River Metabolism Estimation Tools (RiverMET) with Demo in the Illinois River Basin

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Abstract

Ecosystem metabolism quantifies the rate of production, maintenance, and decay of organic matter in terrestrial and aquatic systems. It is a fundamental measure of energy flow associated with biomass production by photosynthesizing organisms and biomass oxidation by respiring plants, animals, algae, and bacteria (Bernhardt et al., 2022) . Ecosystem metabolism also provides an understanding of energy flow to higher trophic levels that supports secondary and tertiary productivity, as well as helping to explain when aquatic ecosystems undergo out-of-balance behaviors such as harmful algal blooms and hypoxia. Recent advances in sensor technology and modeling capabilities have enabled estimation of aquatic system metabolism and gas exchange over long time periods in rivers, streams, ponds, and wetlands where oxygen sensors have been deployed. Here we present RiverMET, a framework for estimation of river metabolism, with workflows to streamline data preparation, run a stream metabolism model, assess the model performance, and flag and censor final output data. The workflows are specifically tailored to use streamMetabolizer, a model for one-station calculations of stream metabolism that calculates gross primary productivity (GPP), ecosystem respiration (ER) and the air-water gas exchange rate constant (K600). We advise potential users of RiverMET to review core publications for the streamMetabolizer model (Appling et al., 2018 a, b, c) to ensure best practices that produce the most useful results. We encourage feedback about our workflows, although issues regarding the streamMetabolizer model itself should be referred to the model authors. We tested RiverMET by calculating GPP, ER, and K600 across 17 river sites in the Illinois River basin (ILRB). Each river had between one and nine years of sensor data appropriate for modeling metabolism. In total, metabolism was modeled on 15,176 days between 2005 and 2020. Overall confidence in the results was rated as high at nine river sites, medium at six river sites, and poor at two river sites. Twenty-nine percent of the total modeled days had performance metrics that triggered flags. Metrics used for daily flagging are provided with the final output, with an option to only retain the censored daily outputs with high confidence (representing 72 %, i.e., 10,938 days, of the total days modeled). This work was completed as part of the U.S. Geological Survey Proxies Project, an effort supported by the Water Mission Area (WMA) Water Quality Processes program to develop estimation methods for harmful algal blooms (HABs), per- and polyfluoroalkyl substances (PFAS), and metals, at multiple spatial and temporal scales.

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Contents

1. Purpose and Scope

Ecosystem metabolism quantifies the rate of production, maintenance, and decay of organic matter in terrestrial and aquatic systems. It is a fundamental measure of energy flow associated with biomass production by photosynthesizing organisms and biomass oxidation by respiring plants, animals, algae, and bacteria (Bernhardt et al., 2022) . Ecosystem metabolism also provides an understanding of energy flow to higher trophic levels that supports secondary and tertiary productivity, as well as helping to explain when aquatic ecosystems undergo out-of-balance behaviors such as harmful algal blooms and hypoxia. Recent advances in sensor technology and modeling capabilities have enabled estimation of aquatic system metabolism and gas exchange over long time periods in rivers, streams, ponds, and wetlands where oxygen sensors have been deployed.

Here we present River*MET*, a framework for estimation of river metabolism, with workflows to streamline data preparation, run a stream metabolism model, assess the model performance, and flag and censor final output data. The workflows are specifically tailored to use *streamMetabolizer*, a model for one-station calculations of stream metabolism that calculates gross primary productivity (GPP), ecosystem respiration (ER) and the air-water gas exchange rate constant (K_{600}). We advise potential users of River*MET* to review core publications for the *streamMetabolizer* model (Appling et al., 2018 a, b, c) to ensure best practices that produce the most useful results. We encourage feedback about our workflows, although issues regarding the *streamMetabolizer* model itself should be referred to the model authors.

We tested River*MET* by calculating GPP, ER, and K_{600} across 17 river sites in the Illinois River basin (ILRB). Each river had between one and nine years of sensor data appropriate for modeling metabolism. In total, metabolism was modeled on 15,176 days between 2005 and 2020. Overall confidence in the results was rated as high at nine river sites, medium at six river sites, and poor at two river sites. Twenty-nine percent of the total modeled days had performance metrics that triggered flags. Metrics used for daily flagging are provided with the final output, with an option to only retain the censored daily outputs with high confidence (representing 72 %, i.e., 10,938 days, of the total days modeled).

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2. Description

This documentation explains theory and tools for data preparation for modeling stream metabolism as well as quality assurance and control of model results. It provides a detailed explanation of the workflows and the inputs and outputs from five R scripts, the criteria and explanation of methods of quality assurance, with examples for an application in the ILRB (Figure 1). It accompanies a data release (Choi et al., 2022) that also provides the following:

- Metadata: includes description of data column headers, units, description of source materials, and brief methods
- Readme file – a .txt file with bare bones advice for getting started

- Scripts: 5 R scripts that are used to prepare the model inputs, to execute model with quality assurance and quality control, and to post-process the model outputs

  1_Process-Data.R

  2_Prepare-Model-InputFiles.R

  3_Verify-Model-InputFiles.R

  4_Run-streamMetabolizer.R

  5_PostProcess-ModelOutputs.R

- Zip file with **input files** to script-2 of the downloaded and reorganized data files (csv format) for 17 Illinois River Basin sites and 1 hydraulic geometry coefficients file (txt format)

  Inputs**/Inputs/**5 csv files for barop.csv, disch_gage.csv, do.csv, sal.csv, temp.csv, and hydraulic_coeffs.txt

- Zip file with **output files** from script-2 and script-5 for 17 Illinois River basin sites

  ***Outputs**/outputs_from_script-2/ **34 csv model input files**, 17 from hgc (hydraulic geometry coefficient) approach and 17 from 3 different field measurement approaches, Ex) bayesInput_[date]_depth-hgc_[site_no].csv*
  */outputs_from_script-5/ outputs-A/ **21 flagged_GPP_ER_K600_[date]_depth-hgc_[site_no].csv***
  */ outputs-B/ **21 censored_ GPP_ER_K600 _[date]_depth-hgc_[site_no].csv***

3. Using Oxygen Dynamics to Estimate GPP, ER, and K_{600}

Metabolism can be estimated by tracking the rate of oxygen production and consumption in the aquatic system. Over time, the measurements of dissolved oxygen concentration can be analyzed to estimate both GPP and ER. Rates of GPP are reported in positive units, adding oxygen and organic carbon to the system, and rates of ER are reported in negative units, subtracting oxygen by consuming organic carbon to fuel organism maintenance and growth. The sum of GPP and ER is the net ecosystem productivity (NEP), a net estimate of whether oxygen and organic carbon are building up or being depleted in the system. In order to use the oxygen balance method to quantify GPP and ER in shallow waters, it is also necessary to quantify the rate of dissolved gas exchange with the atmosphere by accounting for physical effects of surface renewal as well as the dissolved oxygen difference compared to the saturated concentration for a given temperature and atmospheric pressure.

