Appendix A. ASA's WQMAP

WQMAP (Water Quality Mapping and Analysis Program) is a proprietary modeling system developed by Applied Science Associates, Inc. and the University of Rhode Island for water quality mapping and analysis. WQMAP is advertised as an integrated system for modeling the circulation and water quality of estuarine and coastal waters (Spaulding et al. 1999b). The system has a suite of integrated environmental models, including a boundary-conforming grid generation model, a three-dimensional hydrodynamic model, and a set of pollutant transport and fate models (single- and multiple-constituent and WASP5 eutrophication kinetics). All operate on a boundary-conforming grid system and are supported by an embedded geographic information system and environmental data management tools. WQMAP runs on a Windows-based personal computer. Color graphics and animation are used to display model prediction. The system is structured to facilitate application to any geographic area.

WQMAP's hydrodynamic model solves the three-dimensional conservation of water mass, momentum, salt and energy equations on a spherical, non-orthogonal, boundary conforming grid. Relevant equations are presented at the end of this section. The model may be applied to both fresh and salt water systems, and can simulate the effects of tide, river flow, air temperature; solar radiation and wind induced environmental forcing on circulation and water properties including temperature and salinity. Bottom stress is determined from a quadratic law. If sufficient resolution near the bottom boundary is provided, the drag coefficient C_D may be estimated so that velocities match the logarithmic law of the wall. In those cases where bottom boundary layer is not well resolved, C_D may be specified as a constant, typically between 0.002-0.003, or it may be calibrated based on observations. An environmental heat transfer sub-model at the water surface contains an explicit balance of short-wave solar radiation, long-wave atmospheric radiation, long-wave radiation emitted from the water surface, convective (sensible) heat transfer and evaporative (latent) heat transfer between water and air.

There are three separate models within the WQMAP pollutant transport model system, all using the same grid as the hydrodynamic model. The first is a single constituent transport model, which includes first order reaction terms. This model is suitable for a single constituent contaminant that settles or decays, like suspended sediment and fecal coliform bacteria. The second is a multi-constituent transport and fate model with a reaction matrix that can be specified by the user. This can be used to custom design a multi-component water quality model system. The third is a multi-constituent eutrophication model (e.g. nitrogen, phosphorous, dissolved oxygen) that incorporates EPA WASP5 kinetic rate equations. The user can set the parameters of the rate equations via the user interface or select default values.

WQMAP Governing Equations

The WQMAP solves the following set of equations, which govern the conservation of mass, momentum, salt, energy, dissolved constituents, turbulent kinetic energy, and turbulent dissipation. Implicit here are the assumptions of hydrostatics and the Boussinesq approximation.

By employing the following operators:

$$\psi_{x'} = \frac{\partial \psi}{\partial x'},\ \psi_{y'} = \frac{\partial \psi}{\partial y'},\ \psi_{\gamma} = \frac{\partial \psi}{\partial \gamma},\ \psi_{t'} = \frac{\partial \psi}{\partial t'}$$

(1)

differential operators in the (x, y, z, t) system can be expressed in terms of derivatives in the (x', y', γ, t') by

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x'} - \frac{\partial}{\partial \gamma}\frac{\psi_{x'}}{\psi_{\gamma}},\ \frac{\partial}{\partial y} = \frac{\partial}{\partial y'} - \frac{\partial}{\partial \gamma}\frac{\psi_{y'}}{\psi_{\gamma}},\ \frac{\partial}{\partial z} = \frac{\partial}{\partial \gamma}\frac{1}{\psi_{\gamma}},\ \frac{\partial}{\partial t} = \frac{\partial}{\partial t'} - \frac{\partial}{\partial \gamma}\frac{\psi_{t'}}{\psi_{\gamma}}$$

(2)

conservation equations in (x', y', γ, t') can be written as follow (all primes will be fopped for notational convenience).

