

## Appendix C-T7. Surface-water quality models (fate and transport)

<i>Method: Level I</i>		
<p><b>Description:</b> Calculates the equilibrium distribution of a fixed quantity of conserved (i.e., nonreacting) chemical in a closed environment at equilibrium with no degrading reactions, no advective processes, and no intermediate transport processes.</p> <p><b>Equilibrium:</b> 1-dimensional  <b>Version:</b> March 2004  <b>Format:</b> Windows</p> <p><b>References:</b> Mackay 2001  <b>Website:</b>  <a href="http://www.trentu.ca/academic/aminss/envmodel/models/models.html">www.trentu.ca/academic/aminss/envmodel/models/models.html</a></p>	<p><b>Advantages:</b> None reported.</p> <p><b>Disadvantages:</b> None reported.</p>	<p><b>Analyte capability:</b>            Organo-chlorines, other organic compounds</p>
<i>Method: Level II</i>		
<p><b>Description:</b> Models a situation in which a chemical is continuously discharged at a constant rate and achieves a steady-state and equilibrium condition, at which the input and output rates are equal.</p> <p><b>Equilibrium:</b> 1-dimensional  <b>Version/released:</b> February 17, 1999  <b>Format:</b> Windows</p> <p><b>References:</b> Mackay 2001  <b>Website:</b>  <a href="http://www.trentu.ca/academic/aminss/envmodel/models/models.html">www.trentu.ca/academic/aminss/envmodel/models/models.html</a></p>	<p><b>Advantages:</b> None reported.</p> <p><b>Disadvantages:</b> None reported.</p>	<p><b>Analyte capability:</b>            Organo-chlorines, other organic compounds</p>
<i>Method: Level III</i>		
<p><b>Description:</b> Describes the fate of a chemical continuously discharged at a constant rate and has achieved a steady-state condition in which input and output rates are equal but equilibrium between media is not assumed.</p> <p><b>Steady state:</b> 1-dimensional  <b>Version/released:</b> February 7, 2004  <b>Format:</b> Windows</p> <p><b>References:</b> Mackay 2001  <b>Website:</b>  <a href="http://www.trentu.ca/academic/aminss/envmodel/models/models.html">www.trentu.ca/academic/aminss/envmodel/models/models.html</a></p>	<p><b>Advantages:</b> None reported.</p> <p><b>Disadvantages:</b> None reported.</p>	<p><b>Analyte capability:</b>            Organo-chlorines, other organic compounds</p>

<i>Method: Quasi</i>		
<p><b>Description:</b> Describes the steady-state behavior of an organic chemical in a lake subject to chemical inputs by direct discharge, inflow in rivers, and deposition from the atmosphere.</p> <p><b>Steady state:</b> 1-dimensional  <b>Version/released:</b> February 8, 2002  <b>Format:</b> Windows/Basic</p> <p><b>References:</b> Mackay 2001; Mackay, Joy, and Patterson 1983  <b>Website:</b>  <a href="http://www.trentu.ca/academic/aminss/envmodel/models/model_s.html">www.trentu.ca/academic/aminss/envmodel/models/model_s.html</a></p>	<p><b>Advantages:</b> None reported.</p> <p><b>Disadvantages:</b> None reported.</p>	<p><b>Analyte capability:</b>            Organo-chlorines, other organics, metals</p>
<i>Method: Sediment</i>		
<p><b>Description:</b> Calculates the water-sediment exchange characteristics of a chemical based on its physical chemical properties and total water and sediment concentrations.</p> <p><b>Steady state:</b> 1-dimensional  <b>Version/released:</b> February 2004  <b>Format:</b> Windows</p> <p><b>References:</b> Rueber et al. 1987, Mackay 2001  <b>Website:</b>  <a href="http://www.trentu.ca/academic/aminss/envmodel/models/model_s.html">www.trentu.ca/academic/aminss/envmodel/models/model_s.html</a></p>	<p><b>Advantages:</b> Useful for determining the likely fate of a chemical subject to transfer between a water column and a sediment compartment.</p> <p><b>Disadvantages:</b> None reported.</p>	<p><b>Analyte capability:</b>            Organo-chlorines, other organic compounds</p>
<i>Method: Exams</i>		
<p><b>Description:</b> Interactive computer software for formulating aquatic ecosystem models and rapidly evaluating the fate, transport, and exposure concentrations of synthetic organic chemicals.</p> <p><b>Steady state to dynamic:</b> 1-dimensional  <b>Version/released:</b> 2.98.04.06/2005  <b>Format:</b> Fortran</p> <p><b>Website:</b>  <a href="http://www.epa.gov/ceampubl/swater/exams/exams2980406.html">www.epa.gov/ceampubl/swater/exams/exams2980406.html</a></p>	<p><b>Advantages:</b> A “legacy” Fortran routine that is used extensively to model the fate, transport, and exposure concentrations of synthetic organic chemicals, including pesticides, industrial materials, and leachates from disposal sites. Often used to predict hazards of pesticides a priori. Can be integrated seamlessly into other model platforms.</p> <p><b>Disadvantages:</b> Steep learning curve and requires numerous input variables, some of which may have to be assumed.</p>	<p><b>Analyte capability:</b>            Organo-chlorines, other organic compounds</p>

