D. Common Water Quality Models

In this appendix we introduce a few of the common models used in water quality analysis. This is by no means a complete list, but does provide a starting point from which to work. Much of the text in this appendix was copied from the internet home pages describing each of the models. The web page for this course[1] provides links to each of these models in the web.

D.1 One-dimensional models

One-dimensional models are most commonly used in rivers, but can also be used in special cases in estuaries and lakes with large length-to-width ratios. Accept for the ATV model, these models are publicly available free of charge, and most can be downloaded over the internet. The list of models below progresses from steady-state models, to dynamic tanks-in-series models, to fully-dynamic numerical models. Refer to Chapter 7 for an introduction to water quality modeling and its methodology.

D.1.1 QUAL2E: Enhanced stream water quality model

The QUAL2E series of models has a long history in stream water quality modeling. It was primarily developed by the U.S. Environmental Protection Agency (EPA) in the early 1970s. Since, it has gained a broad user base, including applications outside the U.S. in Europe, Asia, and South and Central America.

The Enhanced Stream Water Quality Model (QUAL2E) is applicable to well mixed, dendritic streams. It simulates the major reactions of nutrient cycles, algal production, benthic and carbonaceous demand, atmospheric reaeration and their effects on the dissolved oxygen balance. It can predict up to 15 water quality constituent concentrations. It is intended as a water quality planning tool for developing total maximum daily loads (TMDLs) and can also be used in conjunction with field sampling for identifying the magnitude and quality characteristics of nonpoint sources. By operating the model dynamically, the user can study diurnal dissolved oxygen variations and algal growth. However, the effects of dynamic forcing functions, such as headwater flows or point source loads, cannot be modeled with QUAL2E. QUAL2E-U is an enhancement allowing users to

[1] `http://www.ifh.uni-karlsruhe.de/ifh/studneu/envflu_I/envflu_I.htm`

perform three types of uncertainty analyses: sensitivity analysis, first-order error analysis, and Monte Carlo simulation.

The model only simulates steady-state streamflow and contaminant loading conditions; the reference to dynamic modeling above refers only to water quality forcing functions of climatologic variables (air temperature, solar radiation, among others). The transport scheme in the model is the implicit backward-difference finite difference method.

D.1.2 HSPF: Hydrological Simulation Program–FORTRAN

Developed in the late 1970s by the EPA, HSPF is a union between the Stanford Watershed Model, an advanced, continuous-simulation, process-oriented hydrologic model, and several water quality models developed by the EPA, including the Agricultural Runoff Model (ARM) and the NonPoint Source model (NPS). The model is intended for both conventional and toxic organic pollutants. Contaminant loads are either user-input point sources or nonpoint sources modeled by build-up and wash-off parameterizations. It is the only comprehensive model of watershed hydrology and water quality that allows the integrated simulation of land and soil contaminant runoff processes with in-stream hydraulic and sediment-chemical interactions. However, make no mistake: it is not a three-dimensional model.

An advantage of HSPF is in its software development, which resulted in a complete data-management tool. A disadvantage of HSPF is its large data requirements, which include physical data such as watershed data, river network discretization, soil types, geologic setting, vegetative cover, towns, and other regional data, meteorologic data such as hourly data for precipitation, solar radiation, air temperature, dew-point temperature, and wind speed and daily evapotranspiration. In addition, the model has a wealth of empirical calibration parameters that must be determined from handbook values and by calibrating to field measurements.

The river transport model is a tanks-in-series model that uses flood routing *via* stage-discharge relationships (which must be input by the user from external knowledge).

D.1.3 SWMM: Stormwater Management Model

In urban settings, where pressurized pipe flow in sewer systems is to be modeled, the EPA model SWMM is recommended. The SWMM model is actually a package of models. In one mode, it can function as a design model which undertakes detailed simulations of storm events, using relatively short time steps and as much catchment and drainage system detail as necessary. In another mode it can be used as a routine planning model for an overall assessment of the urban runoff problems and proposed abatement options. The planning mode is typified by continuous simulation for several years using long (e.g. hourly) time steps and minimum detail in the catchment scheme. Like HSPF, the model requires a great deal of input data (both physical and meteorological).