Conservation of water mass:

$$\frac{\partial \psi_{\gamma}}{\partial t} + \frac{\partial u\psi_{\gamma}}{\partial x} + \frac{\partial v\psi_{\gamma}}{\partial y} + \frac{\partial \omega\psi_{\gamma}}{\partial \gamma} = 0$$

(3)

conservation of momentum - x and y

$$\frac{\partial u\psi_{\gamma}}{\partial t} + \frac{\partial u^2\psi_{\gamma}}{\partial x} + \frac{\partial uv\psi_{\gamma}}{\partial y} + \frac{\partial u\omega\psi_{\gamma}}{\partial \gamma} - \psi_{\gamma} f v = \frac{\partial}{\partial \gamma}\left(\frac{K_v}{\psi_{\gamma}}\frac{\partial u}{\partial \gamma}\right) - \frac{\psi_{\gamma}}{\rho_0}\left[\rho g \frac{\partial \eta}{\partial x} - gqD\frac{\partial \bar{\rho}_{\gamma}}{\partial x} + (\rho - \bar{\rho}_{\gamma})g\frac{\partial qD}{\partial x}\right] + \psi_{\gamma} F_x$$

(4)

$$\frac{\partial v\psi_\gamma}{\partial t} + \frac{\partial uv\psi_\gamma}{\partial x} + \frac{\partial v^2\psi_\gamma}{\partial y} + \frac{\partial v\omega\psi_\gamma}{\partial \gamma} + \psi_\gamma fu = \frac{\partial}{\partial \gamma}\left(\frac{K_v}{\psi_\gamma}\frac{\partial v}{\partial \gamma}\right) - \frac{\psi_\gamma}{\rho_0}\left[\rho g\frac{\partial \eta}{\partial y} - gqD\frac{\partial \bar{\rho}_\gamma}{\partial y} + (\rho - \bar{\rho}_\gamma)g\frac{\partial qD}{\partial y}\right] + \psi_\gamma F_v$$

(5)

conservation of salt and energy

$$\frac{\partial S\psi_\gamma}{\partial t} + \frac{\partial uS\psi_\gamma}{\partial x} + \frac{\partial vS\psi_\gamma}{\partial y} + \frac{\partial \omega S\psi_\gamma}{\partial \gamma} = \frac{\partial}{\partial \gamma}\left(\frac{N_v}{\psi_\gamma}\frac{\partial S}{\partial \gamma}\right) + \psi_\gamma F_s$$

(6)

$$\frac{\partial T\psi_\gamma}{\partial t} + \frac{\partial uT\psi_\gamma}{\partial x} + \frac{\partial vT\psi_\gamma}{\partial y} + \frac{\partial \omega T\psi_\gamma}{\partial \gamma} = \frac{\partial}{\partial \gamma}\left(\frac{N_v}{\psi_\gamma}\frac{\partial T}{\partial \gamma}\right) + \psi_\gamma F_T$$

(7)

conservation of pollutant constituent

$$\frac{\partial C\psi_\gamma}{\partial t} + \frac{\partial uC\psi_\gamma}{\partial x} + \frac{\partial vC\psi_\gamma}{\partial y} + \frac{\partial \omega C\psi_\gamma}{\partial \gamma} + \frac{\partial}{\partial \gamma}\left(\frac{N_v}{\psi_\gamma}\frac{\partial C}{\partial \gamma}\right) + \psi_\gamma(F_C + \mathbf{S} + \mathbf{R}C)$$

(8)

κ-ε turbulent closure

$$\frac{\partial k\psi_\gamma}{\partial t} + \frac{\partial uk\psi_\gamma}{\partial x} + \frac{\partial vk\psi_\gamma}{\partial y} + \frac{\partial \omega k\psi_\gamma}{\partial \gamma} = \frac{\partial}{\partial \gamma}\left(\frac{K_v}{\psi_\gamma\sigma_k}\frac{\partial k}{\partial \gamma}\right) + \psi_\gamma(P + G) - \varepsilon\psi_\gamma + \psi_\gamma F_k$$

