

# TROPHICTRACE USERS MANUAL: A TOOL FOR ASSESSING RISKS FROM TROPHIC TRANSFER OF SEDIMENT-ASSOCIATED CONTAMINANTS

## TrophicTrace

Chemicals

Environment

Invertebrates

Fish

Human Exposure

Mammals

Avian

Help

Create Output

### PCBs (Total)

Add New

Edit

Delete

Home

Detail

### Child Angler

Add New

Edit

Delete

Home

Detail

### Summer Flounder

Add New

Edit

Delete

Home

Detail

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## 1 What is *TrophicTrace* ?

*TrophicTrace* is an Excel™ add-in that provides a spreadsheet tool for calculating the potential human health and ecological risks associated with bioaccumulation of contaminants in dredged sediments. This manual provides details on the equations in *TrophicTrace* and provides the Users Manual for the *TrophicTrace* spreadsheet tool. A companion document (von Stackelberg and Bridges, 2003) provides a management guide with a quantitative example of how the model can be used within the United States Army Corps of Engineers (USACE) tiered approach to dredged material management. This tool can be used to provide health- and ecologically-protective estimates of potential risk using results from sediment chemistry tests or 28-day bioaccumulation tests. A prototype of the model is presented for two types of contaminants: metals (arsenic) and chlorinated organics (polychlorinated biphenyls or PCBs and DDD, DDE, and DDT). The model currently incorporates several example datasets for assumptions for human exposure, which are presented and discussed in this paper. The user can edit the demonstration model parameters as well as create new models based on different fish species and/or human and ecological exposure parameters based on site-specific conditions.

All of the algorithms incorporated in *TrophicTrace* follow USEPA and USACE risk assessment guidance (USEPA, 1989; 1997a; USEPA/USACE, 1998; Cura et al., 1999).

*TrophicTrace* contains several human receptor population data libraries built into the demonstration form of the model, including recreational anglers (children and adult) in the New York and New Jersey (NY/NJ) area, and members of the general public (children and adult). The example exposure assumptions used for these demonstration receptor populations are obtained from the USEPA Exposure Factors Handbook (USEPA, 1997a; 1997b) as well as from the New Jersey Department of Health (NJDA, 1994). The values provided in the model are for demonstration purposes only. All model runs should be based on site-specific information. *TrophicTrace* is also parameterized for several ecological receptors, including fish, osprey, bald eagle, mink, and otter. Again, these values are provided for demonstration purposes.

Human and ecological receptors can be exposed to potential contaminants in dredged materials via ingestion of fish. The model estimates expected concentrations in fish using a sediment-based food-web for organic compounds, via trophic transfer factors from invertebrates to fish for certain metals, and via bioconcentration factors from water to fish for the remaining metals and hydrophilic organic compounds. Water concentrations are estimated using a partitioning approach based on the user-specified sediment concentration or the user can input a water concentration directly (the model requires a freely dissolved concentration but can estimate one from an input whole water concentration).

The example food-web that is included in the model is sediment based. It assumes that organic compounds partition from organic carbon in sediment to the lipid fraction of benthic invertebrates. The model is parameterized for a simple sediment-based food web representative of a food web that might be found in the Northeast Region. The invertebrate in *TrophicTrace* is the sandworm (*Nereis verins*). The model assumes that sandworms are consumed by a mid-trophic level fish represented by the mummichog (*Fundulus heteroclitus*), and that mummichog

are consumed by an upper trophic level fish represented by the summer flounder (*Paralichthys dentatus*). The user can create additional food-webs by modifying or adding additional invertebrate and/or fish species, for example, pelagic invertebrates that derive the bulk of their exposure from the water column, and/or fish that consume both benthic and pelagic invertebrates. Appendix C provides the data libraries and example values incorporated in the demonstration model for key food-web and chemical parameters that can be modified by the user.

The model allows for a characterization of uncertainty. *TrophicTrace* allows users to characterize uncertainty using trapezoidal fuzzy numbers (e.g., a minimum, a range of likeliest values, and a maximum). These uncertainties are propagated throughout the analysis using the fuzzy arithmetic principles. Model results are also presented as trapezoidal fuzzy numbers. These results are interpreted as: minimum value, a range of two likeliest values, and a maximum. If there is only data for a single value, then that value must be input for all four cells.

