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Memorandum

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Date: September 17, 2013
Project: SRRTTF
To: SRRTTF
CC:

SUBJECT: **DRAFT: Review of Modeling Tools**

Summary

The Spokane River Regional Toxics Task Force (SRRTTF) is developing a comprehensive plan to reduce toxic pollutants in the Spokane River, and has hired LimnoTech to serve as a technical advisor. This memorandum reviews available modeling tools to describe the in-stream fate and transport of polychlorinated biphenyl (PCB) and polychlorinated dibenzo-*p*-dioxin and dibenzofuran (dioxin) levels in the Spokane River. Several potentially applicable model frameworks are available to support development of this plan. We recommend that primary consideration be given to a linked application of the EFDC hydrodynamic model with the WASP water quality model. This recommendation is based upon the fact that these models:

- are fully capable of simulating all of the environmental processes of concern,
- are supported by U.S. EPA, and
- have a wide history of application.

The AQUATOX model should be considered only if particular focus is desired on assessing bioaccumulation factors.

Introduction

The SRRTTF is developing a comprehensive plan to reduce toxic pollutants in the Spokane River, designed to identify specific management actions that can be undertaken to control pollutant loads such that water quality objectives can be attained. Comprehensive plans of this type typically rely upon mathematical models to describe the relationship between pollutant sources and resulting environmental concentrations.

Several water quality model frameworks exist that are potentially applicable for the Spokane River. Given the nature of this project, this review is focused on public domain, non-proprietary models. The remainder of this memorandum describes each model's capabilities, advantages, and disadvantages. It concludes with a recommendation regarding which modeling tools are most suitable for use in future phases. It is divided into sections of:

- Available Model Frameworks
- Model Recommendations

Available Model Frameworks

Modeling the fate and transport of hydrophobic organic pollutants, such as PCBs and dioxins, requires consideration of hydrodynamics and toxic pollutant kinetic processes. Some models exist that consider both of these aspects as part of an integrated framework; while many applications, in practice, have consisted of a linkage of individual models frameworks specific to each component (i.e. hydrodynamic model results linked to toxic chemical kinetic model). This section provides a review of available public domain models in each category that have been applied for toxic organic chemical modeling at other sites. Model reviews are divided into categories of:

- Hydrodynamic models
- Toxic pollutant kinetic process models
- Integrated model frameworks

Hydrodynamic models

There are four general purpose hydrodynamic modeling frameworks that are commonly used to provide input to toxic chemical kinetic models:

- CH3DZ
- Princeton Ocean Model (POM)
- ECOM-3D
- EFDC

CH3DZ (Curvilinear Hydrodynamics in 3 Dimensions — Z Plane) is a finite-difference model that computes three-dimensional velocity, salinity, and temperature fields in bays, estuaries, lakes, and rivers. CH3DZ was used as the hydrodynamic component of the Chesapeake Bay water quality model, and was also used to provide three-dimensional hydrodynamic inputs to a water quality model of Lake Washington. http://www.ch-t.com/models.shtml.

The Princeton Ocean Model (POM) is modeling code capable of simulating a wide-range of hydrodynamic conditions: circulation and mixing processes in rivers, estuaries, and lakes. POM is a sigma coordinate, free surface model with embedded turbulence and wave sub-models, and wet-dry capability. http://www.aos.princeton.edu/WWWPUBLIC/htdocs.pom/. ECOM-3D is a close relative of the Princeton Ocean Model, and solves the time dependent, three dimensional equations for the conservation of mass, momentum, salt, heat and turbulence quantities in an incompressible hydrostatic fluid. http://pritchard.marine.usf.edu/TBmodel/ecom3d.html.

The Environmental Fluid Dynamics Code (EFDC) is a state-of-the-art hydrodynamic model that can be used to simulate aquatic systems in one, two, and three dimensions. EFDC uses stretched or sigma vertical coordinates and Cartesian or curvilinear, orthogonal horizontal coordinates to represent the physical characteristics of a water body. It solves three-dimensional, vertically hydrostatic, free surface, turbulent averaged equations of motion for a variable-density fluid. Dynamically-coupled transport equations for turbulent kinetic energy, turbulent length scale, salinity and temperature are also solved. http://www.epa.gov/athens/wwqtsc/html/efdc.html.

All four of these models have sufficient capability to accurately simulate the hydrodynamic features of Spokane River and its impoundments. The primary differences between them for purposes of this application are that the EFDC model is EPA-supported and has been more widely applied in TMDL and similar regulatory settings. Also, software linkages have already been developed between EFDC outputs and the inputs of many water quality models.

Toxic pollutant kinetic process models

There are three widely accepted public domain toxic chemical kinetic modeling frameworks:

- WASP
- AQUATOX

- CE-QUAL-ICM

WASP (Water Quality Analysis Simulation Program), developed and supported by USEPA, is a dynamic compartment-modeling program for aquatic systems, including both the water column and the underlying benthos. WASP allows the user to investigate 1, 2, and 3 dimensional systems, and a variety of pollutant types. The time varying processes of advection, dispersion, point and diffuse mass loading and boundary exchange are represented in the model. WASP also can be linked with hydrodynamic and sediment transport models that can provide flows, depths velocities, temperature, salinity and sediment fluxes. http://www.epa.gov/athens/wwqtsc/html/wasp.html. WASP is the most widely used modeling framework for assessing toxic pollutants, and has often been linked to hydrodynamic model outputs at a range of spatial resolutions. Further, the toxic kinetic routines in WASP serve as the basis for many other water quality models.