The instantaneous rate of change in dissolved oxygen [O_2] is modeled as the sum of GPP, ER, and gas exchange (Odum, 1956, expressed in volumetric rates as):

$$\frac{d[O_2]}{dt} = P_t + R_t + D_t \quad (1)$$

where $d[O_2]/dt$ is the rate of change in O_2 [mg O_2 L^{-1} d^{-1}]; P_t is the instantaneous volumetric rate of oxygen addition by gross primary production [mg O_2 L^{-1} d^{-1}]; R_t is the instantaneous volumetric rate of oxygen removal by respiration [mg O_2 L^{-1} d^{-1}]; and D_t is the instantaneous volumetric rate of air-water oxygen exchange [mg O_2 L^{-1} d^{-1}]. By the definition, P_t should be greater than or equal to zero, R_t should be less than or equal to zero, and gas exchange, D_t, can take either sign.

Recent advancements by several scientists (Holtgrieve et al., 2010; Grace et al., 2015; Appling et al., 2018a,b,c) restructured the oxygen balance expressions to facilitate the modeling of a long-term oxygen times series to estimate metabolism:

$$P_t = \boldsymbol{GPP} \times \frac{1}{\bar{z}_t} \times \frac{(t_1 - t_0) \times PPFD_t}{\int_{u=t_0}^{t_1} PPFD_u \; d_u} \tag{2}$$

$$R_t = \boldsymbol{ER} \times \frac{1}{\bar{z}_t} \tag{3}$$

$$D_t = K_{2,t} \times \left(O_{sat,t} - O_{mod,t}\right) \tag{4}$$

$$K_{2,t} = \boldsymbol{K_{600}} \times \left(\frac{S_A + S_B T_t + S_C T_t^2 + S_D T_t^3}{600}\right)^{-0.5} \tag{5}$$

where **GPP** is the daily areal average rate of primary production [g O_2 m^{-2} d^{-1}], **ER** is the daily areal average rate of respiration [g O_2 m^{-2} d^{-1}], and $\mathbf{K_{600}}$ is the daily average gas exchange rate constant normalized for molecular properties and temperature to a Schmidt number of 600 [day^{-1}]. The rate of gas exchange is the product of the rate constant and the deficit between actual and saturated concentrations of dissolved O_2. Variables with subscript *t* are instantaneous values that are typically, estimated from 15 minute interval measurements. Rather than fit $K_{2,t}$ value, the model fits K_{600}, so that only one standardized gas-exchange-related parameter per day need be reported that still captures and reflects the within-day variation in gas exchange rates caused by diel variation in temperature. Additional variables are $\bar{z}_t$, mean water depth across the width and length of the reach [m]; PPFD, photosynthetic photon flux density [µmol photons m^{-2} d^{-1}]; $O_{sat,t}$, saturated O_2 concentration [mg O_2 L^{-1}]; $O_{mod,t}$, model estimated O_2 concentration [mg O_2 L^{-1}]; $K_{2,t}$, O_2-specific and temperature specific gas exchange coefficient [day^{-1}]; T_t , water temperature [°C]; and *S,* Schmidt number coefficients: S_A=1568, S_B=−86.04, S_C=2.142, and S_D=−0.0216.

The equations are solved using a one-station modeling approach that assumes homogenous upstream conditions in GPP, ER, and gas exchange for a "metabolism length" assumed to be proportional to *v*/*K* where *v* is stream velocity and *K* is the gas exchange coefficient. The stream or water body is also assumed to be well-mixed vertically and laterally such that a single dissolved oxygen sensor accurately characterizes oxygen concentration. Also, the approach only quantifies aerobic processes and is not sensitive to anaerobic respiration processes, which may degrade the quality of results if daily average dissolved oxygen concentration declines too far below 2 mg L^{-1}.

streamMetabolizer (https://github.com/USGS-R/streamMetabolizer) and similar models take advantage of the long oxygen time series to separately identify the target variables. Simultaneously

estimating the rate of gas exchange and ER is a challenge because of overlapping sensitivities, which under the worst circumstances may produce poor estimates and also may corrupt the estimation of GPP. In general, results are much better when GPP > K, which produces strong diel variation in dissolved oxygen concentrations that increase the signal-to-noise ratio needed for the model to accurately separate and quantify GPP, ER, and K.

Users of *streamMetabolizer* have the option to use Bayesian estimation techniques that build priors based on the expectation that K_{600} will vary as a function of discharge. Gas exchange is often higher with greater discharge because of the greater stream velocity that increases turbulence and surface renewal. Sometimes the relationships are idiosyncratic with highest gas exchange at low discharge because of the greater influence of bed and bank roughness in lower flows and also because of the shallower depth. The Bayesian approach used by *streamMetabolizer* does not specify a priori the relationship between K_{600} and discharge, and its use often improves model performance (Appling et al., 2018a).

4. Site Information

Seventeen sites in the ILRB with the needed input data were used for the development and testing of metabolism modeling workflow. The upper Illinois River Basin encompasses areas of southern Wisconsin, central and northeastern Illinois, and northwestern Indiana. Site locations are shown in Figure 1 with U.S. Geological Survey National Water Information System (USGS NWIS; U.S. Geological Survey, 2021) site names, numbers, and geographic coordinates detailed in Table 1. The needed data were acquired for time periods beginning in 2005, approximately when optical dissolved oxygen sensors began being routinely deployed.

