# **Exercise 13 – Water Quality Calibration**



**BASINS/HSPF** Application Steps



This exercise is a continuation of Exercise 12, which provided an introduction to modeling nutrients, biochemical oxygen demand (BOD), dissolved oxygen (DO), and algae. In this exercise, we will focus on calibrating these constituents by adjusting key parameter values. Our goal is to 'tune' our model results so that they are similar to available observed data (or to expected/reasonable ranges for parameters for which there aren't field observations).

This exercise will help you gain a better understanding of how the watershed 'works' (as represented by the model) by assessing the degree to which non-point sources, point sources and instream processes account for observed concentrations at the watershed outlet. This exercise is divided into three sections, in which we will attempt to calibrate water quality by: (1) adjusting ONLY non-point sources, (2) adjusting ONLY instream parameters, and (3) adjusting BOTH non-point source loadings and instream parameters.

In Exercise 12, we did a rough sensitivity analysis for some key parameters that affect nutrient, algae, and dissolved oxygen concentrations. In this exercise, we will quantify how well we are simulating various constituents by comparing our results with either observed instream concentrations or export coefficients.

## Questions addressed in this exercise:

- 1.) How do I determine whether I am over-predicting or under-predicting nutrient loads and instream concentrations?
- 2.) How do I calibrate the non-point source loads coming from the watershed?
- 3.) How do I calibrate the instream portion of my model so that simulated instream concentrations are similar to observed instream concentrations?
- 4.) If I am still over-simulating or under-simulating various constituents and I have adjusted instream calibration parameters within their limits, what do I do now?
- 5.) What are the steps required for water quality calibration?

# A. Examining Initial Model Results

# **QUESTION ANSWERED:**

# 1.) How do I determine whether I am over-predicting or under-predicting nutrient loads and instream concentrations?

In this section, we will open a WinHSPF input file, run the HSPF, and then assess the

simulation results by looking at plots, utilizing the "Compare Timeseries" tools to view statistics, and by opening and examining the report files generated by the model. Because of time constraints, we will look primarily at total nitrogen loadings from land use segments and at nitrate concentrations instream. In your own models, you should examine, assess, and calibrate all of the modeled constituents carefully.

To ensure that everybody begins this exercise with the same input values, we will open a new \*.*uci* file. This file is identical to the one you opened in Exercise 12, except that it includes initial estimates for the nutrient-related input parameters.

- 1. If WinHSPF isn't already open, from the **Start** menu under **Programs**, select **BASINS** and then **WinHSPF**.
- 2. From the **File** menu, select **Open**.
- 3. Navigate to *c:\basins\modelout\wq\_cal* and select "*wq\_cal.uci*." Click OPEN.
- 4. Click (Run HSPF).
- 5. Click (View Output through GENSCN).
- 6. Click the "HSPF Output" tab.
- 7. Check the box beside "*c:\basins\modelout\wq\_cal.wdm*."
- 8. Click OK.

A convenient feature of GenScn is the ability to plot multiple water quality constituents at once on multiple plots. This feature is especially useful when performing a water quality calibration, as you will want to see the effect a particular parameter change has on each modeled water quality constituent. To familiarize you with this tool, we will plot various constituents using the "Multiple WQ Plots" option in the following steps.

9. In the "Scenarios" frame, select "OBSERVED" and "WQ\_CAL."

- 10. In the "Constituents" frame, select "NO3," "PO4," and "TW."
- 11. Click the "Add to time series list" button,
- 12. Click (Generate Graphs).
- 13. Click YES when the following window appears.



14. Check the box beside "Multiple WQ Plots."



15. Click GENERATE. The following three plots should appear.





- 16. Close all three plots.
- 17. Click CANCEL.

In the following steps, we will focus only on nitrate. We will plot the simulated and observed instream nitrate in Reach 5. This will help us quantify how well we are simulating nitrate.

