5 STRUCTURE AND METHODS IN RMA-11

5.1 Introduction

RMA-11 has been designed to replicate most of the water quality constituent relations used in QUAL2E. It has also been constructed in a modular form so that additional constituents and associated interactions can be readily added. The sections that follow discuss some of the important features of the implementation aspects of the model.

5.2 Use Of Newton-Raphson Iteration To Accommodate Constituent Interactions.

RMA-11 has been programmed to give the user maximum flexibility when selecting how the model will operate on the constituents. In RMA-4 first order reaction rates were approximated using a single iteration on a projected best estimate from the previous time step. RMA-11 allows the user to select from a variety of options when setting up the solution approach.

Given a governing differential equation for a constituent C:

$$L\,(C^*) = 0$$

where L is a partial differential operator and C* is the set of all active constituents, then the finite element representation of the Newton Raphson iteration for the time dependent, advection and diffusion section [A] and the first order rate term [K] may be written as:

$$[A]\,\{\Delta C\} + [K]\,\{\Delta C\} = -\{S\}$$

where $\{\Delta C\}$ is the vector of changes to the present estimate {C} during the current iteration and [S] is the error vector representing the L evaluated at the current best estimates of all the constituents C*. In this expression, in addition to the geometry. [A] is a function only of the time step, the velocity distribution and the diffusion coefficients. However the first order term [K] depends on the geometry and all the constituents C*. Conventional solution would combine [A] and [K] and solve
If this method were selected then a different set of equations would have to be formed and solved for each constituent. This could lead to very long computer times.

RMA-11 offers several alternatives. A computer efficient method is neglect [K] and solve:

$$[A\,]\,\{\Delta C\} = -\{S\}$$

In this case A is a constant for all constituents and simultaneous solution for all constituents is possible. This is in essence successive iterations Note that the repeated iterations within a time step will update the matrix {S} so that a true solution will be achieved if the method converges. The key to satisfactory convergence in this approach is that [A] be small in magnitude relative to [K]. If this is not satisfied then the solution will converge either very slowly or not all. A typical case where this can occur is in sand transport where the settling rate is often relatively large. RMA-11 provides two alternatives for this case. One is to allow the user to isolate this constituent and solve by successive iteration for this constituent

separately, the other permits the user to separate this constituent and to retain [K] in the global matrix.

In the model these options are implemented through the NPASS variable that is input for each constituent. The NPASS variable defines when and how a constituent appears in the solution scheme. Constituents with the same NPASS number are solved simultaneously. If the NPASS number is set negative, then the alternative in which [K] is active will be used. Note that a given NPASS number may be set negative for only one constituent. In other words if several constituents have important [K] contributions each must be given a separate negative NPASS number.

5.3 Subroutine Structure

The principal finite element coefficient construction routines are as follows

- COEF1 for one-dimensional channel elements.
- COEF2 for two-dimensional depth averaged elements.
- COEFV for two-dimensional laterally averaged elements.
- COEF3 for three-dimensional elements.
- SURCOF for one and two-dimensional surface elements where external boundary conditions are applied

During execution of the model numerical integration (Gaussian quadrature) is undertaken to develop the coefficient matrices for each element. So that, within the coefficient subroutines above the basic equations are evaluated and their contributions summed at a series of Gauss points. This means that values for all the principal variables must developed. The coefficient routines construct the time dependent, advective and dispersive contributions internally. The water quality parameters are developed using a basic call to the same routine MKRATES for all approximations. It, in turn, calls the appropriate subroutine to assemble the reaction rate, settling and source terms for each constituent.
Users wishing to modify the model should examine the subroutines in the MKRATES block for examples of how the logic is constructed and of the variable names used. Water quality data is input in INCON and changes and/or additions to data should be added in that routine.

5.4 Temperature Simulation

The temperature state variable is maintained in metric units only (deg C)! Initial and boundary conditions for temperature must be in degrees C. Atmospheric data may be supplied in metric or English (deg F, etc) units. This data includes atmospheric absorption and pressure, wet bulb and dry bulb air temp, wind speed and elevation of the basin. The METRIC flag in the global system coefficients line identifies whether the atmospheric data is described in English or metric units. Subroutine HEATEX is the main operative routine external to the MKRATES block.

5.5 Routines For Suspended Sediment

Bed accretion and loss are incorporated and recorded in the model for the suspended sediment simulations, either cohesive or non-cohesive. When cohesive

sediments are simulated the model permits consolidation and layered structures for the bed.

When these constituents are simulated separate subroutine blocks are used to update estimates of settling, bed accretion or loss etc. These blocks are called between iterations and keep track of the bed structure on a node by node basis.