## 2 Installation and Running

### 2.1 What do I need to run *TrophicTrace*?

*TrophicTrace* is designed to run on IBM-compatible computers with a 486 or higher processor running Windows 95/98 or higher. The following are hardware and software requirements of *TrophicTrace*:

- 486 or higher processor
- Microsoft Windows 95/98, NT/2000 or Microsoft Windows XP
- Excel 97 or higher
- 5MB of available harddisk space
- VGA or higher-resolution video adapter (Super VGA, 256-color recommended)
- Microsoft Mouse, or compatible pointing device

Important Note: Before installing *TrophicTrace*, it is VERY IMPORTANT to go to Excel, click on “Tools” “Macro” “Security” and select “medium” or “low”. If “high” is selected, *TrophicTrace* will not run properly and will be unable to save any changes.

### 2.2 How do I install *TrophicTrace*?

*TrophicTrace* functions as a Microsoft Excel™ add-in. It is programmed in Visual Basic and runs as a macro. Therefore, it is extremely important to change the macro setting in Excel to “medium” or “low” before installing *TrophicTrace*. To install the program, select Run under the Windows Start Menu and choose “ttsetup.exe”. Excel must not be open during this procedure. The user can select or specify the folder and subdirectory that *TrophicTrace* installs to.

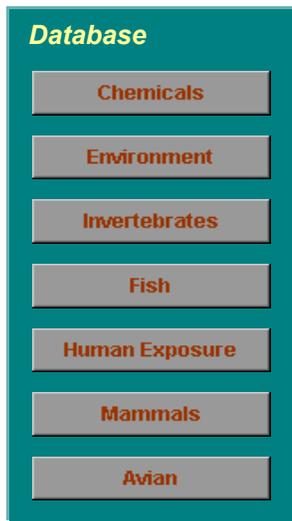
### 2.3 How do I run *TrophicTrace*?

When the installation process is complete, *TrophicTrace* will appear under the “Tools” menu in Excel™. Click on *TrophicTrace* under the “Tools” menu to start the program.

### 3 User Interface

#### 3.1 Main Screen

The main screen provides the gateway to the databases and input screens for specific model runs, as well as output screens and the help file. This screen can be accessed from any of the data library screens by clicking “Home”. There are seven categories of inputs:



- Chemicals (physical, chemical and human toxicity parameters)
- Environment (site-specific sediment and water chemistry)
- Invertebrates (exposure parameters and/or measured concentrations)
- Fish (exposure parameters and/or measured concentrations)
- Human (exposure parameters)
- Mammals (exposure and effects parameters)
- Avian (exposure and effects parameters)

For demonstration purposes, several data libraries are provided as examples of assumptions for specific receptor populations. Users can either add additional receptors, or the demonstration datasets can be directly modified.

#### 3.2 Browsing and editing the databases

All the data libraries have a common format:



Users can add new receptors, chemicals, or environments by clicking on “Add New”. The current data library on the screen can be edited by clicking on “Edit”, or can be deleted by clicking on “Delete”. “Home” takes users back to the main menu screen, and “Detail” provides a text box for adding relevant information, including details on references, calculations, judgments made to reach specific assumptions, and so on.

All the database input screens typically have four input fields for each parameter. This is done to allow *TrophicTrace* to provide estimates of uncertainty in the output. The format is as follows: enter four monotonically increasing numbers, where the first number represents the minimum of the known range of values for that parameter, the next two values represent the likeliest range (e.g., an average and a 95% upper confidence limit. Note that there are a variety of methods and

statistical techniques that can be used to quantify a “likeliest” range. The user can also enter the same number twice if there is no information on a likeliest range; for example, enter the calculated average in both the second and third fields), and the final value represents the maximum of the known range. If there is no information such as minimum and maximum for any parameter, the user should enter the same value four times. If the data are triangular (e.g., a minimum, maximum, and average), then three numbers should be entered and the average is entered twice (in the second and third fields).

