Addendum to EPA-453/R-02-011b September 2002

ADDENDUM

to

TRIM

Total Risk Integrated Methodology

TRIM.FaTE

Technical Support Document Volume II: Description of Chemical Transport and Transformation Algorithms

March 2003

U.S. Environmental Protection Agency Office of Air Quality Planning and Standards Emissions Standards & Air Quality Strategies and Standards Divisions Research Triangle Park, North Carolina

[This page intentionally left blank.]

ADDENDUM

This Addendum to the Technical Support Document, Volume II, for TRIM.FaTE includes three sections. Section 1, Errata, provides a list of corrections for the September 2002 version of the TSD. Section 2, Library Changes, lists a change that was made to the TRIM.FaTE public reference library as a result of test runs after September 2002. Section 3 includes a few points of clarification for the TSD.

1. ERRATA

Page 2-7, Eq. 2-18.... Replace ρ_d with K_d , the correct equation is:

$$\kappa_{\text{solid}} = \rho_{\text{solid}} \times K_d \times CF \tag{Eq. 2-18}$$

Page 4-3, TF 4-12..... Replace E_{ij} with DSP_{ij} in both locations; the correct equation is: **Page 4-4**, E_{ij} **definition**

$$T^{disp}_{SMA \to j} = \frac{DSP_{ij} \times A_{ij}}{L_{ii} \times V_{i}}$$
 TF 4-12

Page 5-18, TF 5-6.Multiply the transfer factor equation by $(1 - I_{dry})$ so that only the
dust particles deposited directly to the surface soil (i.e., not
intercepted by the plant leaves) are available for dry resuspension.
The correct equation is:

$$T_{\underline{Ss} \to \underline{AirP}}^{res} = \frac{A_{\underline{Ss}}}{V_{\underline{Ss}}} \times \frac{res}{\rho_P} \times \frac{Z_{pure_solid}}{Z_{\underline{Iotal_Ss}}} \times \left(1 - I_{dry}\right)$$
(TF 5-6)

where:

 I_{dry} = fraction of dry deposition that is intercepted by plants (unitless) [also defined on top of page 5-16]

Page 6-9, Eq. 6-9..... The equation is missing a units conversion factor of 1 kg/L. The correct equation is:

$$k_{BI,\alpha\alpha-W} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{BIW}}\right] \times K_{BI-W} \times 1\left(\frac{\lg}{L}\right)$$
(Eq. 6-9)

Page 6-9, V_{Sed} variable name in the V_W definition

The variable V_{Sed} in the V_W definition refers to the volume of the sediment compartment in units of liters. TRIM.FaTE assumes units of m³ for the volume of the sediment compartment. Thus, to clarify that the units for V_{Sed} in the definition of V_W are in liters, the name of the variable should be changed to $V_{Sed L}$. Thus:

- V_W = volume of water in the sediment compartment (L) = $V_{Sed_L} \times \theta$, where: V_{Sed_L} = volume of sediment compartment (L)...
- Page 6-10, TF 6-3aThe equation is missing a units conversion factor of 1/1000 to
convert from the sediment volume expressed in L to the sediment
volume expressed in m³, which are the units used in TRIM.FaTE.
Thus, the correct equation is:

$$T_{Sed W \rightarrow BI} = \frac{n_{BI} \times m_{BI} \times k_{BI, acc-Sed W}}{V_{Sed _L}} \times \frac{Fraction_Mass_Dissolved}{\theta}$$
$$= \frac{n_{BI} \times m_{BI} \times k_{BI, acc-Sed W}}{V_{Sed} \times 1000(\frac{L}{m3})} \times f_{ML}$$
(TF 6-3)

where:

$$V_{Sed_L} =$$
 volume of sediment compartment (L), and
 $V_{Sed} =$ volume of sediment compartment (m³).

Page 7-22, $K_{Root-Sr}$ units Replace "m³[soil wet wt]" with "m³[soil]". The correct units are:

 $K_{Root-Sr}$ units = (g[chemical]/m³[root] per g[chemical]/m³[soil])

Page 7-29, Q_{Ph} definition . . . Change "leaves" to "stem from leaves"; the correct definition is

 Q_{Ph} = phloem flux into stem from leaves (...)

