Water Quality Model
Version 1.00

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A.R.M. Loxahatchee National Wildlife Refuge
Water Quality Model Version 1.00

User's Manual

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1. INTRODUCTION

Water quality modeling based on long-term ecosystem monitoring can provide important information for resource managers. Water quality modeling is needed to insure effective management of ecosystems including the A.R.M. Loxahatchee National Wildlife Refuge (Refuge). This user's manual provides the detail description of the implementation of a simple water quality model for the Refuge, or Refuge Water Quality Model (RWQM). The goal is to allow Refuge managers to explore the dynamics of important water quality constituents – chloride, total phosphorus and sulfate in this model – influenced by water management that may cause canal water of high nutrient concentrations to intrude into the soft-water, oligotrophic marsh of the Refuge interior (USFWS, 2007).

1.1. General description of model structure

In the RWQM, the Refuge was classified into four cells (compartments) based on the analysis of the distribution of surface water chloride and phosphorus as a function of distance away from the canal (Arceneaux et al., 2007). These cells consist of the canal (996 acres), and three inner marsh cells. The first marsh cell (Cell 1) encompasses the outer fringe of the Refuge marsh from the canal to 1 km into the interior (22,072 acres). The second marsh cell (Cell 2) encompasses the marsh between 1 km and 4 km from the canal (55,353 acres). The third marsh cell (Cell 3) encompasses the remaining interior marsh area greater than 4 km from the canal (60,901 acres). The RWQM is based on a simple constituent mass balance equation and a water budget model, the Simplified Refuge Stage Model (SRSM), which projects canal and marsh stage (hence, the dynamics of volumes and water exchange) from inflow, outflow, precipitation, and evapotranspiration (Meselhe et al., 2007). The mass balance equation for a 1-dimensional stream used by WASP is shown below (Arceneaux et al., 2007):

$$\frac{\partial}{\partial t}(AC) = \frac{\partial}{\partial x}\left(-U_x AC + E_x A\frac{\partial C}{\partial x}\right) + A\left(S_L + S_B\right) + AS_K$$

where A is the cross-sectional area, m^2; C is the concentration of the water quality constituent, mg/L; t is time in days; U_x is the longitudinal, advective velocities in

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m/day; E_x is the longitudinal diffusion coefficients, m^3/day; S_L is the total of direct loading rates in g/m^3 per day; S_B is the boundary loading rates in g/m^3 per day; and S_K is the total kinetic transformation rate in g/m^3per day.

1.2. Model platform –WASP

The platform of the Refuge's simple water quality modeling is the U.S. Environmental Protection Agency's (EPA) Water Quality Analysis Simulation Program, Version 7.2 (WASP 7.2, hereafter referred to as simply WASP). WASP is a dynamic compartmental model that allows users the ability to interpret and predict water quality responses due to natural and anthropogenic pollution (US EPA, 2006a). The model includes the following data requirements: water body hydrogeometry, advective and dispersive flows, settling and resuspension rates, boundary concentrations, pollutant loadings, and initial conditions (Arceneaux et al., 2007). The area being modeled can be separated into multiple segments or compartments. The segment volumes, connectivity, and type, such as surface water, must be known. Each segment or compartment is modeled independently, with the water quality constituents modeled as spatially constant within each segment.

Some benefits of selecting WASP include: it is free to the public, user friendly (no computer programming experience required), and it has been widely applied for both simple and complex water quality simulations. For example, WASP has been successfully used to examine phosphorus loading to Lake Okeechobee and eutrophication of Tampa Bay in Florida (Jin et al., 1998; Wang et al., 1999). Another major advantage of using WASP is that it has a data preprocessor that allows for quick development of input datasets, and a postprocessor that enables efficient reviewing of model results.

1.3. User's manual objectives

This manual will help users to set up and run the WASP model to simulate the dynamics of chloride (CL), total phosphorus (TP) and sulfate (SO_4) in canal and marsh in the Refuge. The user can generate (in Excel) an input file that imports time series data for water flow and water quality. The user can set up the model by inputting model parameters, and importing time series data through each WASP toolbar icon.

1.4. Caveats

1) Before working with the RWQM, the user should be familiar with the EPA WASP model (USEPA 2006a, b), including its intended uses and limitations. This manual does not cover how to use WASP.

2) Users should not adjust fixed parameters in the RWQM that were determined through model calibration. This manual identifies what parameters that can be changed for a particular simulation time period and water quality constituents.

3) This manual presents an example of modeling CL, TP and SO_4 from 1995-2004 for the Refuge. The user's assumes responsibility (including limitations) of obtaining, organizing and running this WASP model if the period of record (POR) is different from 1995-2004.