### 3.2.1 Chemicals

This screen allows the user to select the chemicals to model. This version of the model contains data libraries for three chemicals: arsenic (a metal), PCBs (an organochlorine), and DDT/DDE/DDD (related organochlorine pesticides). The chemical is selected from a drop-down list at the top of the screen. The program automatically specifies the type of contaminant and the CAS number for these three contaminants; this information must be entered for new contaminants. The user must specify either a  $K_{ow}$  for hydrophobic organic contaminants, and a BCF for the remaining contaminants. The  $K_{ow}$  represents the octanol-water partitioning coefficient, and is used in the food-web model in several of the rate constants used to calculate fish body burdens.  $K_{ow}$  is specified if the contaminant is organic. If the contaminant is an inorganic, then this field represents the BCF. The BCF is a water: organism bioconcentration factor and is used to predict fish body burdens from a water concentration. Several metals (currently copper, cadmium, lead, zinc, and arsenic) can use a trophic transfer factor (TTF) instead of a BCF. The TTF represents the trophic transfer factor from invertebrate (prey) to fish. There is some evidence that these TTF may be appropriate for a wider range of inorganic contaminants.

Human toxicity factors are specified on this screen. The cancer slope factor (CSF), or measure of carcinogenicity, is typically obtained from the Integrated Risk Information System (IRIS), a USEPA database, and is in units of  $(\text{mg}/\text{kg}\text{-day})^{-1}$ . The Reference Dose (RfD), or measure of noncarcinogenic, systemic effects, is in units of  $\text{mg}/\text{kg}\text{-day}$  and is also typically obtained from the IRIS database.

Some sites will have data on measured accumulation factors from sediment to benthos from the 28-day bioaccumulation test results or other field studies. These data can be included on this screen for each chemical. Currently, the model contains a BSAF of 1.7 for hydrophobic organic contaminants following USACE guidance.

Users can add a new chemical by selecting “*Add New*”, edit existing chemicals by selecting “*Edit*”, delete chemicals by selecting “*Delete*” and return to the main screen by selecting “*Home*”. Each input screen also has a button, “*Detail*”, which provides a text box for entering references, or other information necessary to document specific modeling assumptions and revisions that are made to existing assumptions.

### 3.2.2 Environment

To access the environmental attributes input screen, click on “*Environment*” from the main screen. The environment sheet allows the user to specify the site-specific environmental attributes, including sediment and water concentrations, temperature, and organic carbon content in sediment. The only requirement to run the model is a user-specified sediment concentration and organic carbon content, both of which are entered by the user in this screen.

*TrophicTrace* requires a freely dissolved water concentration in ng/L. This value can be entered by the user if site-specific measurements are available. If a whole water measurement is available, it can be entered and the subroutine incorporated in *TrophicTrace* used to estimate a freely dissolved concentration. The subroutine (equation 5) contains several example values that can be edited by the user, including POC and DOC (site-specific), and  $K_{oc}$  (chemical-specific). If no water measurements are available at all, *TrophicTrace* estimates a freely dissolved water concentration from a user-specific sediment concentration assuming equilibrium partitioning. Because of the conservative assumptions inherent in the equilibrium partitioning calculation, this method of obtaining a water concentration is considered an upper-bound (in the absence of additional sources). It is strongly recommended that users carefully consider the appropriate water concentration for modeling purposes. It is likely that mixing calculations using the ADDAMS models or other methods would have been conducted for other aspects of the project to compare to water quality standards; this information can be used in the model.

Two demonstration sites are included in the prototype version of *TrophicTrace*. These are provided as examples only. To add a new site, click on “*Add New*”. Select a site designation or abbreviation. The “*Site*” field can be used to provide additional descriptive information for the site. Temperature (degrees Celsius) and organic carbon content in sediment (percent) are entered next. Finally, select the chemicals to include in the analysis. To add a chemical that is not in the list, return to the main screen and select “*Chemicals*”, and then click on “*Add New*”.

