Response to Reviewer 1 (gmd-2022-222)

The manuscript provides a new global model for water quality assessment (DynQual). The model runs at a daily time step for the grid cell of approximately 10km by 10 km at the equator. The authors made a major effort to develop such a comprehensive dynamic model on a global scale. One of the model's strengths (compared to other existing large-scale water quality models) is the sector contributions (e.g., livestock, irrigation, manufacturing) to surface water pollution per grid and day while considering dynamics in pollutant routing through the river network. The model is process-based and largely uncalibrated. It makes the model more flexible to represent the processes based on characteristics (e.g., livestock number, people, runoff) and less dependent on observations (which are often scarce). In this way, there is an opportunity to apply the model for the future while considering the future characteristics of the areas. Validating the global model is not easy. The authors did a great job here and managed to validate in a good way. The manuscript is well-written, with beautiful maps and graphs. It is easy to follow the description of the model and results.

I suggest a minor revision. Below, I provide suggestions that can be helpful to improve the manuscript:

We thank the reviewer for these suggestions. The overarching theme of the comments is to further increase clarity in some sections (particularly methods and discussion). As noted by the reviewer, some of these additional descriptions are currently contained in the SI. We fully agree that some improvements can be made/ pertinent information can be moved from the SI on these points in order to further strengthen the manuscript.

Please find our point-by-point response to the detailed reviewer comments below. The more substantial additions or changes we will make to the text are indicated in this documents in *"italics".* For the more minor and editorial changes, we indicate the actions we will take in purple. Full details of these changes will be available in a manuscript with tracked changes that we will submit once the discussion period has ended.

1. Abstract: It is a nice abstract, but does not provide any insights that we learn from the model application. Please add the main messages (2-3 sentences) that reflect the two main objectives of the model application:
    1. Pattern and trends
    2. Sector contributions

True. We will add the following text to the abstract:

"Modelled output indicates that multi-pollutant hotspots are especially prevalent across northern India and eastern China, but that surface water quality issues are present across all world regions. Trends towards water quality deterioration are most profound in the developing world, particularly Sub-Saharan Africa."

Given this manuscript is submitted as a model description paper, and due to the broad scope of this manuscript: 1) introducing the DynQual model; and 2) showcasing a variety of potential applications (e.g. spatial patterns, trends, seasonality and sector-specific contributions) for multiple pollutants and at the global scale, we refrain from including more specific (e.g. pollutant specific) results from the model application – preferring the more general outlook as summarised in the text above.

2. Methods: They are described rather concisely. Details are provided in the supplementary materials, which is nice. Nevertheless, I have four suggestions to elaborate on:
    1. Figure 1: please add the legend. The description of what colors and different arrows (dashed and solid) mean is not clear;

Thanks for this. We will add a legend to Figure 1.

    2. Pollutant loadings to streams: this is well described in the supplementary information, but very concisely described in the main methods. Please add a few more sentences to tell the reader how pollutant loadings are calculated (e.g., the summary of the description from the SI). You can elaborate on the text where you mention the mass-balance approach. Here, you can briefly tell that pollutant loadings from livestock activities are simulated as a function of livestock number, excretion rates of pollutants per animal and day, and removal of pollutants during waste management practices while considering runoff from land to streams (see SI Section 1.4 for details). A similar description can be given for other sectors.
    3. Sector contribution: you do mention sectors in the methods, but briefly. Please elaborate more on what sectors exactly include and how. For example, the irrigation sector: what does it include? Which crops? rainfed irrigation? Livestock sector: which animals? I do know that some details are in the SI. But I do feel a need to give a bit more description of the main methods of the manuscript.

As noted by the reviewer, the additional descriptions on pollutant loading estimates (which directly also relate to the sectors) are currently contained in the SI. It was a deliberate choice to keep this section relatively short in the manuscript – due to the fact that pollutant loadings can alternatively be forced directly to DynQual. This provides an option for users who have pre-defined (or prefer to use their own methodology for estimating) pollutant loadings, yet still wants to make use the pollutant routing and in-stream decay components of DynQual (see point 1.2). Nevertheless, we agree with the reviewer that some pertinent information on the estimation of pollutant loadings should indeed be included in the manuscript.