2. DATA PREPARATION

In this section, the user can prepare the necessary hydrological and water quality data for importing data into WASP through the use of an Excel file. The name of the file is: "**WASP_input_file.xls**". There are a total of 13 worksheets in this file. The hydrological data the user needs for the input file are obtained from the Water Budget Model, SRSM (Meselhe et al., 2007; Arceneax et al., 2007). Water quality data can be obtained from DBHYDRO database (http://www.sfwmd.gov/org/ema/dbhydro/), or other sources for water quality constituents. Details for file structure are described according to each worksheet in the Excel input file.

2.1. Basic parameters - the "Constants" worksheet

In the "Constants" worksheet, the user can find basic constants including total area of Refuge, areas of canal and marsh, areas of each individual cells in marsh (m^2); initial volumes of canal and marsh cells (m^3); initial depth in canal and marsh (m); percentage of evaporation and transpiration; concentrations of CL, TP and SO_4 in rainfall (mg/L); dry deposition rates of CL ($g/m^2/yr$), TP, and SO_4 ($mg/m^2/yr$); mass loading rates for TP in canal and marsh ($mg/m^2/day$); and apparent settling coefficients of SO_4 in three marsh cells (in m/yr). **Note: these constants should NOT be changed because they are derived from the calibrated Water Budget Model (SRSM) and calibrated RWQM**.

2.2. Hydrological processes

Time series of hydrological processes are typically copied from the water Mass Balance Model (Arceneaux et al., 2007). In order to assure an overall conservation of water volume, it is essential that these time series are consistent (as they will be if copied from the Mass Balance Model). One may not, for example, adjust the precipitation component here without re-running the mass balance model and replacing all of the hydrological process time series. Hydrological process sheets specify flow, groundwater seepage, precipitation, evaporation and transpiration are given in four Excel worksheets:

"Flow" worksheet. The user is asked to identify the modeling time series for three flows identified and derived from the Water Mass Balance Model:

- inflow pumped into canal, QE;
- exchange flow between canal and marsh (>0 for flow from canal to marsh; <0 for flow from marsh to canal), QMI2; and
- outflow from canal, QRO.

"GW" worksheet. This worksheet determines the time series of total amounts of groundwater seepage in canal and marsh (m^3/day) from groundwater seepage rates (m/day, from the Water Budget Model).

"PT" worksheet. This worksheet gives the time series of precipitation in m/day, and converts them to m^3/day, and finally to m^3/sec.

"ET" worksheet. This worksheet derives time series of evaporation (in m^3/sec) and transpiration (in m^3/day) from ET (m/day, results from Water Budget Model) based on the percentages of evaporation and transpiration ("EvapTranPct" also from Water Budget Model results).

2.3. Boundary concentrations

In the WASP model, the time series of boundary concentrations (in mg/l) for CL, TP and SO_4 are required as inputs into canal. These boundary concentrations are estimated from daily total CL, TP, and SO_4 loads divided by total daily inflow volume into the canal (this is equivalent to the flow weighted mean concentration). Total daily inflow volume is the sum of all the inflows into the canal from all the hydraulic structures along the canal. Total daily loads of CL, TP, and SO_4 are estimated by summing all the loads from each hydraulic structure along the canal. The daily load from each structure is estimated by multiplying daily inflow volume by the observed (or interpolated) concentrations of CL, TP and SO_4 of the inflow at the structure using data from DBHYDRO.

It should be noted that unlike the time series of inflows from each structure, time series of concentrations of CL, TP, and SO_4 of the inflows are usually not available, measurements of these concentrations can be bi-weekly, monthly, or even quarterly. TP at major inflows is typically monitored using composite sampling. In order to calculate daily time series of constituent loads it is necessary to interpolate the incomplete concentration data into complete daily time series. Simple SAS and Excel programs for data interpolation are provided in the Appendix A and B.

2.4. Wet and dry deposition loads

Atmospheric loading (from wet and dry deposition) of CL, TP and SO_4 is required input for the WASP model. Users may find the recent compilation and analysis of deposition data by Guoqing He (2007) helpful in estimating aerial deposition parameters.

"Precip_load" worksheet: The time series of loads (in kg/day) of CL, TP, and SO_4 from precipitation for canal and marsh cells are estimated from the product of concentrations of CL, TP, and SO_4 in precipitation, precipitation amount, and the areas of all four cells. This worksheet updates automatically when the precipitation data is inputted into the "PT" worksheet.

"Dry_dep" worksheet: The loads (in kg/day) of CL, TP, and SO_4 from dry deposition for canal and marsh cells are estimated from the dry deposition rates of CL, TP, and the areas of all four cells. Loads from dry deposition are assumed to be constant over time. This worksheet updates automatically.