- 18. In the "Scenarios" frame, select "OBSERVED" and "WQ\_CAL."
- 19. In the "Constituents" frame, select "NO3."
- 20. Click the "Add to time series list" button,
- 21. Plot the simulated nitrate (NO<sub>3</sub><sup>-</sup>) and the observed nitrate (NO<sub>3</sub><sup>-</sup>) data in for the entire time period and in one-year increments to visually examine how well we are simulating nitrate. Your plots should look similar to the following:





Examine the plots. Are we consistently under-predicting or over-predicting nitrate? Are we doing reasonably well during one season, but over-predicting or under-predicting in another?

The plots indicate that for most years, we are estimating nitrate concentrations fairly well during the summer months (June – September), but that we are overestimating nitrate concentrations during all other seasons. Keep this in mind as you adjust key parameters in the next section.

- 22. Close the plot(s) and the "Graph" window.
- 23. Change the values in the "Dates" frame to the following:

Dates			
Basat	Start	End End	
neset	Jian		
Current	1986 1 1	to 1986 12	31
Common	1985 10 1	to 1988 9	30

24. Highlight both the observed and simulated nitrate timeseries in the "Timeseries" block (if they are not already selected) and click the "Compare Two Timeseries" **木木** but

tton, 🚾, in the "Analysis" frame. The "Gen	enScn Compare" window v	will open:
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GenScn Compare				
Compare Analysis for OBSERVED NO3 at UPMARLBR and WQ_CAL NO3 at RCH5				
Class <u>L</u> imits	Select Statistics	<u>R</u> esults		
Defaults Avail   C Arithmetic 0   Image: Comparity 1.3 1.8   Number: 35 2.3 3.1   Lower: 1 5.3 4   Upper: 10000 1.99   Missing Values -99   Second Time series: -99	able Active Active →>> -2 -2 -2 -2 -2 -2 -2 -2 -2 -2	FORTRAN Compare F90 Compute F90 Results F90 Output File		
S <u>w</u> ap Sa <u>v</u> e Results	Save Specs <u>G</u> et Specs	Clear Specs Close		

The observed nitrate  $(NO_3^{-})$  timeseries contains values for only 29 days in 1986, so there are 336 days for which there are no data values. For each day on which there is no data available, the corresponding record has a value of "-999." as shown in the window below:

🙀 Timeseries Data		۲
<u>File E</u> dit		
Scenario	OBSERVED	•
Location	UPMARLBR	
Constituent	NO3	
1986/01/09	-999.	
1986/01/10	-999.	
1986/01/11	-999.	
1986/01/12	-999.	
1986/01/13	0.403	
1986/01/14	-999.	
1986/01/15	-999.	
1986/01/16	-999.	
1986/01/17	-999.	al
1005/01/10	000	2

Note: This window will **not** appear on your screen. You can view this window by clicking the "List Timeseries" button, [222], in the main GenScn window.

Because the "Compare Timeseries" tool compares values for only days on which both the observed  $NO_3^-$  timeseries and the simulated  $NO_3^-$  timeseries contain values, we must specify the missing value indicator (-999.).

- 25. In the "Missing Values" frame, enter "-999." in the cell corresponding with the observed nitrate time series (see note below). You don't need to change the number in the other cell because it corresponds to the simulated nitrate timeseries, which has no missing values. Leave all other inputs in the "Class Limits" tab as they are because we will not be using any other values here.
  - **Note:** The cell that corresponds with the *observed* nitrate timeseries depends on the order in which the observed and simulated nitrate timeseries appear in the "Time Series" frame in the main GenScn window. In the following example, you would enter "-999" in the "First Time Series" box within the "Missing Values" frame because the *observed* nitrate timeseries is listed above the *simulated* nitrate timeseries.



