knows that data transformation is a common procedure in building empirical/machine learning-based models. In practice, it has been suggested that when implementing supervised learning algorithms, training data and testing data need to be transformed in the same way. However, there is a misconception that data transformation is not necessary for random forest.

To better explain this issue, first, note that random forest is a tree-based model and tree-based models do not care about the absolute value that a feature takes. They only care about the order of the values. Second, note that there is a distinction between the output of the random forest when it is used in classification or regression problems. For classification tasks, the output of the random forest is the class selected by most trees. For regression tasks, the mean or average prediction of the individual trees is returned. By taking these into account, we can say that data normalization, therefore, won't affect the output for random forest classifiers, whereas it will affect the output for random forest regressors. Regarding the regressor, it can be shown that the algorithm will be more affected by the high-end values if the data is not transformed. This means that they will probably be more accurate in predicting high values than low values. Consequently, transformations such as log-transform will reduce the relative importance of these high values, hence generalizing better.

In the context of the present study, the whole purpose of data transformation was to reduce the impacts of the extremely high values on model calibration. This is because those high values often present in extremely low proportions within the data. If those extreme values were left untransformed, they may cause the models to emphasize too much on rare extreme events, and thus largely affect our ability to represent the overall large-scale patterns in water quality. Our transformed model focuses more on proportional errors instead of absolute errors since the latter is less important at high concentrations in practice. Additionally, we presented model evaluation at the transformed scale because the model was calibrated in a transformed scale, and we believe that the transformed scale is most relevant and informative for performance assessments as we presented.

To address this comment, we will add more discussions in Section 2.2 (Data collection and processing) to improve the justification of data transformation. We will also add explanations in Section 4.1 (Model performance assessment) on why model performance evaluations are presented in a transformed scale. While we decided to focus this study on the transformed data, we have noted back-transforming modelled data as a possible option, and we would like to explore the differences between these two approaches in future studies.

I would like to see comparison of this model to benchmark models. For example, how does this compare against a simple linear regression? Against a mixed effects regression? Against simply fitting linear trends independently at each site? Not all of these need to be done, but some sort of well selected benchmarks are needed to contextualize model performance.

There has been extensive theoretical exploration and testing of random forest methods against other methods. By way of example, performance of the random forest algorithm in simulating

groundwater nitrate contamination at the African continent scale was evaluated in comparison to the multiple linear regression by Ouedraogo et al. (2019). Moreover, Chen et al. (2020) compared the water quality prediction performance of several learning models, including logistic regression, linear discriminant analysis, support vector machine, decision tree, random forest, etc., across major rivers and lakes in China. In addition, there has been extensive use of other data-based methods for predicting water quality, especially at a catchment scale (please see Section 1.2 of the paper and references therein). However, the fact that these simpler methods do not appear in the global water quality literature can be taken as being indicative that they are not suitable for that purpose. Some of these methods can be eliminated a priori: the processes are clearly not linear, and sites are not independent, so we would expect any reviewer to dismiss adoption of these methods for such a complex task as being foolish. Hence, we believe this 'model comparison' is beyond the scope of current study.

How to performance metrics compare with similar nitrogen modeling studies? If this model is the core advancement of the paper, its performance relative to other literature has to be clear and impressive. Unclear at this point if that is the case.

Thanks for this comment. To authors' knowledge, there is no parallel in the literature with similar model building approach, in terms of time scale, spatial resolution, and the selected constituent. However, we will add some evaluation of the closest relevant studies in the revised manuscript to discuss the similarity and differences between our findings and that of others.

Model interpretation:

The variable importance feature is interesting, but I want to see the influence of each variable on the outcome to check they make scientific sense. Otherwise the model could be getting it 'right' for the 'wrong' reasons. Partial dependence plots or the like are one way to plot those dependencies and could provide more interesting scientific findings rather than the surficial relationships presented so far in the paper.

Thanks for this suggestion. We believe that the variable importance measure used in this study (i.e., random forest permutation accuracy importance) is statistically advantageous compared to partial dependence plots or other univariate screening methods because it accounts for multivariate interactions.

In fact, partial dependence plots show how the model's predictions are affected by one or two predictors, which is the marginal effect that one or two features have on the predicted outcome of a machine learning model. In contrast, permutation accuracy importance measure covers the impact of each predictor variable individually as well as in multivariate interactions with other predictor variables, which is the combined importance of the variable and all its interactions with

other variables (see, e.g., Lunetta et al., 2004; Hastie et al., 2009; Grömping, 2009; Touw et al., 2013; Boulesteix et al., 2015; etc.). Moreover, partial dependence plots are easy to interpret. In the revised manuscript, we will add these plots and the above-mentioned discussion on their advantages and/or disadvantages when dealing with high-dimensional problems.