2.5. KC load for TP

"TP_KC_load" worksheet: Another source of TP load (kg/day) is defined for canal and marsh. This is the product of K ("settling coefficient") and C* (concentration in background) in Kadlec's model (Kadlec and Knight, 1996; Arceneaux et al., 2007). It is assumed to be constant for canal and marsh cells over time. This worksheet updates automatically.

TP and SO_4 are modeled here as carbonaceous biological oxygen demand 1 (CBOD1) and CBOD 2, respectively using the first order concentration model (the k-c* model) from Kadlec and Knight (1996):

$$\frac{dhC}{dt} = -k(C - C^*) = -kC + kC^*$$

where, h is depth in m, C is the concentration in g/m^3, k is the removal rate constant in m/yr, and C^* is the background pollutant concentration in g/m^3. For TP, the c* value for the canal was calibrated to be 80 μg/L and the interior cells were calibrated to have a value of 8 μg/L (Arceneaux et al., 2007).

2.6. Total loading

"Total_loading" worksheet: The time series of total loads of CL, TP, and SO_4 (kg/day) for the four cells are calculated by summing wet and dry deposition loads (Note: for TP, the KC load component is added) as input into the "loads" module of the WASP model. This worksheet updates automatically, so user does not need to do anything.

2.7. Apparent settling coefficient for SO_4

For SO_4 modeling, the C* (background concentration of sulfate in canal and marsh) is assumed to be zero. Therefore, the loss of SO_4 from the marsh water column is assumed to be estimated by a constant apparent settling coefficient (*K*) for each marsh cell to represent all the mechanisms of loss of SO_4 by biological processes such as sulfate reduction (Wang et al. 2007). The settling coefficient for the canal is set to zero based on the assumption that SO_4 is not settled or lost by biological processes such as SO_4 reduction or plant uptake in the canal.

"S_settling" worksheet: The losses of SO_4 for marsh cells are estimated from the product of the settling coefficient and areas of each marsh cell, and also are assumed constant throughout the modeling period. The data will be used in the "Solid 2" in the "Flows" in WASP model. This worksheet updates automatically, so user does not need to do anything. Settling is entered modeled in WASP analogous to a flow, with units of m^3/day.

3. MODEL SETUP AND DATA INPUT

In this section, you will be guided through each sequential toolbar to set up the model and input the time series of data in the WASP model. Please refer to WASP6 and WASP71 Manuals for details (USEPA 2006a, b). **Note: be sure to save after you finish each toolbar setup**. We recommend saving the model with a different file name from the original model to protect the original integrity of RWQM v.1.00 as released.

3.1. Data set

Parameters you need to adjust: “Description” and “Time Range”.

Fixed parameters (therefore, should not be changed): “Model Type = Eutrophication”, “Restart Option=No Restart File”, “Hydrodynamics=”Gross Flows”, “Bed Volumes= Static”, “Time Step=User Defined”.

3.2 Time step

Define your simulation start and end date, time and value (use 0.1 day in the simulations).

3.3. Print interval

Define your output print start and end date, time and value (can be 1 day).

3.4. Segments

“<u>Segments</u>”: Give the initial volumes for all your segments (canal and three marsh cells). This was done by assuming an initial water depth in the canal of 2 m and a depth in the interior cells of 0.61 m. The water depth in the interior cells was calculated by taking the observed water level in the marsh on January 1, 1995 of 5.23 m and subtracting the average marsh elevation of 4.62 m. The assigned volumes are 8,066,971, 54,509,080, 136,701,113, and 150,402,747 m^3 for canal, cell-1, cell-2, and cell-3, respectively. Note that you need to change the initial volumes if modeling period not starting January 1, 1995. Values consistent with the water balance model should be used.

“**<u>Segment type</u>**” = “Surface”.

“**<u>Parameters</u>**”: No Change

“**<u>Initial Concentrations</u>**”: Give initial concentrations for all segments under “Salinity” for CL, “CBOD1” for TP, and “CBOD2” for SO_4. All the initial concentrations are estimated from field observations.

"**Fraction dissolved**": 1 for CL and TP, 0 for SO_4.

3.5. Systems

Check under "Mass Balance" to confirm the following: CBOD1 for TP, CBOD2 for SO_4, and Salinity for CL.

3.6. Parameters

Not used for this model. Skip this step.

3.7. Constants

The constants used for the Refuge Water Quality Modeling are defined in the input Excel file, and are used in calculating loads for data inputs. Therefore the user needs to do nothing with this toolbar . Skip this step.