26. Click the "Results" tab. The table should look like the following:

Compare Analysis for OBSERVED NO3 at UPMARLBR and WQ_CAL NO3 at RCH5									
$\square$	- Class <u>L</u> ir	nits	ts <u>S</u> elect Statistics				<u>R</u> esults		
Class	Count 1	Count 2	Percent 1	1 Percent 2 Mean 1		Mean 2	Geometric Mean		
Total	29	365	7.95	100.00	0.30	1.29	0.23		

**Note:** Scroll to the right and notice that many typical statistics are displayed. Some of the statistics (count, percent, mean, geometric mean, and standard deviation) are calculated separately for each of the two timeseries. These statistics can be helpful in determining how well you are simulating each constituent. The numbers (1 and 2, next to the headings) correspond to the order of the time series (see above note).

The other statistics (correlation coefficient, coefficient of determination, etc.) compare the two timeseries. These may or may not be useful since water quality data are usually limited in number. The user must determine whether these numbers accurately represent the correlation between the observed and simulated nitrate given the number of observations available for the period of time being simulated.

- **Note:** You may want to look at the standard deviations for each time series. To do this, click on the "Select Statistics" tab. In the "Available" list, hold down the SHIFT key while you select "Std Devation 1" and "Std Devation 2." Click ADD (they will be added to the "Selected" list). Click the "Results" tab to see the calculated standard deviations.
- 27. Close the "GenScn Compare" window.

Now that we have a better understanding of the simulated nitrate in the stream, we will determine whether our total nitrogen loads from the land use segments are reasonable. We will open a report that will display the simulated loading fluxes (lbs/yr/acre) for each land use segment for several constituents. We will compare the values found in the reports to export coefficients to examine how well we are simulating total nitrogen loads from the land use segments.

- 28. From the **Analysis** menu, select **Run Script**.
- 29. Navigate to c:/basins/models/hspf/bin and select "GenScnWatershedSummary.spt."
- 30. Click OPEN.
- 31. In the "Script Arguments" window enter "wq\_cal" in the "CurScenario" box,

"TotalN" in the "gCurConstituent" box, and " $c: BASINS Modelout wq_cal$ " in the "InputDir" box.

**Note:** Be sure to use the same capitalization for the constituent name and include the backslash at the end of the input directory path.

#### 32. Click OK.

When the script completes, a file named "*wq\_cal.TotalN.Watershedsummary.txt*" will open. Among other things, this report shows the annual load (lbs/acre/year) for each land use segment for each constituent.

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<u>E</u> le <u>E</u> dit F <u>o</u> rmat <u>V</u> iew <u>H</u> elp	Elle Edit Format View Help							
Watershed Summary Report for Sc Run Made 2005-08-15 14:53 Average Annual Rates and Tot UCI Created by WinHSPF for w Time Span: 1 yr from 10/01/8	enario [wq als estpat 5 to 10/01	_cal] /86						
TotalN								
Land Use	Perv. lbs/acre	Imperv. lbs/acre	Eff.Imp.	Combined lbs/acre	Area acres	Total lbs	% GrTot.	
UPMARLBR,PI:PETINP=0.8 Forest Land Urban or Built-up La Agricultural Land Barren Land Wetlands	1.634 1.220 5.764 3.957 1.564	0.000 72.713 0.000 0.000 0.000	0% 5 0% 0% 0%	1.634 36.967 5.764 3.957 1.564	17,320 13,414 21,402 1,420 4	28,307 495,869 123,367 5,619 6	4.3% 75.9% 18.9% 0.9% 0.0%	
Seg Wtd Aver/Tot	3.532	72.713	13%	12.195	53,560	653,170	100.0%	
Totals for all Non-Point Source Forest Land Urban or Built-up La Agricultural Land Barren Land Wetlands	Segments 1.634 1.220 5.764 3.957 1.564	72.713	0% 5 0% 0% 0%	1.634 36.967 5.764 3.957 1.564	17,320 13,414 21,402 1,420 4	28,307 495,869 123,367 5,619 6	4.3% 75.9% 18.9% 0.9% 0.0%	
Non-Pnt Wtd Aver/Tot	3.532	72.713	13%	12.195	53,560	653,170	100.0%	
Point Sources WESTERN BRANCH_WWTP						0	0.0%	
Point Wtd Aver/Tot						0	0.0%	
Reaches R1 Upper Western Br R6 North Collington						206,537 66,225	31.6% 10.1%	
<b>   </b>							]	