### 3.2.3 Invertebrate Attributes

The model example invertebrate is a sandworm, which derives its exposure exclusively via sediment. The sandworm was selected because it is a common organism used in the 28-day bioaccumulation tests. Additional invertebrates can be added, including those that derive their exposure from the water column. The model will estimate invertebrate concentrations from water using equilibrium partitioning. There are no required inputs for invertebrates but it is strongly recommended that users evaluate the percent lipid (in wet weight) for invertebrates, as the assumed value, together with TOC in sediment, dictates the predicted invertebrate concentration. There is a database of lipid values available from the ERDC BSAF database.

Users can also enter measured invertebrate concentrations. This is done by selecting a “*Reference Invertebrate*” and specifying a measured concentration, often obtained from the 28-day bioaccumulation tests conducted in Tier 3. The user can also enter a measured sandworm concentration into the output sheet for organic chemicals in order to directly compare these results to the calculated sandworm results. However, entering data into the output sheet does not save this information in the model itself and should only be used as a quick sensitivity analysis.

In addition, when the measured concentration is entered directly into the output worksheet, the model does NOT automatically make the  $K_{ow}$ -dependent steady state adjustment required for the 28-day test results.

### 3.2.4 Fish Attributes

The demonstration food chain that is included in the model is a sediment-based food web. The species included in the model are the mummichog and summer flounder. Required inputs for the fish species include the weight (in grams), the lipid content (in percent wet weight), and the dietary composition (in percentages which sum to one). To add a new species, click on “Add New” and fill in the required fields.

### 3.2.5 Human Exposure

Four demonstration populations are currently included in this version of *TrophicTrace*: General public child (under 6 years old), general public adult, recreational child angler (under 6 years old), and recreational adult angler. The general public ingestion rates were obtained from the USEPA Exposure Factors Handbook for consumption of marine fish. The recreational angler population fish ingestion rates were obtained from the New Jersey Department of Agriculture (NJDA, 1994) and are specific to the NY-NJ harbor region. Neither of these should be considered as default values. Users are urged to consult the Exposure Factors Handbook as well as local Departments of Health and research institutions to determine if there are studies suitable for the specific project being considered.

Click on “*Human Exposure*” from the main screen to access the input screen for human exposure parameters. One of the four example populations can be selected from the top box. A new receptor group can be added by clicking on “Add New”. The model requires the following parameters:

- Body weight in kg
- Number of fish meals per week (#/week)
- Size of fish meal (gr)
- Number of weeks of fish meals (weeks)
- The percentage of fish in the diet obtained from the site (0.01% to 100%)
- Exposure duration (days)
- The type of fish consumed in the diet (for example, summer flounder). The types of fish must sum to 1.0.

The program calculates an annualized fish ingestion rate in g/day based on the number of fish meals consumed per week, the size of the fish meal, and the number of weeks that fish meals are consumed.

Fields are provided to include references for the selected values. In addition, to provide more information on references or assumptions used in developing exposure parameters, click on the “*Details*” button. This button leads the user to a blank text box that can hold additional narrative text documentation. Several demonstration populations have been included in the prototype

version of the model based on exposure factors from the USEPA exposure factor handbook (USEPA, 1997a and 1997b) and for a regional NY/NJ population (NJDA, 1994).

### 3.2.6 Mammals

*TrophicTrace* includes two demonstration data libraries for mammals: mink and otter. Click on “*Mammals*” from the main screen to access the input screen for these receptors. Users can select from the example mammalian receptors from the pull-down list and can edit the values provided for the parameters that are provided by clicking on “*Edit*”. Users can add new receptors by clicking on “*Add New*”.

Exposure parameters for mink and otter are provided in Appendix C with references. For each mammalian receptor, users need to specify a body weight (kg), ingestion rate (kg/day), and foraging factor (unitless fraction). Users also need to specify contaminant- and species-specific TRVs. The TRVs provided in *TrophicTrace* were estimated based on studies obtained from the primary literature following the methodology described earlier.

Fields are provided to include references for the selected values. In addition, to provide more information on references or assumptions used in developing exposure parameters, click on the button “*Details*”. This button leads the user to a text box that can hold additional narrative text and documentation.