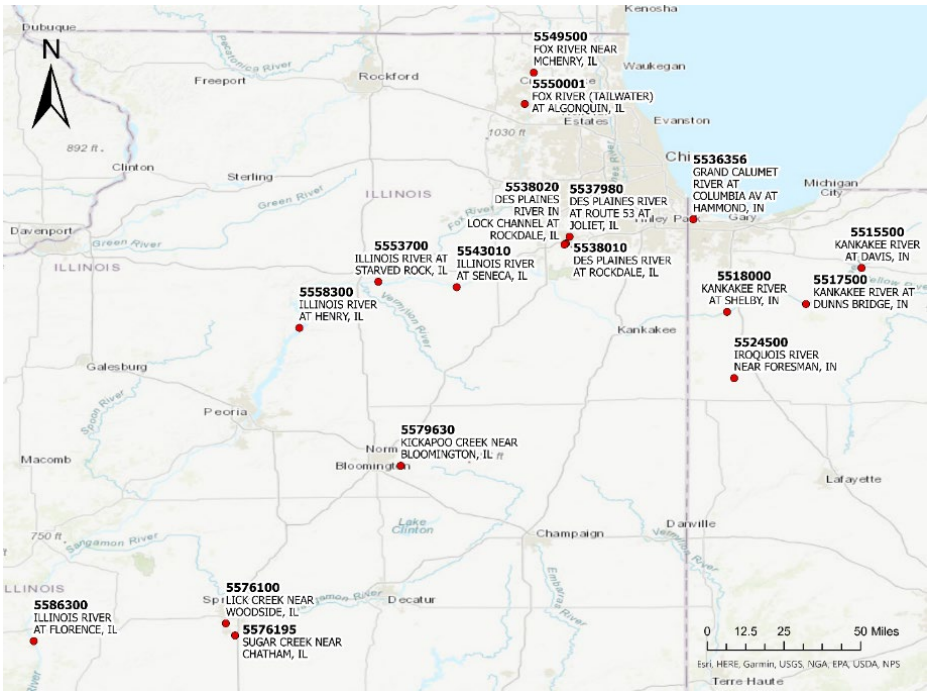

Figure 1. Seventeen sites in the Illinois River Basin (ILRB) selected for development and testing of workflows for metabolism modeling. Sites are identified by U.S. Geological Survey National Water Information System site name and number (U.S. Geological Survey 2021).

Table 1. Site name, USGS National Water Information System (NWIS) site number, and geographic coordinates of 17 study sites (U.S. Geological Survey 2021).

NWIS Site Name	NWIS Site Number	Latitude	Longitude
KANKAKEE RIVER AT DAVIS, IN	05515500	41.38964	-86.70617
KANKAKEE RIVER AT DUNNS BRIDGE, IN	05517500	41.22004	-86.96836
KANKAKEE RIVER AT SHELBY, IN	05518000	41.18281	-87.34031
IROQUOIS RIVER NEAR FORESMAN, IN	05524500	40.87059	-87.30669
GRAND CALUMET RIVER AT COLUMBIA AV AT HAMMOND, IN	05536356	41.61861	-87.49983
DES PLAINES RIVER AT ROUTE 53 AT JOLIET, IL	05537980	41.53639	-88.08250
DES PLAINES RIVER AT ROCKDALE, IL	05538010	41.50500	-88.09972
DES PLAINES RIVER IN LOCK CHANNEL AT ROCKDALE, IL	05538020	41.50000	-88.10694
ILLINOIS RIVER AT SENECA, IL	05543010	41.29972	-88.61417
FOX RIVER NEAR MCHENRY, IL	05549500	42.31002	-88.25147
FOX RIVER (TAILWATER) AT ALGONQUIN, IL	05550001	42.16194	-88.29389
ILLINOIS RIVER AT STARVED ROCK, IL	05553700	41.32476	-88.98397
ILLINOIS RIVER AT HENRY, IL	05558300	41.10722	-89.35611
LICK CREEK NEAR WOODSIDE, IL	05576100	39.71554	-89.70244
SUGAR CREEK NEAR CHATHAM, IL	05576195	39.65908	-89.65894
KICKAPOO CREEK NEAR BLOOMINGTON, IL	05579630	40.45833	-88.8775
ILLINOIS RIVER AT FLORENCE, IL	05586300	39.63278	-90.60778

5. Metabolism Modeling

A broad-brush description of the main steps in the workflow are provided here, beginning with 1) data fetching and preparation of model inputs, 2) modeling, and 3) performance assessment and censoring and flagging of model results. Figure 2 shows a flow path for the main steps, including downloading data from the USGS NWIS (U.S. Geological Survey, 2021) and from National Oceanic and Atmospheric Administration Local Climatological Data (NOAA, National Oceanic and Atmospheric Administration National Centers for Environmental Information, 2021). Included with the workflows are **Scripts 1** through **3** for processing to prepare an input date file compatible with *streamMetabolizer*, **Script 4** for modeling metabolism using *streamMetabolizer*, and **Script 5** for assessing the results to evaluate confidence, and to flag and censor the output. Also included are input and output files for the ILRB that may be used as examples for testing the workflows.

The field data were downloaded as described above from USGS NWIS and NOAA and hydraulic geometry coefficients were obtained from published literature (e.g., Gomez-Velez et al., 2015). Data were processed to create model inputs according to the format and time interval requirements of *streamMetabolizer*. Before executing *streamMetabolizer* model, the input data were validated by comparing with downloaded raw data. Both as a part of the model execution and afterwards, the model

outputs were analyzed to produce performance metrics that were assessed relative to threshold criteria to produce a rating of confidence for the overall simulation. Additional performance metrics were assessed on a daily basis and used to flag days that can be censored from final output based on criteria explained in Section 5.3.

Our workflows were developed during an application at seventeen USGS surface-water sites in the ILRB. A user who wishes to apply these scripts to other sites will need to revise them. Filenames and folder locations may need changes in several places throughout the scripts. Also, based on data availability, the approach for estimating water depth using field measurements of gage height or using hydraulic geometry equations may have to be adapted. Finally, a user should be aware that, depending on the availability of field measurements, it is sometimes beneficial to pair measurements from one site with another nearby site. For example, sites of interest with dissolved oxygen measurements in the ILRB sometimes sometimes did not have discharge measurements, and where appropriate we used discharge measurements from a "replacement" site, e.g., a nearby site on the same river without major tributaries between the locations.