In order to evaluate how well we are modeling water quality, we need to compare the values found in the reports to either observed values or export coefficients. Export coefficients are values, usually obtained from literature, that represent typical or average loadings for various constituents within specific regions and for specific land use categories. There are two types of export coefficients: (1) *edge of field loads* (loads at the land segment) and (2) *delivered loads* (loads delivered to the stream channel; these values take into account such variables as travel time, travel distance, dilution, and so forth). For this model, we are interested in the delivered loads since we wish to assess instream water quality. The documentation of export coefficients should specify what type the values are (edge of field loads or delivered loads) and the method in which the values were determined.

The following export coefficients for nitrogen were taken from *Estimating Nutrient Exports* to *Estuaries* (Frink, 1991).

Land use category	Total Nitrogen (lbs/acre/yr)		
Urban	$12.0 \pm 2.3$		
Agriculture	$6.8\ \pm 2.0$		
Forest	$2.1 \hspace{0.1in} \pm 0.4$		

- 33. In the report file (wq\_cal.TotalN.Watershedsummary.txt), scroll to the section for water year 1987 (10/01/86 to 10/01/87).
- 34. Compare the total nitrogen loads for 1987 (the year in our simulation period during which the annual rainfall was closest to the average annual rainfall) to the export coefficients in the table above for each land use. Are we overestimating or underestimating total nitrogen loads?
  - **Note:** Because there is a land use category for both pervious urban land and impervious urban land, you need to look at the values in the "Combined lbs/acre" column. These values represent the area-weighted average of the simulated pervious and impervious total nitrogen loads.

Notice that we are underestimating nitrogen loads from forest land, overestimating loads from urban land, and estimating loads for agriculture land within the typical range. Keep this in mind as you adjust loading rates in the next section.

- 35. Close "wq\_cal.TotalN.Watershedsummary.txt."
- 36. Close GenScn and return to WinHSPF.

In the following section, we will adjust key calibration parameters in an attempt to 'tune' our simulated nitrate to the observed nitrate. The statistics in GenScn indicate that we are fairly consistently over-predicting nitrate concentrations instream. This could be due to either the loads we are predicting from the watershed (i.e., overestimating the amount of nitrate entering the stream from the land use segments) or the rate of nitrification occurring in the stream.

Recall the plots of the simulated and observed values we made previously and the conclusions you made. Was there a seasonal trend?

# **B.** Adjusting Watershed Loading Parameters

## **QUESTION ANSWERED:**

#### 2.) How do I calibrate the nonpoint source loads coming from the watershed?

Recall that in this exercise, we will change key calibration parameters first for watershed loading, second for instream processes, and finally for a combination of watershed loading and instream processes. This final step requires an iterative approach to determine the best possible combination of parameters that results in both reasonable loads and reasonable instream concentrations of each constituent.

In this section, we will begin the water quality calibration procedure for nitrate by adjusting key watershed loading calibration parameters. We will then examine the results by looking at plots and calculating statistics.

- 1. Click the "Input Data Editor" button,
- 2. **Double click** PERLND  $\rightarrow$  PQUAL  $\rightarrow$  MON-ACCUM

**Note:** Recall that there are three occurrences that correspond to the following: Occurrence 1: Ammonia/ammonium (NH<sub>3</sub>+NH<sub>4</sub><sup>+</sup>) Occurrence 2: Nitrate (NO<sub>3</sub><sup>-</sup>) Occurrence 3: Biochemical oxygen demand (BOD)

Remember that "Orthophosphate" was associated with sediment and therefore, will not have a MON-ACCUM table.