### 3.2.7 Avian

*TrophicTrace* includes two demonstration avian populations: osprey and eagle. Click on “*Avian*” from the main screen to access the input screen for these receptors. Users can select from the example avian receptors from the pull-down list and can edit the values for the parameters that are provided by clicking on “*Edit*”. Users can add new receptors by clicking on “*Add New*”.

Exposure parameters for osprey and eagle were obtained from USEPA (1993). For each avian receptor, users need to specify a body weight (kg), ingestion rate (kg/day), and foraging factor (unitless fraction). Users also need to specify contaminant- and species-specific TRVs. The TRVs provided in *TrophicTrace* were estimated based on studies obtained from the primary literature following the methodology described earlier.

Fields are provided to include references for the selected values. In addition, to provide more information on references or assumptions used in developing exposure parameters, click on the button “*Details*”. This button leads the user to a text box to which additional narrative text and documentation can be added.

## 3.3 Model Run screen

After completing and verifying all the input screens, run the *TrophicTrace* model by selecting “*Create Output*” from the main screen. There are several choices for how the model is run, and a dialog box will pop up asking the user to select from among them. One approach uses

equilibrium partitioning from sediment to invertebrates and the Gobas Model to estimate fish concentrations for organic contaminants and a BCF approach to estimate fish concentrations for inorganic and hydrophilic organic contaminants. Another approach uses the 28-day bioaccumulation test results and applies a TTF for those contaminants for which there is enough information to develop TTFs (arsenic in this example) and uses the measured invertebrate concentrations directly in the Gobas Model for organic contaminants. Note that the model will notify the user of an error if a measured concentration is included for organic contaminants, or if a TTF has not been specified. The user must use the Gobas model option for hydrophobic organic contaminants, even if sandworm concentrations are specified from the 28-day bioaccumulation test results.

### 3.4 Model Output

The model provides output consisting of the following:

- A summary of input parameters for the selected “environment”;
- The ability to plot results;
- A risk summary for the population of interest;
- The input parameters for each human population;
- Exposure concentrations at each trophic level;
- Input parameters for each fish species;
- Rate constants for each fish calculated by the model;
- Input parameters for invertebrates;
- Input parameters for each of the avian and mammalian ecological receptors;
- Summary of the physical-chemical properties for each chemical; and,
- Site-specific environmental properties.

Users can edit the white fields in the output sheets. Although this information will not be saved in the model database, it can be useful to quickly gauge the impact of changes in particular variables in a quick sensitivity analysis. For example, one could quickly see how much different predicted child angler risks would be under an assumption of 100% of fish caught from site instead of 80%. However, to save these changes in the underlying database that corresponds to this receptor population, one must return to the Main Menu, select “*Human Exposure*”, and click on “*Edit*” for that population to make and save changes.

Results, or input parameters, can be plotted by clicking on “*Plot*”. A dialog box will come up and the user should enter the name of the plot, select the range of results to be plotted, and finally select whether the results will be plotted in a new chart or an existing chart. Charts can be exported or saved for use in other graphics programs. The trapezoidal fuzzy number shows the likeliest range (or probable range) and the full range (or possible range) of values.

## 4 Modeling Framework in *TrophicTrace*

### 4.1 Gobas Model for organics

The model used to estimate fish body burdens for hydrophobic organic compounds relies on a steady-state uptake model based on the approach of Gobas (1993 and 1995):

$$C_f = \frac{k_1 * C_{wd} + k_d * C_{diet}}{k_2 + k_e + k_m + k_g} \quad (1)$$

$k_1$	= gill uptake rate (L/Kg/d)
$C_{wd}$	= freely dissolved concentration in water (ng/L)
$k_d$	= dietary uptake rate ( $d^{-1}$ )
$C_{diet}$	= concentration in the diet ( $\mu\text{g}/\text{kg}$ )
$k_2$	= gill elimination rate ( $d^{-1}$ )
$k_e$	= fecal egestion rate ( $d^{-1}$ )
$k_m$	= metabolic rate ( $d^{-1}$ )
$k_g$	= growth rate ( $d^{-1}$ )
$C_f$	= concentration in fish ( $\mu\text{g}/\text{kg}$ )

Several sources provide equations for the rate constants ( $k_2$ ,  $k_e$ ,  $k_m$  and  $k_g$ ) and these are described in greater detail in von Stackelberg et al. (2002).