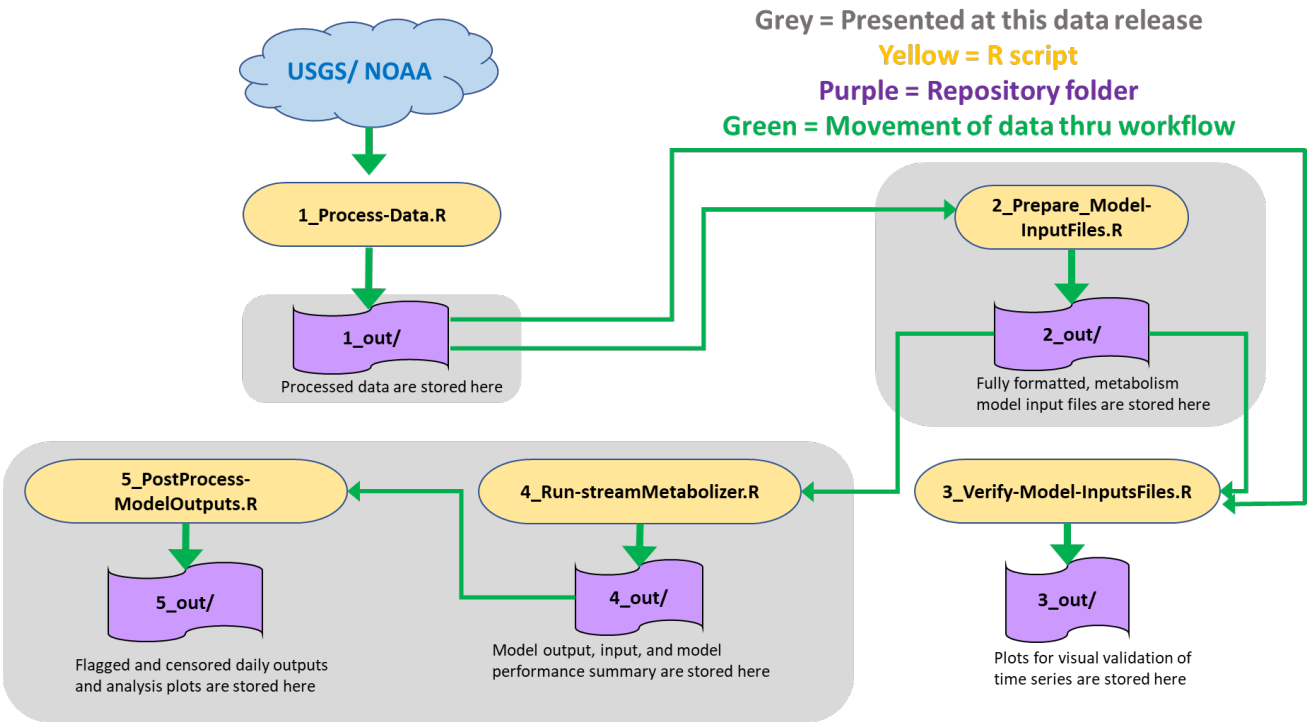

Figure 2. Workflow overview of data acquisition, preparation of input files, model execution, analysis of model results. **Scripts** are shown in yellow, and **repository folders** are shown in purple. The green arrows show **the flow of data through workflow**. This data release includes input/outputs only for grey-shaded portion of workflow.

5.1 Getting Started

- Note: All scripts provided, input/output files provided only for script-2, 4, and 5. To test and learn the scripts, we suggest that the user run script-2, 4, and 5, which is shown in Figure 3. Other scripts are optional for user's testing. Detailed explanation on all scripts can be found in Table 2. To apply these scripts to new site, user will likely run all of the scripts,

recognizing script-2 may need revision to apply to sites outside of the Illinois River Basin (see the script's comments where sites have been hard-wired in the code).

- To test script-1, first download raw data and save to folder.
    - Download these parameters from NWIS (https://waterdata.usgs.gov/nwis):
        - Dissolved Oxygen (uv): data_00300_uv
        - Temperature (uv): data_00010_uv
        - Specific Conductivity (uv): data_00095_uv
        - Discharge (uv): data_00060_uv
        - Gage height (uv, dv): data_00065_uv, data_00065_dv
    - Download pressure data from NOAA (https://www.ncei.noaa.gov/maps/lcd/)
        1. Select nearest station to NWIS site
        2. Choose "LCD CSV" (local climatological data in .csv format) and enter the desired date range
        3. Enter email address and download when complete
- To test scripts, create *user-specified folder* on local drive and download 5 scripts to *user-specified folder*:
    - 1_Process-Data.R *(optional, not used for this test)*
    - 2_Prepare-Model-InputFiles.R
    - 3_Verify-Model-InputFiles.R *(optional, not used for this test)*
    - 4_Run-streamMetabolizer.R
    - 5_PostProcess-ModelOutputs.R

  and 5 csv files and 1 text file to *user-specified folder*:
    - barop.csv
    - disch_gage.csv
    - do.csv
    - sal.csv
    - temp.csv
    - hydraulic_coeffs.txt
- Then, create following sub-folders under *user-specified folder:*