**Note:** Total nitrogen is the sum of total ammonia  $(NH_3+NH_4^+)$ , nitrate, nitrite, and organic nitrogen (labile and refractory). We are assuming that all nitrite is converted to nitrate in this application, so we will disregard the nitrite component. We are estimating both total ammonia and nitrate loads as indicated by the MON-ACCUM and MON-SQOLIM tables. Where is the organic nitrogen component coming from?

We are also assuming that the BOD/organic loads coming from the land surface are comprised of both a labile and refractory component. Because a percentage of the organic matter (the labile component) contributes to the biochemical oxygen demand within the stream and is stoichiometrically partitioned into organic nitrogen, phosphorus and carbon, we can control the loading of organic nitrogen by adjusting the biochemical oxygen demand (BOD) loads.

3. Make sure the "Occurrence" is "1" (for ammonia/ammonium, NH<sub>3</sub>+NH<sub>4</sub><sup>+</sup>). Adjust the monthly accumulation factors **according to what you observed in the reports**. (Hint: Recall that the reports indicated that we were underestimating nitrogen loads from forestland, overestimating loads from urban land, and estimating loads for agriculture land within the typical range.) The following table shows the report values and the export coefficients:

Land use category	Total Nitrogen - Simulated (lbs/acre/year)	Total Nitrogen - Export Coefficients (lbs/acre/yr) (Frink, 1991)
Urban	44.91 (too high)	$12.0\pm2.3$

Agriculture	5.67 (about right)	$6.8\ \pm 2.0$		
Forest	1.31 (too low)	$2.1 \pm 0.4$		

- 4. Click APPLY.
- 5. From the "Occurrence" list, select "2" (for nitrate,  $NO_3$ ). Adjust the monthly accumulation factors **according to what you observed in the reports**.
- 6. Click APPLY.
- 7. From the "Occurrence" list, select "3" (for biochemical oxygen demand). Adjust the monthly accumulation factors **according to what you observed in the reports**.
- 8. Click APPLY.
- 9. Click OK.
- Double click PERLND → PQUAL → MON-SQOLIM. Adjust the monthly values of the limiting storage according to what you observed in the reports for ammonia/ammonium (Occurrence 1), nitrate (Occurrence 2), and biochemical oxygen demand (Occurrence 3).
- 11. Click APPLY.
- 12. Click OK.
- 13. Double click IMPLND →IQUAL → QUAL-INPUTS. Make sure the "Occurrence" is "1." Adjust the value of ACQOP and SQOLIM for ammonia/ammonium according to what you observed in the reports. Keep in mind that the model was significantly overestimating total nitrogen loads for impervious urban land.

**Note:** If you take the value for SQOLIM divided by ACQOP (or MON-ACCUM), you can determine the approximate number of days that you are allowing a constituent to build up or accumulate.

- 14. Click APPLY.
- 15. Repeat steps (13-14) for nitrate (Occurrence 2) and biochemical oxygen demand (Occurrence 3).
- 16. Click (Run HSPF).
- 17. Click (View Output through GENSCN).

- 18. From the Analysis menu, select Run Script.
- 19. Navigate to c:/basins/models/hspf/bin and select "GenScnWatershedSummary.spt."
- 20. Click OPEN.
- 21. In the "Script Arguments" window enter "wq\_cal" in the "CurScenario" box, "TotalN" in the "gCurConstituent" box, and "*c:\BASINS\Modelout\wq\_cal*\" in the "InputDir" box.
- 22. Click OK.

Have you improved the loads from each land use?

- 23. Repeat these steps until you feel you are adequately predicting total nitrogen loads for these three land use categories.
  - **Note:** You may want to adjust the MON-ACCUM and MON-SQOLIM factors for the other land use segments. Because we do not have export coefficients to which to calibrate for these land use categories, you will need to make sure the loads from these land use segments are reasonable.