Biota-sediment accumulation factors (BSAFs) are ratios that describe the relationship between the concentration of a nonpolar organic chemical in the lipid phase in tissue of a sediment-dwelling organism to the concentration in the sediment organic carbon phase to which the organism is exposed. BSAFs are defined as:

$$BSAF = (C_B / f_L) / (C_S / f_{OC}) \quad (2)$$

where

$C_B$	= concentration of contaminant in biota, mg/kg wet weight
$f_L$	= the fraction lipid of the biota, kg lipid/kg wet weight
$C_S$	= the concentration of contaminant in sediment, mg/kg dry weight
$f_{OC}$	= the fraction organic carbon in sediment, kg organic carbon/kg dry weight

$$C_B = C_S * (f_L / f_{OC}) * BSAF \quad (3)$$

where

$C_B$	= concentration of contaminant in biota, mg/kg wet weight
$f_L$	= the fraction lipid of the biota, kg lipid/kg wet weight
$C_S$	= the concentration of contaminant in sediment, mg/kg dry weight

$f_{OC}$  = the fraction organic carbon in sediment, kg organic carbon/kg dry weight

BSAF = biota-sediment accumulation factor (typical assumption is 1.0) obtained from site-specific measurements or literature sources

The model can also accept a measured invertebrate concentration resulting from the standard Tier 3 28-day bioaccumulation test results. To account for the fact that these measured concentrations may not have achieved steady-state, a  $K_{ow}$ -dependent adjustment is made (McFarland, 1984; Connell and Hawker, 1988) automatically within *TrophicTrace* based on the following formula:

$$\log t_{ss} = 6.9 \times 10^{-3}(\log K_{ow})^4 - 1.85 \times 10^{-1}(\log K_{ow})^3 + 1.65(\log K_{ow})^2 - 5.34(\log K_{ow}) + 5.93 \quad (4)$$

where:

$t_{ss}$  = time required to reach steady-state

#### 4.2 Trophic Transfer (TTF) and Bioconcentration Factor (BCF)

Estimates of fish burdens for inorganic and hydrophilic organic compounds rely on two different approaches, depending on data availability. The first approach is a trophic transfer factor (TTF) from prey to predator approach, and the second is a bioconcentration factor (BCF) approach. For some chemicals, there are data available on bioaccumulation from invertebrates to fish (Dillon, 1995). Currently, TTF are available for copper, cadmium, lead, zinc, and arsenic. In the BCF approach, water concentrations are multiplied by a bioconcentration factor to estimate fish body burdens. Water concentrations can either be provided by the user or estimated by the model assuming equilibrium partitioning from sediment. Table 2 provides the chemical-specific BCFs and TTFs obtained from the literature.

Both the food web model for hydrophobic organic compounds and the BCF approach for inorganic and hydrophilic organic compounds require a freely dissolved water concentration as an input. *TrophicTrace* incorporates two approaches for estimating a freely dissolved water concentration: 1) a user-specified freely dissolved water concentration from site-specific data; 2) from a subroutine (equation 2) using either a user-specified whole water concentration or an estimated whole water concentration (calculated by assuming equilibrium partitioning from a user-specified sediment concentration). The subroutine that estimates a freely dissolved water concentration is shown in equation 2:

$$C_{wd} = \frac{1}{(1 + 0.1 * DOC * DE_{oc} * K_{oc} + POC * DE_{oc} * K_{oc})} * C_{ww} \quad (5)$$

where:

$C_{wd}$  = freely dissolved concentration in water (ng/L)

$DOC$  = dissolved organic carbon (mg/L)

$DE_{oc}$  = density of organic carbon (0.041 mg OC/mg)

$K_{oc}$  = organic carbon/water partition coefficient (L/kg OC)

$POC$  = particulate organic carbon (mg/L)

$C_{ww}$  = whole water concentration (ng/L)

Demonstration values for DOC, POC and chemical-specific  $K_{oc}$  (organic carbon to water partition coefficients) are provided in Appendix C. These can be edited by the user if site-specific information is available.