AQUATOX, developed and supported by USEPA, predicts the fate of a wide range of pollutants and their effects on the ecosystem. AQUATOX is an ecosystem model, and includes numerous types of plants, invertebrates and fish. AQUATOX, in contrast to the other models described here treats the biota as interacting with the chemical/physical system. http://water.epa.gov/scitech/datait/models/aquatox/index.cfm. The primary advantage to AQUATOX is its unique ability to simulate bioaccumulation and biological effects. Its primary disadvantage is that it is not commonly linked to hydrodynamic models, and is most commonly applied at a coarse segmentation scale where detailed hydrodynamics are not considered.

CE-QUAL-ICM was developed by the US Army Corps of Engineers, and initially developed as a component of the model package employed to study eutrophication processes in Chesapeake Bay. Subsequent to employment in the Bay study, the model code was generalized to include consideration of toxics. The toxics model (ICM/TOXI) resulted from incorporating the toxic chemical routines from EPA's WASP model into the transport code for ICM, incorporating a more detailed benthic sediment model, and enhancing linkages to sediment transport models. ICM/TOXI includes: physical processes such as sorption to DOC and three solid classes, volatilization, and sedimentation; and chemical processes such as ionization, hydrolysis, photolysis, oxidation, and biodegradation. http://el.erdc.usace.army.mil/elmodels/icminfo.html. The advantages to ICM/TOXI are that is readily linked to hydrodynamic model outputs at a range of spatial resolutions, and that it possesses the capability to simulate benthic sediment processes at a greater level of detail than the other two models discussed here. Its disadvantages are that it requires use of the CH3DZ hydrodynamic model and that it has not been as widely applied as the WASP model framework.

Integrated Model Frameworks

The EFDC model, in addition to the hydrodynamic capabilities discussed above, also possesses the capability to simulate sediment transport and toxic kinetic processes. As such, it has the capability to meet all Spokane-specific needs in a single integrated modeling framework. Another advantage to applying EFDC in an integrated fashion is that its capabilities of simulating sediment transport processes are superior to those contained in WASP or AQUATOX.

There are two disadvantages to using the integrated EFDC modeling package. First, hydrodynamic and water quality calculations are fully coupled, such that every model simulation must conduct calculations for both components. This is in contrast to a linked model framework such as EFDC-WASP where, once the hydrodynamic model is calibrated, future water quality simulations can be conducted without the need for re-rerunning model hydrodynamics. Because hydrodynamic calculations are much more computationally intensive than water quality calculations, it is much more computationally efficient to use a linked model framework in situations like Spokane where the influence of sediment transport dynamics or other water quality variables on hydrodynamic predictions can be considered to be insignificant (or marginal) relative to other factors.

Model Recommendations

This section begins by assessing the available models in each of the three categories (hydrodynamic, water quality, integrated framework), and then provides overall recommendations for moving forward.

EFDC is the preferred hydrodynamic modeling framework, because

- It is fully capable of simulating the key hydrodynamic features of the Spokane River and its impoundments
- It has been much more widely applied than the other hydrodynamic models
- It is officially supported by USEPA
- None of the other hydrodynamic models offer unique capabilities that override the advantages listed above

Each of the water quality models considered have unique features that merit their consideration. AQUATOX provides a detailed description of bioaccumulation and biological effects of toxic pollutants, but is less well suited for considering finer-scale hydrodynamics. CE-QUAL-ICM/TOXI possesses the capability to simulate benthic sediment processes at a greater level of detail than the other two stand-alone water quality models, but requires linkage to the CH3DZ hydrodynamic model. WASP is widely applied and contains kinetics that serve as the basis for most other toxic models, but has lesser capabilities in describing benthic sediment transport.

Application of EFDC in an integrated manner provides a detailed description of benthic sediment transport, but this integrated framework is not as widely applied and will be computationally inefficient.

The linked EFDC-WASP framework is recommended for this project, as it meets all project needs, is widely applied, and is EPA supported. Its primary limitations (less rigorous simulation of benthic sediment transport than EFDC or ICM/TOXI, and less rigorous simulation of bioaccumulation and biological effects) are not considered significant detriments, because:

- Resuspension of buried historical contamination is not a major issue in Spokane. Sediments in the riverine segment are scoured downstream during periods of high flow. Historical sediment contamination in Lake Spokane is located at sufficient water depths that resuspension is not an important process to consider.
- The environmental endpoint of concern for this project is the water quality standard. EFDC-WASP is capable of predicting water column concentrations for comparison to these standards, and can provide estimated fish tissue concentrations through the use of established bioaccumulation factors.

The use of AQUATOX should be considered only if the SRRTTF desires detailed assessment of bioaccumulation processes in the Spokane River system.