# C. Adjusting Instream Process Parameters

#### **QUESTION ANSWERED:**

3.) How do I calibrate the instream portion of my model so that simulated instream concentrations are similar to observed instream concentrations?

Now that we have improved the simulation of total nitrogen loads delivered to the stream in the watershed, we need to determine how well we are predicting instream concentrations. Recall that because of time constraints, we look at only nitrate concentrations instream; however, for your own projects, you should also look at total ammonia, BOD, and DO concentrations, as well as phytoplankton growth and decay. This is necessary because these constituents' concentrations are interdependent.

- 1. Click (View Output through GENSCN).
- 2. Plot the nitrate results and calculate the statistics (following the steps in the previous section) to determine whether the model simulation has improved. The simulated nitrate concentrations will probably still be too high. Remember that our focus in the previous section was to calibrate the loads from each land use segment. Are we consistently underestimating or overestimating nitrate?
- 3. Close all plots and GenScn to return to WinHSPF.

4. Click the "Input Data Editor" button, **III**. Adjust the following parameters **one at a time** within their respective typical value ranges and then plot the results in GenScn. Continue to adjust these instream parameters until the results look reasonable.

Parameter	Location	<b>Typical Range</b>	<b>Constituents to Plot</b>
KNO320	RCHRES $\rightarrow$ NUTRX $\rightarrow$ NUT-	0.001-0.4 hr <sup>-1</sup>	$NH_3$ , $NO_3^-$ , DO
	NITDENIT		
KBOD20	RCHRES $\rightarrow$ OXRX $\rightarrow$ OX-GENPARM	$0.00004-0.04 \text{ hr}^{-1}$	DO and BOD
MALGR	RCHRES $\rightarrow$ PLANK $\rightarrow$ PLNK-PARM1	0.008-0.3 hr <sup>-1</sup>	$PO_4$ , TAM, $NO_3$ , DO,
			Chl-a

# **D.** Overall Watershed Calibration

# **QUESTION ANSWERED:**

4.) If I am still over-simulating or under-simulating various constituents and I a have adjusted instream calibration parameters within their limits, what do I do now?

Water quality calibration is often an iterative process of adjusting watershed loads within limits and then adjusting various instream parameters within other limits. In this section, we will retrace some of the steps taken previously in an attempt to improve our calibration. Keep in mind that because nutrient loads, nutrient cycling, and phytoplankton growth, death, and decay rates are highly interdependent, there are many possible reasons that a particular nutrient may not be represented well by the model.

- 1. Make sure your land use loads are reasonable by looking at the loading report. Continue to adjust loading parameters until the loads are reasonable.
- 2. Look at instream concentrations by plotting simulated concentrations with the observed concentrations in GenScn. Continue to adjust key calibration parameters within range until simulated instream concentrations match up with the observed concentrations.
- 3. If the instream concentrations are still too high or too low given the watershed loads, you may need to decrease watershed loads within expected ranges.
- 4. Iterate until you are able to predict instream concentrations well using acceptable loadings and parameter values.

# E. Summary of Water Quality Calibration Steps

# **QUESTION ANSWERED:**

5.) What are the steps required for water quality calibration?

• Estimate all model parameters, including land use specific accumulation and

depletion/removal rates, washoff rates, and subsurface concentrations.

- Tabulate, analyze, and compare simulated nonpoint loadings with expected range of nonpoint loadings from each land use and adjust loading parameters when necessary.
- Calibrate instream water temperature.
- Compare simulated and observed instream concentrations at each of the calibration stations.
- Analyze the results of comparisons in steps 3, 4, and 5 to determine appropriate instream and/or nonpoint parameter adjustments.

## Reference:

Frink, C. R. 1991. Estimating Nutrient Exports to Estuaries. J. Environ. Qual. 20(4): 717 - 724.