(9)

$$\frac{\partial \varepsilon\psi_\gamma}{\partial t} + \frac{\partial u\varepsilon\psi_\gamma}{\partial x} + \frac{\partial v\varepsilon\psi_\gamma}{\partial y} + \frac{\partial \omega\varepsilon\psi_\gamma}{\partial \gamma} = \frac{\partial}{\partial \gamma}\left(\frac{K_v}{\psi_\gamma\sigma^\varepsilon}\frac{\partial \varepsilon}{\partial \gamma}\right) + \psi_\gamma\left[C_1\frac{\varepsilon}{k}(P + C_3G) - C_2\frac{\varepsilon^2}{k}\right] + \psi_\gamma F_\varepsilon$$

(10)

where

$$q = \gamma - a\frac{D}{D_r}\sin 2\pi\gamma$$

(11)

and ρ_γ is defined as a vertically averaged density at a depth of γ

$$\bar{\rho}_\gamma = \frac{1}{\eta - z}\int_z^\eta \rho\, dz = -\frac{1}{q}\int_\gamma^0 \rho \frac{\partial q}{\partial \gamma} d\gamma$$

(12)

t = time; S = salinity; T = temperature; C represents concentration of a dissolved constituent; ρ = density; ρ_0 = mean density; g = gravity; (u, v) = components of velocity in the (x, y) directions, respectively; (K_v, N_v) = vertical eddy viscosity and diffusivity, respectively; f = Coriolis parameter ($2\Omega \sin \theta$), in which Ω is the earth's rotation rate and θ is the latitude; P is turbulent production; G is the buoyancy generation; **R** is a reaction matrix; and **S** represents sources and sinks of constituent material which are detailed in Thomann and Mueller (1988). The following recommended empirical constants (Laulder and Spalding 1974; Rodi 1980) are adopted: $C_\mu = 0.09$, $\sigma_t = 0.7$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $C_{1\varepsilon} = 1.43$, $C_{2\varepsilon} = 1.92$, $C_{3\varepsilon} = 0.2$.

The vertical eddy viscosity and diffusivity are expressed as

$$K_v = f_1 C_\mu \frac{k^2}{\varepsilon}; \quad N_v = f_2 \frac{K_v}{\sigma_t}$$

(13)

where f_1 and f_2 = empirical functions (Munk and Anderson 1948) dependent on Richardson number R to account for the buoyant effect

$$f_1 = (1 + 10\mathrm{R})^{-0.5}; \quad f_2 = (1 + 3.33\mathrm{R})^{-1.5}; \quad \mathrm{R} = -\frac{g}{\rho}\frac{\frac{\partial \rho}{\partial z}}{\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2}$$

(14)

the horizontal diffusion terms (Mellor and Blumberg 1985) are expressed as

$$\psi_\gamma F_x = \frac{\partial}{\partial x}\left(2\psi_\gamma K_h \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left[\psi_\gamma K_h \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)\right]$$

(15)

$$\psi_\gamma F_y = \frac{\partial}{\partial x}\left[\left(\psi_\gamma K_h \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left(2\psi_\gamma K_h \frac{\partial v}{\partial y}\right); \quad \psi_\gamma F_{q_i} = \frac{\partial}{\partial x}\left(\psi_\gamma K_h \frac{\partial q_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(\psi_\gamma K_h \frac{\partial q_i}{\partial y}\right)$$

(16)

where q_i represents S, T, C, k, and ε; and $\left(K_h, N_h\right)$ = horizontal eddy viscosity and diffusivity, respectively.

