Title

Data and Scripts Associated with the Manuscript "Water Column Respiration in the Yakima River Basin is Explained by Temperature, Nutrients and Suspended Solids"

Summary

This data package is associated with the publication "Water Column Respiration in the Yakima River Basin is Explained by Temperature, Nutrients and Suspended Solids" submitted to EGU Biogeochemistry (Laan et al. 2025). In this research, water column respiration (ERwc) data, surface water chemistry data, organic matter (OM) chemistry data, and publicly available geospatial data were used in analysis to evaluate the variability in ERwc at 47 sites across the Yakima River basin in Washington, USA.

Brief Overview of Methods

The sensor data and surface water chemistry data are associated with the previously published 2021 spatial study data packages (Fulton et al. 2022; Grieger et al. 2022); the raw data and associated metadata (including geographic locations, methods information, and protocols) can be found within each associated data package. For full references for these data packages, refer to the Citations and Acknowledgment section below. Water column respiration (ERwc) data and surface water chemistry samples were collected in triplicate at 47 sites in the Yakima River basin distributed across Strahler stream orders 2 through 7 and different biophysical settings during summer baseflow conditions in 2021. To test the transferability of study results to catchments throughout the Columbia River basin, we used cluster analysis to group catchments in the Columbia River basin into six classes sharing similar landscape characteristics using key biophysical attributes selected from readily available spatial datasets. The results were used to guide site selection. Watershed characteristics and surface water chemistry data were used to explain spatial variation in ERwc across the Yakima River basin. Please refer to Methods section in the publication for more information on the data and analyses described in the publication.

Critical Details

- 1) This data package is associated with the public GitHub repository "rcsfa-RC2-SPS-ERwc" found at https://github.com/river-corridors-sfa/rcsfa-RC2-SPS-ERwc. The repository contains all of the code (R scripts) and data to run the analyses, interpret the results, and plot the figures (excluding Figure 1) as presented in the publication. Please see the Methods section in the publication for more information on the data processing steps used to run the statistical analyses for this research.
- 2) The sensor data collection field protocol and dissolved oxygen sensor dataset used to generate water column respiration rates (ERwc) for the Yakima River basin (this study) are from the published dataset described in Fulton et al. (2022) (https://data.ess-dive.lbl.gov/view/doi:10.15485/1892052).
- 3) The surface water chemistry sample collection field protocol and water chemistry dataset (including organic matter (OM) chemistry data) used in the multiple linear regression analysis to evaluate the primary drivers of spatial variation in water column respiration rates (ERwc) across the Yakima River basin (this study) are from the published dataset described in Grieger et al. (2022) (https://data.ess-dive.lbl.gov/view/doi:10.15485/1898914).

- 4) Please see Methods sections 2.4 and 2.5 of the publication for detailed information on the analytical methods used to characterize the surface water chemistry and OM chemistry samples, respectively.
- 5) The OM biogeochemical transformation analysis was performed following methods described in Garayburu-Caruso et al. (2020) https://doi.org/10.3390/metabo10120518).
- 6) Please see the Methods section in the publication for more information on the sources for the publicly available data that were used in the cluster analysis to group Columbia River basin catchments into classes sharing key biophysical and hydrological characteristics.
- 7) The Appling et al. (2018b and 2018c) and Bernhardt et al., (2022) stream metabolism dataset was used to generate reach-scale ecosystem respiration (ERtot) data in volumetric units to compare to the water column respiration rate. Data from this research can be found at https://github.com/streampulse/metabolism_synthesis/blob/master/output_data/lotic_gap_filled.r_ds.

Data Package Structure

In addition to this readme, this data package also includes a file-level metadata (FLMD) file that describes each file and a data dictionary (DD) that describes all column/row headers and variable definitions.

The data package includes the data inputs, and outputs, and R scripts to reproduce all the analyses performed in the manuscript and create manuscript figures. The data package is comprised of three main folders (Code, Data, and Figures). The Code folder is comprised of four scripts and three analysis-specific subfolders that contain the R scripts to perform the analyses described in the publication and create publication figures. The Data folder is comprised of two ".csv" files and four subfolders that contain data input and output files. The Published_Data folder contains a readme that directs the user to download the appropriate files and add to this folder when using scripts. The Figures folder includes figures from the manuscript in ".pdf" and ".png" formats and a folder with intermediate figure files. This data package is associated with a GitHub repository which can be found at https://github.com/river-corridors-sfa/rcsfa-RC2-SPS-ERwc.

Citations, Acknowledgements, and License

Acknowledgements

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Cite this data package with the appropriate DOI. Cite the associated manuscript in any work that that uses analyses or conclusions presented in the manuscript. To cite the preprint:

Laan, M. M., Fulton, S. G., Garayburu-Caruso, V. A., Barnes, M. E., Borton, M. A., Chen, X., Farris, Y., Forbes, B., Goldman, A. E., Grieger, S., Hall Jr., R. O., Kaufman, M. H., Lin, X., Zionce, E. L. M., McKever, S. A., Myers-Pigg, A., Otenburg, O., Pelly, A. C., Ren, H., Renteria, L., Scheibe, T. D., Son, K., Tagestad, J., Torgeson, J. M., and Stegen, J. C.: Water Column Respiration in the Yakima River Basin is Explained by Temperature, Nutrients and Suspended Solids, EGUsphere [preprint], https://doi.org/10.5194/egusphere-2025-1109, 2025.