The modular nature of SWMM allows it to simulate diverse situations. Both single-event and continuous simulation can be performed on catchments having storm sewers, or combined sewers and natural drainage, for prediction of flows, stages and pollutant concentrations. The Extran Block solves complete dynamic flow routing equations (St. Venant equations) for accurate simulation of backwater, looped connections, surcharging, and pressure flow. The modeler can simulate all aspects of the urban hydrologic and quality cycles, including rainfall, snowmelt, surface and subsurface runoff, flow routing through drainage networks, storage and treatment. Statistical analyses can be performed on long-term precipitation data and on output from continuous simulation.

The strength of this model is in its hydrodynamics. The transport modules, which are also quite flexible, use simple tanks-in-series formulation, and are not available in the Extran Block (where the complete dynamic flow equations are solved).

D.1.4 DYRESM-WQ: Dynamic reservoir water quality model

The model DYRESM-WQ is a one-dimensional hydrodynamics model for predicting the vertical distribution of temperature, salinity and density in lakes and reservoirs. It is assumed that the water bodies comply with the one-dimensional approximation in that the destabilizing forcing variables (wind, surface cooling, and plunging inflows) do not act over prolonged periods of time. DYRESM-WQ has been used for simulation periods extending from weeks to decades. Thus, the model provides a means of predicting seasonal and inter-annual variation in lakes and reservoirs, as well as sensitivity testing to long term changes in environmental factors or watershed properties.

DYRESM-WQ can be run either in isolation, for hydrodynamic studies, or coupled to CAEDYM for investigations involving biological and chemical processes. The computational demands of DYRESM-WQ are quite modest and multi-year simulations can be performed on PC platforms under Windows operating systems. The code is written in modular fashion to support future updates and improvements.

D.1.5 CE-QUAL-RIV1: A one-dimensional, dynamic flow and water quality model for streams

Administered and developed by the U.S. Army Corps of Engineers, CE-QUAL-RIV1, or more commonly just RIV1, is a fully dynamic (flow and water quality) one-dimensional model. The hydrodynamic portion is computed first, solving the St. Venant equations using the four-point implicit finite difference scheme. The hydrodynamic model does not allow for super-critical flow. This can lead to problems for natural streams under low flow where steep river sections form cataracts. Following the hydrodynamics, the transport equation is solved using an explicit two-point, fourth-order accurate Holly-Preissman scheme. The Holly-Preissman scheme is a backward method of characteristics; however, because the search routine in RIV1 for finding the feet of the characteristic lines only searches the upstream segment, the Courant number restriction still applies. The water quality model can predict variations in each of 12 state variables: temperature, carbonaceous biochemical oxygen demand (CBOD), organic nitrogen, ammonia nitrogen, nitrate + nitrite nitrogen, dissolved oxygen, organic phosphorus, dissolved phosphates, algae, dissolved iron, dissolved manganese, and coliform bacteria. In addition, the impacts of macrophytes can be simulated. Because of the use of the characteristic method, numerical accuracy for the advection of sharp gradients is preserved.

D.1.6 ATV Gewässergütemodell

The ATV Gewässergütemodell, also called the AVG (allgemein verfügbares Gewässergütemodell) or in English the ATV water quality model, was developed in Germany as a new model to bridge the problems (limitations) inherent in some of the models listed above. It is designed as a series of building blocks, each building block to be implemented as needed. The first building block is the hydrodynamic model, which solves the St. Venant equations for either the steady or unsteady case. The remaining building blocks can be added to the hydraulics as needed, including water temperature, conservative tracers, (C)BOD, phosphorus, nitrogen cycle, silicon, algae, zooplankton, sediment/water exchange, suspended sediment transport, oxygen dynamics, pH dynamics, heavy metals, and organic chemicals. The solution to the transport equation uses the method of characteristics and does not have a Courant number constraint. Because of the model's modular design, simulations can be made as simple or as complicated as desired; however, the numerical expense of the hydrodynamic routine should not be underestimated.

D.2 Two- and three-dimensional models

Two- and three-dimensional models are typically used in reservoirs, lakes, and estuaries. They are almost exclusively finite element, finite volume, or finite difference. Because large water bodies are generally stratified, they must simulate buoyancy effects; thus, the hydrodynamic and transport equations are coupled. Because buoyancy effects are a major complication in these models (and the subject of next semester) this section briefly summarizes each model without discussing the details.

