

The Texas A&M University and U.S. Bureau of Reclamation Hydrologic Modeling Inventory (HMI) Questionnaire

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Name of Model, Date, Version Number:

OTEQ (One-dimensional Transport with EQUilibrium chemistry), 2010 release

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<http://water.usgs.gov/software/OTEQ/>

Brief Description:

OTEQ is a mathematical simulation model used to characterize the fate and transport of waterborne solutes in streams and rivers. The model is formed by coupling a solute transport model with a chemical equilibrium submodel. The solute transport model is based on OTIS, a model that considers the physical processes of advection, dispersion, lateral inflow, and transient storage. The equilibrium submodel is based on MINTEQA2, a model that considers the speciation and complexation of aqueous species, acid-base reactions, precipitation/dissolution, and sorption.

Within OTEQ, reactions in the water column may result in the formation of solid phases (precipitates and sorbed species) that are subject to downstream transport and settling processes. Solid phases on the streambed may also interact with the water column through dissolution and sorption/desorption reactions. Consideration of both mobile (waterborne) and immobile (streambed) solid phases requires a unique set of governing differential equations and solution techniques that are developed herein. The partial differential equations describing physical transport and the algebraic equations describing chemical equilibria are coupled using the sequential iteration approach. The model's ability to simulate pH, precipitation/dissolution, and pH-dependent sorption provides a means of evaluating the complex interactions between instream chemistry and hydrologic transport at the field scale.

Model Type:

Water quality

Model Objective(s):

Simulate the fate and transport of inorganic constituents, especially metals

Model Structure or Mathematical Basis:

Mass transport as simulated with the advection-dispersion equation

Spatial Scale Employed in the Model:

One-dimensional stream system (transport in the longitudinal direction) with multiple stream reaches; length of stream system is user defined.

Temporal Scale Employed in the Model:

dynamic or steady-state simulations

Input Data Requirement:

stream system configuration (number and lengths of reaches), list of chemical components (e.g. sodium, sulfate, aluminum, etc.), types of reactions (precipitation, sorption/desorption), and hydrologic/hydraulic information (streamflow, dispersion, etc.).

Model Output:

Component (constituent) concentrations as a function of time and/or space.

Input Data Format:

flat ASCII files

Output Data Format:

flat ASCII files

Parameter Estimation/Model Calibration:

manual

Model Testing and Verification:

see model documentation and references at <http://water.usgs.gov/software/OTEQ/apps/>

Model Sensitivity:**Model Reliability:****Model Application/Case Studies:**

<http://water.usgs.gov/software/OTEQ/apps/>

Platform/Operating System:

Linux, Solaris

Programming language and software:

Fortran 77

Web-based or desk-top application?

Desktop

Is the application flexible to couple with external programs and user created executables?

Input flexibility includes ability to link with flow routing models for consideration of solute transport under unsteady flow regimes.

Are system and user documentation available? (Web site)

<http://water.usgs.gov/software/OTEQ/doc/>

Are example applications available? (Web site)

see model documentation and references at <http://water.usgs.gov/software/OTEQ/apps/>

Is there a user group or hotline-type support? (Website)