If a whole water concentration is not available, the program uses equilibrium partitioning with sediment to estimate a freely dissolved water concentration. The equation for organic contaminants is:

$$C_w = \left( \frac{C_{oc}}{K_{oc}} \right) \quad (6)$$

where

$C_w$  = concentration of freely dissolved chemical in the water ( $\mu\text{g/L}$ )

$C_{oc}$  = the organic carbon-normalized sediment concentration ( $\mu\text{g/kg}$  dry wt sediment) and

$K_{oc}$  = organic carbon-water partition coefficient (L/kg organic carbon)

The  $K_{oc}$  for each chemical can be estimated from its octanol-water partition coefficient,  $K_{ow}$ , according to the following regression relationship (Connell and Hawker, 1988):

$$\log K_{oc} = 0.00028 + 0.983 \log_{10} K_{ow} \quad (7)$$

## 5 Risk Assessment Formulas in the *TrophicTrace* Program

### 5.1 Human health risk model

The estimates of fish body burdens represent point estimates of concentrations to which humans are exposed via fish ingestion. These fish tissue concentrations are used along with exposure assumptions specific to each human receptor population to calculate carcinogenic risk and noncarcinogenic hazard indices. Carcinogenic risk (men and women, or boys and girls, combined) is calculated as follows:

$$Risk = \frac{CSF * IR_f * C_f * ED}{BW * 1000000 * AT} \quad (8)$$

where:

- Risk = incremental lifetime cancer risk
- CSF = cancer slope factor (mg/kg-day)<sup>-1</sup>
- IR<sub>f</sub> = annualized fish ingestion rate (g/day)
- C<sub>f</sub> = concentration in fish (µg/kg)
- ED = exposure duration (days)
- BW = body weight (kg)
- AT = averaging time (days)

Noncarcinogenic hazard indices are calculated as follows:

$$HI = \frac{IR_f * C_f * ED}{RfD * BW * 1000000 * AT} \quad (9)$$

where:

- HI = hazard index
- RfD = Reference dose (mg/kg-day)
- IR<sub>f</sub> = annualized fish ingestion rate (g/day)
- C<sub>f</sub> = concentration in fish (µg/kg)
- ED = exposure duration (days)
- BW = body weight (kg)
- AT = averaging time (days)

The example exposure assumptions for human receptor populations provided in *TrophicTrace* are shown in Table 3 of Appendix C, and the toxicity values (CSF and RfD) for individual chemicals are shown in Table 2 of Appendix C. It is often easier to think of annualized ingestion rates as meals per week assuming a particular meal size (10 oz for adults and 5 oz for children is presented in the table).

Currently, four distinct receptor populations are included in *TrophicTrace*: General public child under 6, general public adult, recreational child angler, and recreational adult angler. The

primary difference between these two populations is that the recreational anglers, both children and adults, incorporate fish ingestion rates specific to the NY-NJ harbor region (NJDA, 1994). The general public ingestion values assume a smaller recreational marine fish ingestion rate, and a smaller proportion of fish obtained from one particular site. The recreational angler scenario assumes that there is a population of anglers who routinely return to a favorite fishing spot and, in a health-protective assumption, this spot is considered to be in the vicinity of the proposed disposal site.

## 5.2 Ecological risk model

Potential ecological risks are evaluated by comparing predicted contaminant concentrations in tissue and/or daily dose estimates to appropriate toxicity reference values (TRVs). These comparisons are based on predicted tissue concentrations in mg/kg for fish, and on predicted daily dose estimates for the higher order ecological receptors. Currently, the model is parameterized for osprey and bald eagle (avian receptors) and mink and otter (mammalian receptors).

TRVs are levels of exposure associated with either Lowest Observed Adverse Effects Levels (LOAELs) or No Observed Adverse Effects Levels (NOAELs). They provide a basis for judging the potential effects of measured or predicted exposures that are above or below these levels. TRVs are contaminant- and species-specific and are developed based on laboratory or field studies.