D.2.1 CORMIX: Cornell Mixing-Zone Model

Begun at Cornell and currently under continued development at the Oregon Graduate Institute, the CORMIX system is a near-field model for the analysis, prediction, and design of aqueous toxic or conventional pollutant discharges into diverse water bodies. Major emphasis is on computation of plume geometry and dilution characteristics within a receiving water's initial mixing zone so that compliance with regulatory constraints can be judged. It also computes discharge plume behavior at larger distances. The model has three modules: CORMIX1 for submerged single-point discharges, CORMIX2 for submerged multi-port diffuser discharges, and CORMIX3 for buoyant surface discharges. As implied by the title, the model predicts mixing (dilution) of the input chemicals, but does not allow for interaction among multiple chemicals (though first-order decay of a single species is implemented).

The model equations are based on jets and plumes, which traditionally are modeled using integral equations. Integral equations rely on self-similarity to reduce the three-dimensional equations to a one-dimensional ODE. The model then solves for the three-dimensional trajectory of the plume centerline using the one-dimensional integral equations. Hydrodynamic conditions (though allowed to be unsteady) must be supplied as input to the model.

D.2.2 WASP: Water Quality Analysis Simulation Program

The WASP system is a generalized framework for modeling contaminant fate and transport in surface waters. The model does not solve a set of multi-dimensional dynamical equations, but rather is based on the flexible compartment modeling approach. WASP can be applied in one, two, or three dimensions. Problems that have been studied using the WASP framework include biochemical oxygen demand and dissolved oxygen dynamics, nutrients and eutrophication, bacterial contamination, and organic chemical and heavy metal contamination.

Because WASP in an EPA model, input and output linkages also have been provided to other stand-alone models. Flows and volumes predicted by the link-node hydrodynamic model DYNHYD can be read and used by WASP. Loading files from PRZM and HSPF can be reformatted and read by WASP. Toxicant concentrations predicted by TOXI can be read and used by both the WASP Food Chain Model and the fish bioaccumulation model FGETS.

A body of water is represented in WASP as a series of computational elements or segments. Environmental properties and chemical concentrations are modeled as spatially constant within segments. Segment volumes and type (surface water, subsurface water, surface benthic, subsurface benthic) must be specified, along with hydraulic coefficients for riverine networks.

D.2.3 POM: Princeton ocean model

POM is the precursor to ECOM-si (see the next section), and was developed in the late 1970s. It is a fully three-dimensional hydrodynamic numerical model, designed to predict ocean circulation. The POM model is freely available to non-commercial applications.

The POM model contains an imbedded second moment turbulence closure sub-model to provide vertical mixing coefficients. It is a sigma coordinate model in that the vertical coordinate is scaled on the water column depth. The horizontal grid uses curvilinear orthogonal coordinates. The horizontal time differencing is explicit whereas the vertical differencing is implicit. The latter eliminates time constraints for the vertical coordinate and permits the use of fine vertical resolution in the surface and bottom boundary layers. The model has a free surface and a split time step. The external mode portion of the model is two-dimensional and uses a short time step. The internal mode is three-dimensional and uses a long time step. Complete thermodynamics have been implemented.

D.2.4 ECOM-si: Estuarine, coastal and ocean model

Ecom-si is a three-dimensional ocean circulation model developed principally by Alan Blumberg of HydroQual. It is similar to the pom model, but incorporates a semi-implicit scheme for solving the gravity wave so that the need for separate barotropic (external) and baroclinic (internal) time steps is eliminated. The ecom-si model is not freely available, but must be obtained through HydroQual.

Ecom-si includes a free surface, nonlinear advective terms, coupled density and velocity fields, river runoff, heating and cooling of the sea surface, a 2.5 level turbulence closure scheme to represent vertical mixing, and is designed to easily allow "realistic" simulations. In addition, the combination of orthogonal curvilinear coordinates in the horizontal plane and sigma-coordinates in the vertical dimension allows grid refinement in regions of interest without sacrificing the well-known characteristics of Cartesian grid schemes. For water quality modeling, both pom and ecom-si must be combined with a transport model.