We will substantially expand section 2.3 to summarise the key information with respect to pollutant loading estimates for each sector, with the following text:

"Loadings from the domestic sector are estimated by multiplying gridded population numbers with region-specific per capita excretion rates. For the manufacturing sector, a mean effluent concentration is multiplied by gridded estimates of return flows from the manufacturing sector. Gridcell specific urban surface return flows are simulated directly by PCR-GLOBWB2 and are multiplied by a region specific mean urban surface runoff effluent concentration. Gridded livestock numbers for buffalo, chickens, cows, ducks, goats, horses, pigs and sheep are multiplied by pollutant excretion rates per livestock type and by region. The livestock sector is sub-divided into 'intensive' and 'extensive' production systems based on livestock densities, in order to better account for differences in the paths by which waste enters the stream network. TDS loadings from the irrigation sector are estimated by multiplying irrigation return flows simulated by PCR-GLOBWB2 with spatially-explicit mean irrigation drainage concentrations based on electrical conductivity over the top- and sub-soil. Return flows from thermo-electric powerplants are included as a source of heat pollution by considering the temperature difference between these flows and ambient conditions."

Through also including a new table in the manuscript as per your suggestion (Table 2, see below), we hope also make the required input data for estimating pollutant loadings within a DynQual run more clear.

4. Downscaling: for example, some of the input data (e.g., livestock numbers) is regional, but DynQual requires the grid cell data. How did the authors go from regional to the grid cell, but also from annual to daily levels? Which model inputs require scaling (e.g., annual->daily; regional -> grid cell)? and which did not. This is not well elaborated. I suggest adding a few sentences on this in the main methods and giving more details in the SI. I suggest adding an overview table showing the list of model inputs and indicating which ones were aggregated from region to grid and from annual to daily.

We agree that an overview table that describes: 1) the list of model inputs per water use sector; 2) data source and 3) spatio-temporal resolution is a valuable addition to the manuscript, with the elaborated details per sector in the SI (sections 1.1 – 1.6).

We will include this in the manuscript:

Table 2. Summary of key input data used for the estimation of pollutant loadings in the presented application

Sector	**Data**	**Source**	**Spatio-temporal resolution**
Domestic	Population	(Lange and Geiger, 2020)	5 arc-min; annual
	Excretion rates	(UNEP, 2016; Van Vliet et al., 2021)	Regional; constant
Manufacturing	Manufacturing return flows	PCR-GLOBWB2 (*simulated*)	5 arc-min; daily
	Effluent concentrations	(UNEP, 2016; Van Vliet et al., 2021)	Global; constant
Urban surface runoff	Urban surface runoff	PCR-GLOBWB2 (*simulated*)	5 arc-min; daily
	Effluent concentrations	(UNEP, 2016)	Regional; constant
Livestock	Livestock populations	(Gilbert et al., 2018)	5 arc-min; annual
	Excretion rates	(Weaver et al., 2005; Wilcock, 2006; Robinson et al., 2011; Wen et al., 2017; Vigiak et al., 2019; Van Vliet et al., 2021)	Regional; constant
Irrigation	Irrigation return flows	PCR-GLOBWB2 (*simulated*)	5 arc-min; daily
	Effluent concentrations	(Batjes, 2005)	30 arc-min; constant
Power	Power return flows	(Lohrmann et al., 2019)	5 arc-min; annual
	ΔT	(Van Vliet et al., 2012a)	Global; constant

We will add some small clarifications to these sections in line with the reviewers suggestions – such as for the downscaling procedure (where appropriate).

With respect to livestock numbers explicitly, these were sourced at 5 arc-min resolution directly from Gilbert et al., (2018) for a reference year of 2010. Thus, no additional downscaling was required on this data. What was required was to account for temporal changes to livestock numbers over past years, for which we had to make a coarse assumption (regional-scale percentage changes applied equally across all gridcells within that region) based on FAO data on changes to livestock numbers in the past decades (Thomson, 2003). We will more explicitly state this in the SI and acknowledge this as an uncertainty in both the manuscript and SI.

3. Discussion: It is very concise and to the point. Some aspects can be expanded and a few aspects can be added:

1. Comparison with other studies: the authors do this for the pollutants that they consider. I also think that the manuscript will benefit if the authors add comparisons in terms of modeling approaches, pollution hotspots, and sector contributions (what new aspects are added in this DynQual model and what new aspects we learn from the model application compared to other models). The authors may consider expanding the discussion (a few sentences) on comparing their pollution hotspots not only for TDS, BOD, and FC but also for other pollutants as well because pollution hotpots often match between pollutants.

Thanks for this suggestion. We agree that a short section comparing the results from our model application (e.g. pollution hotspots) to other studies is a valuable addition to the manuscript, and will add the following text:

"Overall, our modelled spatial patterns in surface water quality match well with previous regional and global assessments – displaying multi-pollutant hotspots (e.g. TDS, BOD, FC) to be located across northern India and eastern China in particular (UNEP, 2016; Wen et al., 2017; Van Vliet et al., 2021). As demonstrated here, DynQual can be used to further enhance the understanding of the main drivers of pollutant via (dynamic) sectoral attribution. The dynamic nature of DynQual also facilitates analysis of intra- and inter- annual trends in surface water quality. Consistent with a recent data driven approach (Desbureaux et al., 2022), albeit for different water quality constituents (e.g. total phosphorus) we find a general trend towards surface water quality improvement in development countries and deterioration in developing countries."