3.8. Loads

"**Loads":** scroll the pull-down menu to add the 4 segments (canal, cell-1, cell-2, and cell-3) for CBOD1 for TP, CBOD2 for SO_4, and Salinity for CL. Then import the time series of loads for TP, SO_4 and CL from the "Total Loading" worksheet in the input Excel file.

"**Scale and Conversion Factors**": No change for the default.

3.9.Time functions

Not used for this model. Skip this step.

3.10. Exchanges

Define the dispersion coefficients for the exchanges between each segment pair. The cross sectional areas were calculated using the perimeter of each cell and an estimated typical depth of 0.5 m for the interior cells and a depth of 2 m for the canal. The lengths are calculated using the center point of adjoining segments (cells). Longitudinal dispersion was calibrated to be equal to 22 m^2/hr (6.1E-3 m^2/sec) (Arceneaux et al., 2007). The set values should not be changed, however the user needs to change the start and ending dates to reflect the time period being simulated.

3.11. Flows

"Flow Fields": check for surface water, Solid 1 for TP, Solid 2 for SO_4, Evaporation/Precipitation. All flows should be in m^3/sec (conversion factor = 1). If flows are in m^3/day, then conversion factor = 0.0000116.

"Functions": Define the hydrological processes including transpiration, outflow from canal, inflow to canal, canal seepage, marsh seepage, exchange flow between canal and marsh (QMI2).

"Segment Pair": define the fraction of flow for each segment pair under each function. Do not change the fractions.

"Time/Volume pairs": import the time series of hydrological processes from the input Excel file. Define the "apparent settling" amounts of TP and SO_4 under Solid 1 and Solid 2 also from the input Excel file.

3.12. Boundaries

"**Boundaries":** scroll the pull-down menu to add canal for CBOD1 for TP, CBOD2 for SO_4, and Salinity for CL. Then import the time series of inflow concentrations (mg/L) for CL, TP, and SO_4 from the "CL_boundary", "TP_boundary", and "SO4_boundary" worksheets in the input Excel file, respectively.

"**Scale and Conversion Factors**": No change for the default.

3.13. Output control

Check both "Output" and "CSV" for Salinity as CL, CBOD1 (ultimate) as TP, and CBOD2 (ultimate) as SO_4. You may also want to model export results for other model calculated items such as volume, depth, etc.

After this step, the user is ready to execute the Refuge Water Quality Model. Be sure the model is saved.

4. MODEL EXECUTION and TROUBLE SHOOTING

Click the "Execute Model" button to run simulations. Pay close attention to the result display window to see if your simulated parameters show error calculations. Your simulations may have errors or even have crashed during the execution. Below are common things to check to resolve runtime errors or crashes.

1) Data period match check

One of the reasons for a model crash is that the data periods in the input data are not consistent for all parameters. Check all the time series data to see if they match the same simulation period, especially for all the time series of water flows in "Flow" screen.

2) Initial volume check

A possible limitation with this modeling program is that WASP does not allow the cells to go completely dry (US EPA, 2006a). Model crashes related to this can be checked by examining the initial volume settings for the segments.

5. POST-PROCESSING

Simulation results can be displayed using the "Visual Graphics" in the "post-processor" (US EPA, 2006b), or open the result .CSV file(s) in Excel to analyze the water budget and water quality dynamics as well as the assessment of model performance and sensitivity/uncertainty analysis.

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7. For more information contact:

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Appendix A1. Interpolation using SAS Proc EXPAND

```
/*-----------------------------------------------------------------------------*/
/* This SAS program is to use Proc EXPAND to                    */
/* 1. Convert time series data with different frequency;        */
/* 2. Convert irregular observations to periodic estimates; and    */
/* 3. Interpolate linearly missing values in time series.         */
/*-----------------------------------------------------------------------------*/

/* -----------  Read in data and variables     ---------------------------*/
data samples;
  infile 'g94c.txt';
  input date mmddyy10. measure;
  format date mmddyy10.;
run;

/* -----------  Interpolate missing data       -----------------------------*/
proc expand data=samples out=daily to=day;
  id date;
/* -----------  Using Linear interpolation: method=join ------------*/
  convert measure = interpol / method=join;
run;

/* -----------  Merge interpolated data and observed data ----------*/
data daily;
  merge daily samples;
  by date;
run;

/* -----------  Write out complete timeseries in a file   -------------*/
 data _null_; set daily;
file 'g94c.dat';
put date yymmdd10. interpol 13-23 .3;
run;

quit;
```

Appendix A2. Interpolation using Excel VLOOKUP

An example of interpolation using the Excel function VLOOKUP is available from Dr. Mike Waldon.