  User-specified/2_out
  /4_out
  /5_out

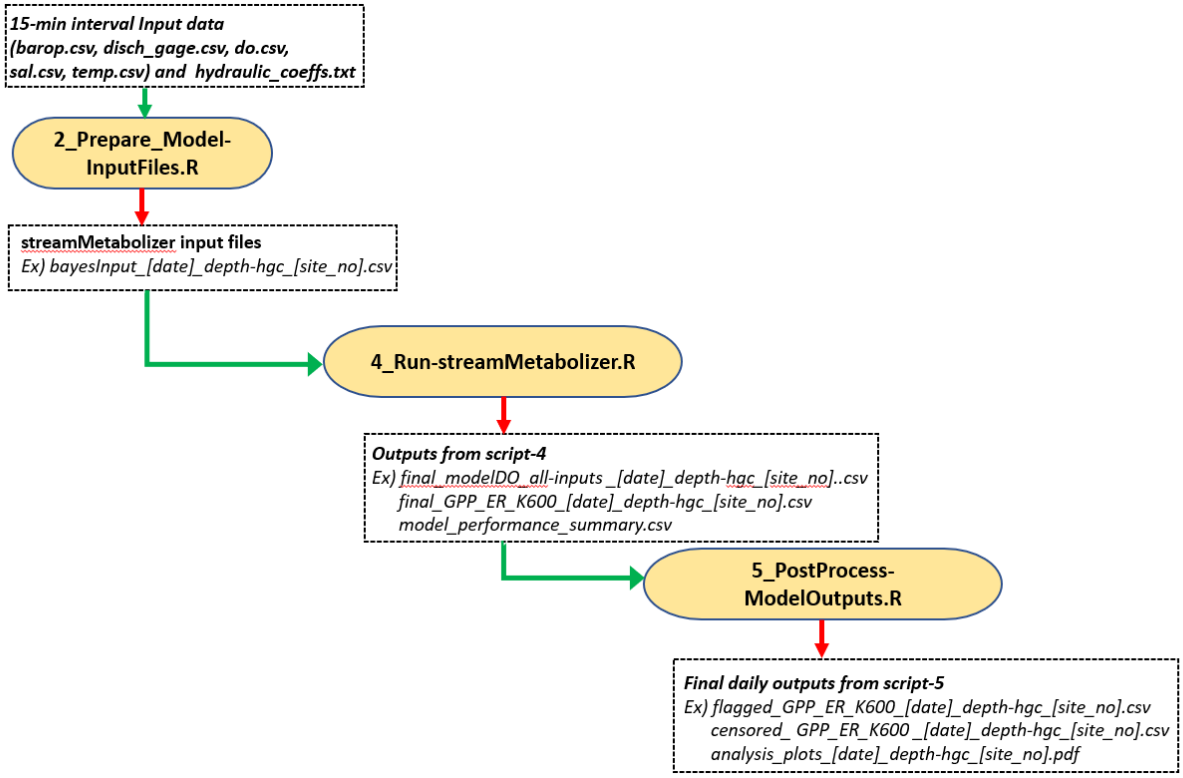

Figure 3. Flow chart explains the input/output structure with corresponding scripts and presents examples (Ex) of output files from each script.

Table 2. Summary table of the descriptions of 5 scripts

Script	Task	When to run	Details
1_Process-Data.R	Data processing & general formatting	First script to be run in the workflow to process raw data into input parameter time series	• Raw data from NWIS with multiple data streams are simplified into single entities ○ Dissolved oxygen (uv): 00300 ○ Temperature (uv): 00010 ○ Specific conductivity (uv): 00095 ○ Discharge (uv): 00060 ○ Gage height (uv,dv): 00065 • Salinity is calculated from specific conductance • Joins daily (dv) gage to gage dataframe for sites where it is the only gage data available for a site • Pressure data from NOAA is also formatted • Fills gaps that are < 3 hours with linear approximation

			• Rounds time steps of data and time matches to 15-minute timesteps beginning on the hour • Converts data to metric units when applicable
2_Prepare-Model-InputFiles.R	Model-specific formatting & calculations	Second script to be run in workflow to combine the processed time series into *streamMetabolizer* input format	• Merges dissolved oxygen, water temperature, salinity, discharge, gage height, and barometric pressure data into one data frame • Depth is calculated using two main methods: field measurements and hydraulic geometric coefficients • Convert Coordinated Universal Time (UTC) to solar time • Calculate saturated concentration of dissolved oxygen and light intensity • Visualize and export model input files
3_Verify-Model-InputFiles.R *(optional)*	Plot formatted data and processed data	Third script to be run in workflow to visually check metabolism model input time series generated from script-2	• Reads in the processed data of DO, temperature, and discharge (do.csv. temp.csv, disch_gage.csv) • Reads in data of *streamMetabolizer* input files • Plots processed data and input file data on y-axis for DO, temperature, and discharge
4_Run-streamMetabolizer.R	Run *streamMetabolizer* model	Fourth script to be run in workflow to model the site's metabolism using *streamMetabolizer* model with improving convergence through QA/QC	• Reads in the input file • Reads in the the lnQ min and max for the site's partial pooling • Runs *streamMetabolizer* model • Model re-runs if R^2 of ER-K_{600} > 0.5 (high ER-K_{600} correlation) or if Rhat > 1.1 (outside of model convergence threshold) • Exports applied input data with modeled DO, final model daily outputs, and model_performance_summary.csv
5_PostProcess-ModelOutputs.R	Flag/censor modeled outputs based on criteria and create plots for analysis	Fifth script to be run in workflow to provide cleaned modeled outputs and create plots for analysis	• Reads in model input and output file • Flags daily output that are unreliable or unrealistic

			• Exports model output .csv of flagged days and .csv where flagged days are removed • Exports pdf of plots that include GPP, ER, NEP, K_{600}, discharge, and depth; DO daily range, DO fraction saturation range, and temperature for analysis • Additional plots can be enabled

5.2 How to run the scripts

5.2.1 Prepare the input file for *streamMetabolizer*

- Open **2_Prepare-Model-InputFiles.R**.
- Set the working directory in R to the *user-specified folder*.
- If needed, edit the replacement site scheme on lines 234-236 and 276-283. If needed, edit the site for field measurements without "poor" filtering on line 333.
- Run the script.
- This script exports *parameter_summary.csv* under *User-specified/2_out/* that will be used in **4_Run-streamMetabolizer.R** for K_{600} pooling used in the model.
- The script creates 4 sub-folders under *User-specified/2_out/* using these methods to calculate water depth, described in Table 3:
    1. field measurements ('depth-fieldmeas')
    2. hydraulic geometry coefficients ('depth-hgc')
    3. field measurements from a replacement site ('depth-repfieldmeas')
    4. field measurements without "poor" rating filtering ('depth-poorfieldmeas')
- The script processes the various field collected data according to the format and time interval suitable for *streamMetabolizer*, shown in Figure 4. The resultant *streamMetabolizer* input files (csv) will then be stored in above 4 sub-folders according to the applied water depth estimation approaches. Plots of the parameters can also be exported with the input files if chosen.