2. Implications of the limitations: any models have limitations. DynQual has as well. Examples are livestock numbers in extensive and intensive production systems that do not vary among days, excretions rates of pollutants in manure, and human waste that are constant across the days and within the regions. I understand that sources such as open defecation, and direct discharges of manure to rivers are not considered. It is fine, but this needs to be discussed. It is important to give examples of the main limitations and reflect critically on their implications on the main conclusions of the manuscript.

Thanks for this comment. We will expand our section on model uncertainties to include more examples, including the example suggested by the reviewer with respect to constant livestock numbers.

"Being a global model, DynQual is inherently unable to represent all aspects relevant to the local context. For example, the lack of information on TDS emissions from mining activities and road de-icing. Livestock numbers in both intensive and extensive production systems are constant across the days of the year, with changes to livestock numbers only applied annually and based on regional averages, without consideration of pollutant retention in soils. Spatial mismatches between the generation of pollutant loadings and the location of discharge to the stream network can result in the simulation of unrealistic concentrations, particularly in gridcells with very low water availability (i.e. headwater streams). This can occur, for example, where the drivers of point-source pollutant emissions (e.g. population) do not directly coincide with the location of wastewater treatment plant outlets."

We will also include a section to more critically evaluate the overarching purpose and applications of these type of global scale models, providing examples of the main type of research questions that DynQual can help to investigate (see #3.3).

3. The usefulness of the model: DynQual has many useful applications (e.g., trends, patterns, future analyses, etc). The authors briefly mention this in paragraph 545. I think the authors can better emphasize how useful their model is compared to other models. For example: which scientific questions we can answer with this model that we could not answer with the previous models? The authors could add a few sentences on this in paragraph 545.

Agreed. We will include some more text in the discussion to further emphasise the types of research questions DynQual can help to address, with specific reference to the results (Figures) we present in the manuscript:

"The presented application of DynQual allows for the investigation of research questions that only large-scale modelling efforts can address, including: global hotspot identification (Figures 4 - 6), the relative importance of different sectors across the globe (Figure 7) and meta-trends in water quality dynamics (Figures 10 – 11). Our approach has particular value for simulating surface water quality in ungauged catchments, and our use of a globally consistent input data facilitates meaningful comparisons of surface water quality across different world regions."

4. Supplementary information: It is well written. I have three suggestions:
   1. Units: they are missed in some equations. For example, units are not included for the following variables: $R_{dom,i,n}$ and Pop_n (population per km^2? Total population?) in equation [1], $L_{man,i,n}$ and $R_{man,i,n}$ in equation [2], $L_{urb,i,n}$ and $R_{USR,i,n}$ in equation [3]. Please also check the variables in equations [4] and [5] and add units for every variable. This will avoid misinterpretation.

Thanks for highlighting this. We will thoroughly go through both the manuscript and the SI to check this. We will also make some small corrections to remove inconsistencies in terms used across the two documents (e.g. in the manuscript equations we denoted pollutant using *i* but in the SI using *p* – we now consistently use *p* across both documents).

We will also add the equations for estimating removal of pollutants at wastewater treatment facilities per sector (e.g. $R_{dom,i,n,}$ $R_{man,i,n}$). As these have been described extensively in previous work, we refrain from providing a full detailed description of these again here - yet we agree it is important to present the equations with the terms again here. We will also amend equations 3 and 4 as necessary to avoid misinterpretation.

   2. Livestock activities: is the number of livestock the same per day? Is this number per km^2 or ha? Did you consider soil processes and associated retentions of the pollutant in soil when you calculate loadings into the streams? All this was not very clear to me. Please clarify the description of equation 4.

Gilbert et al., (2010) provide a snapshot of global livestock numbers (for the 8 livestock types considered) with a reference year of 2010. We then apply estimates of annual change (at regional spatial scale) to livestock numbers in the past and future based on statistics from the FAO to estimate livestock numbers for the other timesteps. We will alter our sentence in the SI to make this more explicit.

Thus, yes, the number of livestock remains constant per day throughout the year. Soil processes and associated retentions of pollutants in soil are not explicitly accounted for, only the transport of pollution from this sector to streams via surface runoff. These are limitations which we will also now explicitly state in the discussion section of the manuscript (as per review comment #3.2), and areas for improvement in estimates of pollutant loadings from the livestock sector within DynQual.

3. Scaling: please elaborate on which input data required to be scaled from region to grid and from annual to daily, and how this was done.

Due to the significant overlap, we have addressed this comment in our response to comment #2.4 (i.e. Table 2). Please see above.