An equation of state for seawater relating salinity and temperature to density (Eckert 1958) closes the system. The vertical velocity ω in γ space is defined as

$$\omega = \frac{1}{\psi_\gamma}\left[w - \psi'_t - \psi'_x u - \psi'_y v\right]$$

(17)

ω can be determined by solving the conservation equation of water mass in the transformed γ space, (3). The vertical velocity w in (x, y, z) space is then calculated from (17). Vertical velocity and eddy viscosity/diffusivity are specified in the layer interface while other flow quantities (S, T, C, κ, ε) are located in the center of each layer.

Boundary conditions:

At the free surface, the boundary conditions are as follows:

$$\omega(x', y', 0, t') = 0; \quad [\tau_{wx}, \tau_{wy}] = \rho_a C_d [u_w, v_w][u_w^2 + v_w^2]^{1/2} \qquad (18)$$

$$\frac{\rho_0 N_v}{\psi_\gamma}\left(\frac{\partial T}{\partial \gamma}, \frac{\partial S}{\partial \gamma}, \frac{\partial C}{\partial y}\right) = (\dot{T}, 0, 0); \quad \frac{\partial (k, \varepsilon)}{\partial \gamma} = 0 \qquad (19)$$

where $\left(\tau_{wx}, \tau_{wy}\right)$ = wind stress components in the x- and y- directions, respectively; $\left(u_w, v_w\right)$ = wind velocity components in the x- and y- direction, respectively; ρ_{air} = air density; C_d = air-water drag coefficient; and T = net ocean surface heat flux. Eq. (19) is used when no wind stress is applied. Otherwise, the surface turbulent kinetic energy κ_s and dissipation ε_s are estimated by the following relations (Rodi 1980; ASCE Task Committee 1988)

$$k_s = \frac{u_*^2}{\sqrt{C_\mu}}; \quad \varepsilon_s = \frac{|u_*|^3}{\kappa \Delta z} \tag{20}$$

where u_* = surface velocity shear; Δz = distance to the surface at the first grid point below surface, as suggested by Raithby et al.(1988).

At all solid boundaries, no normal flux of momentum, salt, energy, and dissolved constituent is allowed. The bottom stress is determined from a quadratic law similar to that at the surface and is given by

$$[\tau_{bx}, \tau_{by}] = \rho_0 C_f [u_b, v_b][u_b^2 + v_b^2]^{1/2} \tag{21}$$

where $\left(\tau_{bx}, \tau_{by}\right)$ = bottom stress components in the x- and y-directions, respectively; u_b, v_b =bottom velocity components in the x- and y-directions, respectively; ρ_0 = mean water density; and C_f = empirical coefficient for bottom friction. if sufficient resolution near the bottom boundary is provided, C_d was estimated so that velocities match the logarithmic law of the wall

$$C_d = \left[\frac{1}{\kappa}\ln(\Delta z_b)/z_0\right]^{-2}$$

(22)

where the karman constant κ = 0.42; Δz_b = distance from the bottom in the grid point nearest the bottom; and z_0 = parameter dependent on the local bottom roughness and set to 1 cm (Blumberg and Mellor 1987).

The bottom turbulent kinetic energy κ_b and dissipation ε_b are determined from relations in the form of (20) with the bottom velocity shear u_* and the distance $\Delta z = \Delta z_0$ at the grid point nearest the bottom.

At inflow boundaries, κ and ε can be prescribed from fully developed channel flow data (Demuren and Rodi 1983) as

$$k_d = 0.004u_d^2;\ \varepsilon_d = C_\mu^{3/4}\frac{k_d^{3/2}}{0.09b} \qquad (23)$$

where u_d = inflow velocity; and b = inflow inlet width.

At open boundaries, the surface elevation or mass flux is required as are fluxes of salt, energy, dissolved constituent in to the system. On outflow simplified conservation equations, using only the advection terms, are used to transport salt, heart, turbulent kinetic energy and dissipation

$$\frac{\partial(S, T, C, k, \varepsilon)}{\partial t} + V_n\frac{\partial(S, T, C, k, \varepsilon)}{\partial x_n} = 0 \qquad (24)$$

where V_n = velocity normal to the open boundary.