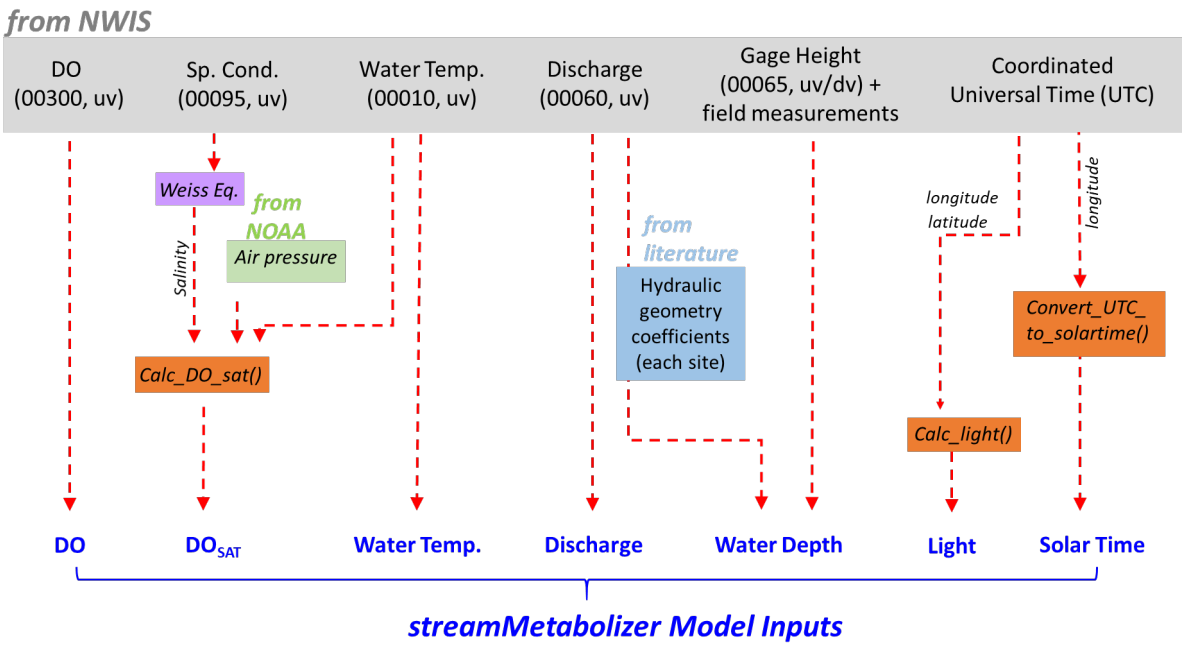

Figure 4. Activities of Script **2_Prepare-Model-InputFiles.R** in preparing the input file for **4_Run-streamMetabolizer.R** by assembling downloaded data and applying functions to estimate the input parameters and final input time series for model execution. Numbers are parameter codes and dv and uv are the data types that refer to daily and instantaneous values, respectively, from the National Water Information System (NWIS).

Table 3. Summary of water depth estimation methods in script 2

Water depth estimation	**Description**
depth-fieldmeas	Where local gage height reflects upstream conditions, use linear regression between field measurements of water depth and gage (poorly rated and negative-value field measurements are excluded) to estimate depth based on measured gage height
depth-hgc	Where local gage height does not reflect well the upstream conditions, e.g., channel at gage height location often is narrower than upstream channel, use hydraulic geometry coefficients (*C* and *F* from hydraulic_coeffs.txt) $Water\ Depth = C \cdot (discharge)^F$
depth-repfieldmeas	When no field measurements are available for a site, same linear regression as depth-fieldmeas is used, but field measurements are from a nearby NWIS site on same river where field measurements are available
depth-poorfieldmeas	When only poorly rated field measurements are available for a site and a nearby alternative with representative field measurements is not available, same linear regression as depth-fieldmeas is used, but poorly rated field measurements are not excluded

5.2.2 Run *streamMetabolizer*

- Open **4_Run-streamMetabolizer.R**.
- Set the working directory in R to the *user-specified folder*.
- Change the file name on line 88 to: *[sub-folder name under 2_out]/[input file name.csv].* We recommend using: *[depth-hgc/…depth-hgc_05536356.csv] for a test input file.*
- Run the script.
- The script exports the applied input data with modeled DO, final model daily outputs (GPP, ER, K_{600}), and model_performance_summary.csv to *User-specified/4_out/.*
- NOTE: For site 05576100, we used the absolute value of discharge for the input file 'bayesInput_2021-12-23_depth-fieldmeas_05576100.csv' to have more valid days for modeling.

5.2.3 Flag/censor model outputs & Create plots to analyze metabolism estimates

- Open **5_PostProcess-ModelOutputs.R**.
- Set the working directory in R to the *user-specified folder*.
- Specify the file names of exported files from script **4_Run-streamMetabolizer.R** on line 43 and 44 for the site you want to analyze the model results. For example: *'final_modelDO_all-inputs_2022-01-24_depth-hgc_05536356.csv'* at line 43 and *'final_GPP_ER_K600_2022-01-24_depth-hgc_05536356.csv'* at line 44.
- Plots of the inputs and modeled outputs can be enabled starting at line 116 to the end. If you wish to plot censored daily output instead of flagged daily output, enable line 126 and 280.
- Run the script.
- The flagged and censored model daily output (csv) and optional analysis plots (pdf) will be stored in *User-specified/5_out/*. The description of flagging and censoring is presented in Section 5.3.3.

5.3 Model Confidence Assessment, and Flagging and Censoring of Results

5.3.1 Evaluation of overall model confidence using performance metrics

The confidence in model performance was rated Low, Medium, or High based on assessment of performance metrics that were calculated within script-4 and that are reported in the **model_performance_summary** output file. The performance metrics are defined and summarized below with further explanation of the thresholds and scoring of performance given in Table 4.

- **coefficient of determination of modeled oxygen, R^2_{det},** is an estimation of signal strength relative to noise, where noise includes both process and observation error:

$$R^2_{det} = 1 - \frac{\sum_j^N \left(O_{det,j} - O_{obs,j}\right)^2}{\sum_j^N \left(O_{obs,j} - \frac{1}{N}\sum_j^N O_{obs,j}\right)^2}$$

where O_{det} is model's prediction and O_{obs} is observation. R^2_{det} was computed daily and then summarized as the percentage of days with $R^2_{det} < 0.5$.

- **biologically unrealistic estimates of GPP, e.g., negative GPP**. GPP was estimated daily and its magnitude was summarized as the percentage of days with GPP < -0.5.

- **biologically unrealistic estimates of ER, e.g., positive ER.** ER was estimated daily and its magnitude was summarized as the percentage of days with ER > 0.5.

- **physically unrealistic values of estimated K_{600}.** K_{600} was estimated daily and its magnitude was summarized in two ways to assess model confidence for a river of a given size. The metrics were (1) 90th percentile of estimated K_{600} and (2) difference between 90^{th} and 10^{th} percentile K_{600}, both of which were compared with threshold values.

- **Potential scale reduction statistics (Rhat)** indicates whether the chains of an MCMC (Markov Chain Monte Carlo) algorithm have converged. This is a measure of whether there is similar variance within and among chains after discarding the warmup samples (Brooks & Gelman, 1998; Gelman & Rubin, 1992). We used the maximum value of 2 different Rhat values associated with K_{600} (Rhat_K600_sigma) and process-error (Rhat_process_error), and compared it with a threshold Rhat value of 1.2 to assess confidence.

- **Presence of flow regulation near the site**, such as dams, locks, flow reversals, aeration bubblers, and water retention features. For each site, we used the type of flow regulation located upstream and distance to monitoring site to evaluate the confidence level.