Page 7-35, TF 7-17b

Equation is incorrect. It should be the same as TF 7-17b on page 7-40. The correct equation from page 7-40 is:

$$T_{\text{SrW} \to \text{Worm}} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{\text{WSrW}}}\right] \times K_{\text{Worm}-\text{SrW}} \times \frac{M_{\text{Worm}}}{V_{\text{Sr}} \times 1000} \times \frac{Z_{\text{pure}_water}}{Z_{\text{Total}}}$$
(TF 7-17b)

Page 7-49, IN_W definition Replace "m³[air]" with "m³[water]"; the correct definition is:

$$IN_W$$
 = water ingestion rate normalized to body weight
(m³[water]/kg[body wet wt]-day)

Page B-2; *m*_{BI} units Replace "g[BI wet wt]" with "kg[BI wet wt]", i.e.:

 m_{BI} units = (kg[BI wet wt]/individual)

Page B-2;1/1000 definition . .Replace "kg/g" with "m³/L" for the units conversion factor, i.e.:

1/1000 = units conversion factor (**m**³/**L**)

Page B-2: Eq. B-4..... Replace multiplication with division operator. The correct equation is:

$$Fraction_Mass_Dissolved = N_W / N_{Total}$$
(Eq. B-4)

Page B-3, TF B-1.... Replace V_{SedW} with V_{Sed} ; the variable in TF B-1 refers to the volume of the entire sediment compartment, not just the sediment pore water. The correct equation is:

$$T_{\textit{SedW} \rightarrow \textit{BI}} = n_{\textit{BI}} \times m_{\textit{BI}} \times \frac{CL_u}{V_{\textit{Sed}}} \times \frac{1}{1000} \times 24 \times f_{\textit{MI}} \tag{TF B-1}$$

Appendix D	There are a few corrections and clarifications of the names,		
	units, and descriptions of the input properties listed in the		
	tables in Appendix D. Refer to the most recent version of		
	the TRIM.FaTE user guidance for the revised tables.		

2. LIBRARY CHANGES

Testing of both the Bioenergetic-based Kinetic Fish Model (Section 6.4.1 of TSD Vol. II) and the Time-to-equilibrium-based Kinetic Fish Model (Section 6.4.2 of TSD Vol. II) in TRIM.FaTE after September 2002 indicated that the second model was very sensitive to the time required to reach 95 percent of the mass or concentration of chemical that would be in each biotic receptor at equilibrium with its source compartment. This time period is a property for which accurate data are difficult to

find. The time-to-equilibrium option for modeling fish bioaccumulation is therefore not included in the current TRIM.FaTE public reference library.

3. CLARIFICATION

Two sets of variable names are provided in TSD Volume II for properties related to the phase distribution of a chemical within a compartment. The initial designation of Greek letters for the variable names in Chapter 2 (page 2-10) follows one set of modeling conventions. However, the use of Greek letters proved confusing to some. Thus, the Greek letter designations in the TRIM.FaTE library were converted to variable names that described the property. In the TSD, the conversion from Greek letters to the explicit property names occurs implicitly at the end of Chapter 2 (pages 2-21 to 2-22). We therefore provide the equivalence of these property names below:

θ	=	Volume_Fraction_Liquid;
e	=	Volume_Fraction_Vapor;
φ	=	<i>Porosity</i> (i.e., 1 - <i>Volume_Fraction_Solid</i>); and
φ	=	Mass_Fraction_Sorbed.

In addition,

 $1 - \theta - \epsilon = Volume_Fraction_Solid.$

There are a few equations in later chapters in TSD Volume II in which the Greek letter is still used (i.e., θ is used instead of *Volume_Fraction_Liquid*).

Also note the equivalence of the following variable names in TSD Volume II:

Fraction_Mass_Dissolved	=	Mass_Fraction_Dissolved
Fraction_Mass_Sorbed	=	Mass_Fraction_Sorbed
Fraction_Mass_Vapor	=	Mass_Fraction_Vapor
Fraction_Mass_Algae	=	Mass_Fraction_Algae