Response to Reviewer 2

Critical:

R2-C1

According to GMD code and data availability policy: "Where the authors cannot, for reasons beyond their control, publicly archive part or all of the code and data associated with a paper, they must clearly state the restrictions" (https://doi.org/10.5194/gmd-12-2215-2019). In the supplement python file, HydroFATE_v09.py, the imported library arcpy is not publicly available. Please state the restrictions in the code and data availability section. For example: "A license of the software provided by ... is required to run the provided scripts."

A: We acknowledge the important issue about the arcpy library not being publicly available. We updated the code and data availability section to clearly state this restriction at line 667:

"*A license of the software ArcGIS Pro provided by ESRI is required to run the provided scripts.*"

R2-C2

The method presented in Section S.1 of the supplementary material is crucial to reproducing the modeling result of HydroFATE v1.0. In essence, Section S.1 details the generation algorithm of the WWTP service area. Section S.1 should be moved to the main manuscript, perhaps in the Appendix.

A: We agree that the generation algorithm of the WWTP service area (Section S.1) is crucial to reproducing our modeling results (we originally had placed the descriptions into the SI only for space considerations). We now moved this section to the main manuscript as an appendix, to make it more accessible to readers.

R2-C3

Follow up on the previous comment on the generation of the WWTP service area. Line 242, which is in Section 3.1, reported a "successive trial-and-error approach in which intermediate results were mapped, visually inspected for plausibility, and statistically tested to verify whether they led to further improvements." I understand the difficulty of the service area generation, and it is acceptable to inspect the model visually. However, the realization of the WWTP service area is a critical part of the HydroFATE model. Hence, it is within the scope of the GMD code and data availability policy. I urge the authors to provide the scripts you use to generate the

service area since I cannot find them in HydroFATE_v09.py. (Please review Section 3.2 of the GMD editorial: https://doi.org/10.5194/gmd-12-2215-2019.) Furthermore, the sensitivity analysis in Section S.3 does not provide the sensitivity of different realizations of the WWTP service area. Therefore, it is necessary to make the service area generation process more transparent by providing the script.

A: We thank the reviewer for this comment. We understand the concern about the transparency of the WWTP service area generation process. To address this, in the revised version of the paper we will provide the script used to generate the WWTP service areas, as suggested in Section 3.2 of the GMD editorial. This will enhance the reproducibility and transparency of our work. As such, we added the following sentence at line 659:

"The code for the WWTP delineation and its output is also available under at the same URL."

Suggestions:

R2-C4

Figure 2 provides an example of the generated WWTP service area used in this study. It would be helpful to show examples of intermediate iteration results and explain why this iteration is rejected or accepted so the readers can have a gist of the visually inspected acceptance criteria.

A: We have thoroughly considered this interesting comment. While we understand the value of a more comprehensive representation of the iterative steps involved, we struggled in finding representative in-between stages that are easy to explain yet illustrative and representative for the broad range of issues that we encountered. We felt that either the figure and explanations would get overly complex, or the simplifications may cause further confusion for the reader. To stay within reasonable limitations in terms of space and detail in this publication, we therefore hope that including the script and the output in the revised paper (see previous comment and answer) will be sufficient to help readers who have an interest in applying our methodology in their own work, or to experiment with modifications to the algorithms to study the associated effects.

R2-C5

In equation (1), the removal efficiencies of wastewater treatment plants (WWTP), $e_{WWTP, j}$, contain three treatment levels, which are primary, secondary, and advanced. However, the parameters of the case study do not include such complexity. Only one removal efficiency is

used in each scenario. During the review, I have always considered WWTP treatment levels spatially varying, and they can be sensitive to the modeling result. I find the presentation of Figure 2 a bit misleading. Therefore, I suggest adding another figure in Section 4, which is based on Figure 2, but the WWTP areas are only color-coded once to represent the model better.

A: We understand and appreciate this concern. Our goal is not to mislead the reader by presenting different WWTP types in Figure 2. But we would like to emphasize that our case study, presented in Section 4, serves only as a test application of the model. In that case, regrettably, certain parameters essential for the selected substance were unavailable for inclusion in the study and some aspects of the analysis presented in Section 4 may not fully capture the complete scope of the model's capabilities. Therefore, we believe that adding another, simplified figure would not do justice to presenting the comprehensive and accurate features of the model. The model has explicitly been developed to be able to distinguish different WWTP types, it is only in the test study where we could not implement this distinction. We therefore hope that it is acceptable to leave the presentation of Section 4 as is. We would also like to point to Figure 4 which presents the WWTPs used in India, all visualized without their specific type.

Minor:

R1-C6

The unit in Figure 4 should be presented as $m^3 \, s^{-1}$.

A: As requested, we corrected the units in the caption of Figure 4 to be presented as $m^3 \, s^{-1}$.

R1-C7

Fix the unit in Figure S-3: $ng \, L^{-1}$.

A: We fixed the units in the caption of Figure S-3 to be $ng \, L^{-1}$.

R1-C8

Fix the reference error in Table S-5 of the supplement.

A: We corrected the reference error in Table S-5 of the supplementary materials.