Using the performance metrics described above, we built 7 criteria with thresholds and score weighting that resulted in low, medium, and high confidence assessments for each criterion (Table 4). Some of the selected criteria follow those used by Appling et al. (2018b), e.g., Appling et al.'s criteria using presence of biologically unrealistic GPP and ER values, variation in predicted K_{600}, and model convergence statistics (Rhat) (criteria 2, 3, 5, and 6 in Table 4). However, in the case of percent of days with biologically unrealistic GPP and ER, we applied more stringent thresholds (Table 4). In addition, we added criteria concerning the presence of days with low R^2_{det}, unrealistically high K_{600}, and proximity to flow regulation (criteria 1, 4, and 7 in Table 4). Based on a pre-determined score weighting assigned to each criterion, we summed the 7 criteria to classify overall model performance as either Low (total score < 3.75), medium (3.8 ≤ total score ≤ 5.6), or high (total score > 5.6).

Table 4. 7 Model performance metrics with score weighting and thresholds for low, medium, and high confidence for each metric and for overall confidence assessment.

Model assessment criteria:	Score weighting	Low confidence	Medium confidence	High confidence
Criteria 1: Percent of days where $R^2_{det,d}$ < 0.5	1.0	>75%	50-75%	< 50%
Criteria 2: Percent of days with Gross Primary Productivity (GPP) < -0.5	1.0	>33%	10-33%	<10%
Criteria 3: Percent of days with Ecosystem Respiration (ER) > 0.5	0.5	>33%	10-33%	<10%

Criteria 4: 90th percentile of K_{600} , air-water gas exchange constant	1.0	>20	Large river: 4-20; stream/small river: 10-20	large river: <4; stream/small river: <10
Criteria 5: Range [90th-10th percentile] of K_{600}, air-water gas exchange constant	1.0	>50	15-50	<15
Criteria 6: Max(Rhat_K600_sigma, Rhat_process_error), see section 5.3.1 for explanation	1.0	>1.2		≤1.2
Criteria 7: Near flow regulation flag	2.0	Structure within 2 miles up/down stream of site	Structure within 2-10 miles up/down stream of site	No structure within 10 miles up/down stream of site
Overall Confidence: **High**: Report results with a high level of confidence **Medium**: exercise judgement before reporting **Low**: disqualify results or report with caution	7.5	<3.8 (<50% of 7.5)	3.8-5.6 (50-75% of 7.5)	>5.6 (>75% of 7.5)

5.3.2 Final Confidence assessment on ILRB model output at 17 sites

The results of the confidence assessment for the 17 ILRB sites are presented below (Table 5). Confidence is based on the weighted sum of scores generated using 7 performance metrics and associated thresholds. The resulting color coding indicates high-confidence (green), medium-confidence (yellow), and low confidence (red). Comments are provided to explain factors that were particularly important in scoring and that may affect use of the final results.

Table 5. Summary of model confidence assessment for the modeled 17 sites in ILRB

NWIS Site Name	NWIS Site Number	Water depth estimation method	Discharge estimation notes	Comment
KANKAKEE RIVER AT DAVIS, IN	05515500	Field measurements		High confidence: Report results with a high level of confidence
KANKAKEE RIVER AT DUNNS BRIDGE, IN	05517500	Field measurements		High confidence: Report results with a high level of confidence
KANKAKEE RIVER AT SHELBY, IN	05518000	Field measurements		High confidence: Report results with a high level of confidence
IROQUOIS RIVER NEAR FORESMAN, IN	05524500	Field measurements		High confidence: Report results with a high level of confidence

GRAND CALUMET RIVER AT COLUMBIA AV AT HAMMOND, IN	**05536356**	Hydraulic geometry coefficients	Calculated discharge from regression of discrete gage and discharge	**High confidence**: Report results with a high level of confidence
DES PLAINES RIVER AT ROUTE 53 AT JOLIET, IL	**05537980**	Field measurements		**Medium confidence: Exercise judgement** (most metrics good but low signal:noise ratio of input data was indicated)
DES PLAINES RIVER AT ROCKDALE, IL	**05538010**	Hydraulic geometry coefficients	Replacement discharge used (05537980)	**Medium confidence: Exercise judgement** (above threshold % of days with positive ER)
DES PLAINES RIVER IN LOCK CHANNEL AT ROCKDALE, IL	05538020	Hydraulic geometry coefficients	Calculated discharge from regression of discrete gage and discharge	**Low confidence: Recommend Disqualification** (dam has a significant spillway located a short distance upstream that reaerates water column)
ILLINOIS RIVER AT SENECA, IL	05543010	Replacement field measurements used (05543500)	Replacement discharge used (05543500)	**Low confidence: Use with Caution** (above threshold % of days with positive ER and unrealistically high gas exchange; those days can be censored but quality of remaining results may be compromised)
FOX RIVER NEAR MCHENRY, IL	**05549500**	Field measurements	Calculated discharge from regression of discrete gage and discharge	**Medium confidence: Exercise judgement** (potential difficulty with model convergence)
FOX RIVER (TAILWATER) AT ALGONQUIN, IL	**05550001**	Field measurements		**Medium confidence: Exercise judgement** (flow regulation 2 km upstream is a potential concern)
ILLINOIS RIVER AT STARVED ROCK, IL	**05553700**	Hydraulic geometry coefficients	Replacement discharge used (05543500)	**Medium confidence: Exercise judgement** (most metrics good but low signal:noise ratio of input data was indicated)
ILLINOIS RIVER AT HENRY, IL	**05558300**	Hydraulic geometry coefficients		**High confidence**: metrics good but potential for channel exchange with large upstream ponds noted
LICK CREEK NEAR WOODSIDE, IL	**05576100**	Field measurements		**High confidence**: metrics good but low flow, and frequent reversals of flow direction, may indicate mixing with downstream pond

SUGAR CREEK NEAR CHATHAM, IL	**05576195**	Field measurements		**High confidence: Report results with a high level of confidence**
KICKAPOO CREEK NEAR BLOOMINGTON, IL	**05579630**	Field measurements		**Medium confidence: Exercise judgement** (potential difficulty with model convergence. Also, potential for channel exchange with wetland through upstream diversion)
ILLINOIS RIVER AT FLORENCE, IL	**05586300**	Field measurements	Calculated discharge from regression of discrete gage and discharge	**High confidence: Report results with a high level of confidence**

5.3.3 Flagging/censoring on daily model output

The model daily outputs (GPP, ER, K_{600}) from *streamMetabolizer* were evaluated using 4 criteria that are reported daily (Table 6) for potential flagging and censoring. For each criterion, we flagged daily output for violating the described conditions, and we provide censored daily output that eliminates days with any flag.