Citations

- Appling, A. P., Hall, R. O., Yackulic, C. B., and Arroita, M., 2018a. Overcoming Equifinality: Leveraging Long Time Series for Stream Metabolism Estimation, Journal of Geophysical Research: Biogeosciences, 123, 624-645. https://doi.org/10.1002/2017jg004140
- Appling, A. P., Read, J. S., Winslow, L. A., Arroita, M., Bernhardt, E. S., Griffiths, N. A., Hall, R. O., Jr., Harvey, J. W., Heffernan, J. B., Stanley, E. H., Stets, E. G., and Yackulic, C. B., 2018b. The metabolic regimes of 356 rivers in the United States, Scientific Data, 5, 180292. https://doi.org/10.1038/sdata.2018.292
- Appling, A. P., Read, J. S., Winslow, L. A., Arroita, M., Bernhardt, E. S., Griffiths, N. A., Hall, R. O., Jr., Harvey, J. W., Heffernan, J. B., Stanley, E. H., Stets, E. G., and Yackulic, C. B., 2018c. Metabolism estimates for 356 U.S. rivers (2007-2017): U.S. Geological Survey data release [dataset]. https://doi.org/10.5066/F70864KX
- Bernhardt, E. S., Savoy, P., Vlah, M. J., Appling, A. P., Koenig, L. E., Hall, R. O., Arroita, M., Blaszczak, J. R., Carter, A. M., Cohen, M., Harvey, J. W., Heffernan, J. B., Helton, A. M., Hosen, J. D., Kirk, L., McDowell, W. H., Stanley, E. H., Yackulic, C. B., and Grimm, N. B., 2022. Light and flow regimes regulate the metabolism of rivers, Proceedings of the National Academy of Sciences, 119, e2121976119. https://doi.org/10.1073/pnas.2121976119
- Fulton, S. G., Barnes, M., Borton, M. A., Chen, X., Farris, Y., Forbes, B., Garayburu-Caruso, V. A., Goldman, A. E., Grieger, S., Kaufman, M. H., Lin, X., McKever, S. A., Myers-Pigg, A., Otenburg, O., Pelly, A., Ren, H., Renteria, L., Scheibe, T. D., Son, K., Torgeson, J. M., and Stegen, J. C., 2022. Spatial Study 2021: Sensor-Based Time Series of Surface Water Temperature, Specific Conductance, Total Dissolved Solids, Turbidity, pH, and Dissolved Oxygen from across Multiple Watersheds in the Yakima River Basin, Washington, USA (v2) [dataset]. https://doi.org/10.15485/1892052
- Garayburu-Caruso, V. A., Danczak, R. E., Stegen, J. C., Renteria, L., McCall, M., Goldman, A. E., Chu, R. K., Toyoda, J., Resch, C. T., Torgeson, J. M., Wells, J., Fansler, S., Kumar, S., and Graham, E. B., 2020. Using Community Science to Reveal the Global Chemogeography of River Metabolomes, Metabolites, 10, 518. https://doi.org/10.3390/metabo10120518
- Grieger, S., Barnes, M., Borton, M. A., Chen, X., Chu, R., Farris, Y., Forbes, B., Fulton, S. G., Garayburu-Caruso, V. A., Goldman, A. E., Gonzalez, B. I., Kaufman, M. H., McKever, S. A., Myers-Pigg, A., Otenburg, O., Pelly, A., Renteria, L., Scheibe, T. D., Son, K., Torgeson, J. M., Toyoda, J. G., and

- Stegen, J. C., 2022. Spatial Study 2021: Sample-Based Surface Water Chemistry and Organic Matter Characterization across Watersheds in the Yakima River Basin, Washington, USA (v2) [dataset]. https://doi.org/10.15485/1898914
- Kaufman, M. H., Barnes, M., Chen, X., Forbes, B., Garayburu-Caruso, V. A., Goldman, A. E., Stegen, J. C., Myers-Pigg, A., and Scheibe, T. D., 2023. Geospatial Information, Metadata, and Maps for Global River Corridor Science Focus Area Sites (v2) [dataset]. https://doi.org/10.15485/1971251
- Laan, M. M., Fulton, S. G., Garayburu-Caruso, V. A., Barnes, M. E., Borton, M. A., Chen, X., Farris, Y., Forbes, B., Goldman, A. E., Grieger, S., Hall Jr., R. O., Kaufman, M. H., Lin, X., Zionce, E. L. M., McKever, S. A., Myers-Pigg, A., Otenburg, O., Pelly, A. C., Ren, H., Renteria, L., Scheibe, T. D., Son, K., Tagestad, J., Torgeson, J. M., and Stegen, J. C.: Water Column Respiration in the Yakima River Basin is Explained by Temperature, Nutrients and Suspended Solids, EGUsphere [preprint], https://doi.org/10.5194/egusphere-2025-1109, 2025
- McKay, L., Bondelid, T., Dewald, T., Johnston, J., Moore, R., and Rea, A., 2012. NHDPlus Version 2: User Guide
- Wieczorek, M. E., Jackson, S. E., and Schwarz, G. E., 2018. Select Attributes for NHDPlus Version 2.1
 Reach Catchments and Modified Network Routed Upstream Watersheds for the Conterminous
 United States (ver. 3.0, January 2021), https://doi.org/10.5066/F7765D7V

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Change History

Data Package Version	Changes
Version 1	Original data package publication
January 2024	
Version 2	Many changes were made during reprocessing and re-analyzing data prior to
July 2025	publishing the manuscript. See the GitHub commit history for details.