Literature discussion:

Overall it did not seem like the results were sufficiently contextualized in the literature. This goes for the performance metrics and the identification of increasing/decreasing trends in certain regions. Several of these regions have already been identified as having increasing/decreasing trends so how do these results build off of (or contradict) the prior literature?

We believe that our paper has been sufficiently contextualized and historicized, particularly in the Introduction section by (i) placing our research topic within its larger setting, (ii) providing important perspective by citing similar examples or relevant background, (iii) explaining what historical circumstances led up to the topic we are discussing, (iv) citing other scholars who have recently contributed to the field, and (v) exploring how our analysis fits into a larger discussion about the field. Also, we agree that the regional observations would benefit from further contextualization in relation to previous regional studies, which we will do in the revised manuscript.

Figure 3 is not helpful, perhaps move to SI if authors feel it is relevant.

This figure schematically shows the structure of the proposed random forest model. We believe it can help readers who are less experienced with the method to better understand how our WQ model works. From this perspective, the authors feel comfortable that the current place of Fig. 3 is appropriate.

Figures 4 and 5: What do the observed and predicted look like in original units? If this model and data outputs will ultimately be useful, it has to perform well in the original units. Figure 5 (test data) is more relevant than Figure 4 (training data), so Fig 4 could go to the SI.

To resolve this comment, we will add a new figure showing model performance in original units (not in transformed space), while keeping Figure 4 in the main text. For detailed discussion on why we presented results in box-cox transformed space, please see our response to your previous comment regarding presenting results in log-log space.

Figures 6-8 I worry considerably about extrapolation, so I do not trust the majority of locations shown. Also, how about accompanying uncertainty maps?

We understand that the reviewer is concerned about the spatial overfitting of the model. As proposed in our response to the second comment regarding extrapolation issue, apart from the conventional out-of-sample validation strategy discussed in the paper (Fig. 5) where the datasets which does not belong to the 1992-2010 period was used for out-of-sample testing, <u>we will implement a 'target-oriented' validation strategy to address this concern in the revised manuscript. We are currently running Leave-Time-and-Location-Out Cross-Validation (LLTOCV) process, and we will update the relevant results and discussions in the revised manuscript.</u>

Regarding the uncertainty analysis, we will add a new 'Discussion' section to better explain caveats/limitations of our approach and will thoroughly discuss the possible sources of uncertainty in our study.

Figure 8: Adds little not shown elsewhere.

Thanks for this comment. The purpose of this demonstration of latitudinal distribution of average (annual) estimated NOx—N concentrations is twofold. First, it helps us characterize the dominant regions of nitrogen concentrations. In addition, this figure shows that, in specific regions, high nitrogen fertilizer use does not necessarily correspond with equally high nitrogen concentration (e.g., the upstream region of the Yangtze River, upstream region of the Yellow River (China), upstream region of the Mississippi River (U.S.A), Murray River (Australia), Nelson River (Canada), midstream region of the Amur River (Russia, China), etc.). On the other hand, as can be seen from this figure there are some regions with relatively low nitrogen fertilizer use but high nitrogen concentration (e.g., downstream region of the Amazon River, and the midstream region of Congo River). This clearly indicates that the processes of the nitrogen cycle are complex, and dynamics of in-stream nitrogen concentration is controlled by nitrogen load input, hydrometeorological conditions, and management practices. Second, this figure can be used to validate our random forest model based on previous works that reported similar findings in these latitudes which correspond to the high agricultural activity and high livestock densities (see, e.g., Potter and Ramankutty, 2009; Lu and Tian, 2017; He et al., 2011). To address this comment, we will expand relevant discussions in Section 4.2 (Patterns of nitrogen concentrations and global hotspots).

Figure 9: Why do they find time series is more relevant? Is that surprising?

We are unclear on the interpretation of this comment, and don't understand why reviewer anticipates a "*surprise*". As we mentioned in the manuscript, time-related variables, namely Cumulative Month since 1992 (CM) and Month of the Year (MOY), have been included in our model to represent 'distance' in the time domain, particularly to capture the long-term trends (CM) and to model seasonality effects (MOY). Furthermore, CM somehow can compensate for biogeochemical legacy and the long travel time between N input and riverine N export signals. Variable importance results shown in Fig. 9 indicate that the most important covariate for predicting monthly nitrogen concentration given the utilized global datasets is: **time**, i.e., cumulative and/or month of the year. These covariates allow the random forest model to fit different spatial patterns for each month underpinning that the observed nitrogen level is different from month to month.

Is it interesting that cattle is ranked where it is? The 'so what?' is missing here.

Yes, we believe it is an important finding. The direct inclusion of the livestock-related variables in data-driven, empirical water quality models is not common. To our knowledge, there is no machine learning-based water quality model that explicitly accounts for various livestock categories at global scale. Although it has been often argued that livestock, and in particular cattle population, play a key role in water pollution, we could not identify any similar study to confirm this argument using model-based evidence. This explains why our research was needed and highlights the significance of our paper.

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