Table 6. Criteria on flagging /censoring of daily output (GPP, ER, and K_{600})

Flag	Description	Conditions
Flag 1	low SNR and/or poor fit	flag and censor daily values if (15th percentile of daily R^2_{det} < 0) and ($R^2_{det,d}$ < 15th percentile of daily $R^2_{det,d}$ values)
Flag 2	biologically unrealistic GPP	flag and censor daily values with GPP_d < -0.5
Flag 3	biologically unrealistic ER	flag and censor daily values with ER_d > +0.5
Flag 4	too high K_{600}	flag and censor daily values if $K_{600,d}$ > 20

5.4 Results

Metabolism results are summarized for sixteen sites for time periods ranging between a half a year and five years (Table 7). Most sites tended toward heterotrophy, where the average magnitude of ecosystem respiration (ER) exceeded the gross primary productivity (GPP). Heterotrophy is a common condition for streams and small rivers where light may be limited and where abundant inputs of organic carbon from the surrounding landscape fuel respiration. Notably there was a site in one river (Fox River near McHenry, Il) where autotrophic conditions were typical, with more organic carbon produced by photosynthesis than was consumed by respiration. Another Fox River site and several Illinois River mainstem sites had indicators that they were at times autotrophic. Autotrophy occurs in rivers especially if they are wide and therefore unshaded, and if at times they have a water clarity that is conducive to blooms of planktonic algae. A more in-depth examination of metabolism patterns in the Illinois River basin may reveal indicators of excessive algal blooms and associated harms such as hypoxia.

Table 7. Censored metabolism model results summary table showing number of days modeled, average and standard deviation of GPP, ER and K_{600} of 16 sites

NWIS Site Name	NWIS Site Number	Number of days modeled	Average GPP (standard deviation)	Average ER (standard deviation)	Average K_{600} (standard deviation)
KANKAKEE RIVER AT DAVIS, IN	05515500	1629	1.01 (0.85)	-5.42 (2.11)	2.30 (0.79)
KANKAKEE RIVER AT DUNNS BRIDGE, IN	05517500	554	0.59 (0.51)	-4.23 (1.90)	2.47 (1.40)
KANKAKEE RIVER AT SHELBY, IN	05518000	1314	0.45 (0.69)	-3.78 (2.28)	1.73 (0.47)
IROQUOIS RIVER NEAR FORESMAN, IN	05524500	437	2.48 (3.56)	-5.78 (3.84)	2.10 (0.82)
GRAND CALUMET RIVER AT COLUMBIA AV AT HAMMOND, IN	05536356	167	1.64 (0.79)	-2.56 (0.96)	1.38 (0.70)
DES PLAINES RIVER AT ROUTE 53 AT JOLIET, IL	05537980	767	3.76 (2.07)	-8.78 (2.21)	1.57 (0.28)
DES PLAINES RIVER AT ROCKDALE, IL	05538010	174	0.70 (1.15)	-7.57 (3.06)	3.85 (1.10)
ILLINOIS RIVER AT SENECA, IL	05543010	337	4.14 (3.49)	-8.01 (6.06)	7.88 (5.69)
FOX RIVER NEAR MCHENRY, IL	05549500	351	8.64 (5.04)	-7.79 (4.22)	1.67 (0.09)
FOX RIVER (TAILWATER) AT ALGONQUIN, IL	05550001	351	5.62 (3.01)	-6.83 (4.19)	3.13 (1.26)
ILLINOIS RIVER AT STARVED ROCK, IL	05553700	398	4.87 (4.33)	-5.17 (4.82)	6.80 (4.67)
ILLINOIS RIVER AT HENRY, IL	05558300	444	2.46 (2.29)	-7.44 (4.55)	3.65 (1.09)
LICK CREEK NEAR WOODSIDE, IL	05576100	417	2.89 (3.03)	-7.62 (3.39)	0.49 (0.22)
SUGAR CREEK NEAR CHATHAM, IL	05576195	234	2.39 (2.29)	-7.46 (4.54)	1.57 (0.68)
KICKAPOO CREEK NEAR BLOOMINGTON, IL	05579630	1158	2.32 (2.35)	-3.61 (2.85)	6.24 (2.18)
ILLINOIS RIVER AT FLORENCE, IL	05586300	1851	2.26 (2.28)	-6.18 (4.37)	0.72 (0.17)

6. Appendix

6.1 Parameters & Pcodes

* A complete list of USGS pcodes can be found here.

Parameter	Pcode	Definition	Utilization by *streamMetabolizer*
Dissolved Oxygen	00300	Dissolved oxygen, water, unfiltered, milligrams per liter	• Estimate GPP and ER
Specific Conductance	00095	Specific conductance, water, unfiltered, microsiemens per centimeter at 25 degrees Celsius	• Convert to salinity, then used to calculate dissolved oxygen saturation
Water Temperature	00010	Temperature, water, degrees Celsius	• Calculate dissolved oxygen saturation
Discharge	00060	Discharge, cubic feet per second	• Optional parameter • Binning K_{600} estimates
Gage Height	00065	Gage height, feet	• Estimate depth

6.2 Calculated Parameters

Parameters	Units	Calculation description and package::function(s) used	Required Inputs
Oxygen Saturation	percent (%)	streamMetabolizer::calc_DO_sat()	water temperature, air pressure (from NOAA), salinity
Light Intensity	photon density ($\mu mol\ m^{-2}\ s^{-1}$)	streamMetabolizer::calc_light()	solar time, latitude, longitude
Solar Time	Mean solar (exactly 24 hours between solar noons)	streamMetabolizer::convert_UTC_to_solartime()	time in Coordinated Universal Time (UTC), longitude
Water Depth	meters	Linear rating curve relating field measurements (obtained from dataRetieval::readNWISmeas()) of depth and stage height or using the Harvey Equation ($d = c*(Q)^f$) where c and f are hydraulic geometry coefficients and Q is continuous discharge	Required for dataRetieval::readNWISmeas(): 1. USGS site number 2. start date 3. end date Required for rating curve (result of dataRetieval::readNWISmeas()) 1. channel width 2. channel depth 3. channel discharge 4. channel velocity 5. gage height

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