<i>Method: SMPTOX4</i>		
<b>Description:</b> SMPTOX is a steady-state flow model that simulates transport and fate of chemical pollutants in suspended solids, dissolved in the water column, and in sediments.  <b>Steady state:</b> 1-dimensional <b>Version/released:</b> 1995 <b>Format:</b> DOS  <b>Supporting agency/developer:</b> USEPA Center for Exposure Assessment Modeling  <b>Reference:</b> USEPA 1995b	<b>Advantages:</b> None reported.  <b>Disadvantages:</b> Steady-state predictions only. Nonpoint source loadings cannot be simulated. Does not consider daughter products or processes. Process kinetics is not simulated.	<b>Analyte capability:</b> Organo-chlorines, metals
<i>Method: MIKE11-WQMIKE21-WQMIKE3W</i>		
<b>Description:</b> Generalized modeling package-1D(/2D/3D) water quality module.  <b>Dynamic:</b> 1-dimensional to 3-dimensional <b>Format:</b> Geographic information system (GIS)  <b>Supporting agency/developer:</b> Danish Hydraulic Institute  <b>Website:</b> <a href="http://www.mikebydhi.com">www.mikebydhi.com</a>	<b>Advantages:</b> None reported.  <b>Disadvantages:</b> None reported.	<b>Analyte capability:</b> Hydraulic models of rivers and floodplains
<i>Method: RATECON (Great Lakes Rate Constant Model)</i>		
<b>Description:</b> Rate constant model for chemical dynamics, designed to predict the fate and recovery times of contaminants in the Great Lakes; similar to QWASI but not using the fugacity concept.  <b>Dynamic:</b> 1-dimensional <b>Version/released:</b> 1991 <b>Format:</b> Basic  <b>References:</b> Mackay et al. 1994 <b>Website:</b> <a href="http://www.trentu.ca/academic/aminss/envmodel/models/models.html">www.trentu.ca/academic/aminss/envmodel/models/models.html</a>	<b>Advantages:</b> None reported.  <b>Disadvantages:</b> None reported.	<b>Analyte capability:</b> Developing a complete quantification of all processes, thus providing a decision support tool to improve management and remediation of aquatic systems by linking loading to concentration
<i>Method: Watershed Analysis Risk Management Framework (WARMF)</i>		
<b>Description:</b> Provides a roadmap to calculate total maximum daily loads for most conventional pollutants.  <b>Dynamic:</b> 1-dimensional to 2-dimensional <b>Version:</b> 6.1/September 1, 2005 <b>Format:</b> Windows 95/98/ME/2000xp  <b>Website:</b> <a href="http://www.epa.gov/athens/wwqtsc/html/warmf.html">www.epa.gov/athens/wwqtsc/html/warmf.html</a>	<b>Advantages:</b> See website.  <b>Disadvantages:</b> None reported.	<b>Analyte capability:</b> Coliform, TSS, biological oxygen demand, nutrients

<b>Method: Water Quality Analysis Simulation Program (WASP6)</b>		
<b>Description:</b> Helps users interpret and predict water-quality responses to natural phenomena and man-made pollution for various pollution management decisions.  <b>Dynamic:</b> 1-dimensional to 3-dimensional <b>Version/released:</b> 7.41/June 7, 2010 <b>Format:</b> Windows 95/98/ME/2000xp  <b>Website:</b> <a href="http://www.epa.gov/athens/wwqtsc/html/wasp.html">www.epa.gov/athens/wwqtsc/html/wasp.html</a>	<b>Advantages:</b> None reported.  <b>Disadvantages:</b> None reported.	<b>Analyte capability:</b> Metals (Hg), organo-chlorines, other organics
<b>Method: AQUATOX–Dynamic, with food web</b>		
<b>Description:</b> Predicts the fate of various pollutants, such as nutrients and organic chemicals, and their effects on the ecosystem, including fish, invertebrates, and aquatic plants.  <b>Steady state to dynamic:</b> 2-dimensional <b>Version/released:</b> 3.0 <b>Format:</b> Windows  <b>Website:</b> <a href="http://www.epa.gov/waterscience/models/aquatox/">www.epa.gov/waterscience/models/aquatox/</a>	<b>Advantages:</b> None reported.  <b>Disadvantages:</b> None reported.	<b>Analyte capability:</b> Organo-chlorines, other organics
<b>Method: ECOFATE</b>		
<b>Description:</b> Includes a steady-state and a time-dependent model of the mass transport and food-web bioaccumulation of organic chemicals in aquatic ecosystems. It can be used to assess the distribution of chemical concentrations in water, sediment, and aquatic biota in real-world aquatic ecosystems.  <b>Steady state to dynamic:</b> 1-dimensional to 2-dimensional <b>Version/released:</b> 1998 <b>Format:</b> Visual Basic for Windows 3.x platform  <b>Website:</b> <a href="http://research.rem.sfu.ca/toxicology/models/models.htm#ecofate">http://research.rem.sfu.ca/toxicology/models/models.htm#ecofate</a>	<b>Advantages:</b> None reported.  <b>Disadvantages:</b> None reported.	<b>Analyte capability:</b> Organics