Use of both LOAELs and NOAELs provides perspective on the potential for risk as a result of exposure to contaminants in dredged materials. LOAELs are values at which effects have been observed in either laboratory or field studies, while the NOAEL represents the lowest dose or body burden at which an ecologically relevant effect was not observed. Exceedance of a LOAEL indicates a greater potential for risk.

Some studies examine toxicity endpoints (such as lethality, growth, and reproduction) that are thought to have greater potential for adverse effects on populations of organisms than other studies. Other studies examine toxicity endpoints such as behavior, disease, cell structure, or biochemical changes that affect individual organisms, but may not result in adverse effects at the population level. For example, toxic effects such as enzyme induction may or may not result in adverse effects to individual animals or populations. The procedure in *TrophicTrace* is to develop TRVs from studies that examine the effects of contaminants on lethality, growth or reproduction. Studies that examined the effects of contaminants on other sublethal endpoints are not used to select TRVs unless no other studies are available. Lethality, growth, and reproductive-based endpoints typically present the greatest risk to the viability of the individual organism and therefore of the population's survival. Thus, these are considered to be the endpoints of greatest concern.

When exposures are expected to be long-term, data from studies of chronic exposure are preferable to data from medium-term (subchronic), short-term (acute), or single-exposure studies (USEPA, 1997c). Bioaccumulative substances are by definition persistent, and exposure of ecological receptors to these contaminants from dredged materials is expected to be long-term,

and therefore studies of chronic exposure are preferentially used to select TRVs. Long-term studies are also preferred since reproductive effects of contaminants are typically studied after long-term exposure.

Dose-response studies compare the response of organisms exposed to a range of doses to that of a control group. Ideally, doses that are below and above the threshold level that causes adverse effects are examined. Toxicity endpoints determined in dose-response and other studies include:

- NOAEL (No-Observed-Adverse-Effect-Level) is the highest exposure level shown to be without adverse effect in organisms exposed to a range of doses. NOAELs may be expressed as dietary doses (e.g., mg contaminant consumed/kg body weight/d), as concentrations in external media (e.g., mg contaminant/kg food), or as concentrations in tissue of the affected organisms (e.g., mg chemical/kg egg).
- LOAEL (Lowest-Observed-Adverse-Effect-Level) is the lowest exposure level shown to produce adverse effect in organisms exposed to a range of doses. LOAELs may also be expressed as dietary doses (e.g., mg contaminant consumed/kg body weight/d), as concentrations in external media (e.g., mg contaminant/kg food), or as concentrations in tissue of the effected organisms (e.g., mg chemical/kg egg).
- LD<sub>50</sub> is the Lethal Dose that results in death of 50% of the exposed organisms. Expressed in units of dose (e.g., mg contaminant administered/kg body weight of test organism/d).
- LC<sub>50</sub> is the Lethal Concentration in some external media (e.g., food, water, or sediment) that results in death of 50% of the exposed organisms. Expressed in units of concentration (e.g., mg contaminant/kg wet weight food).
- ED<sub>50</sub> is the Effective Dose that results in a sublethal effect in 50% of the exposed organisms (mg/kg/d).
- EC<sub>50</sub> is the Effective Concentration in some external media that results in a sublethal effect in 50% of the exposed organisms (mg/kg).
- CBR or Critical Body Residue is the concentration in the organism (e.g., whole body, liver, or egg) that is associated with an adverse effect (mg contaminant/kg wet wt tissue).
- EL-effect is the effect level that results in an adverse effect in organisms exposed to a single dose, rather than a range of doses. Expressed in units of dose (mg/kg/d) or concentration (mg/kg).
- EL-no effect is the effect level that does not result in an adverse effect in organisms exposed to a single dose, rather than a range of doses. Expressed in units of dose (mg/kg/d) or concentration (mg/kg).

Most USEPA risk assessments typically estimate risk by comparing the exposure of receptors of concern to TRVs that are based on NOAELs. Example TRVs included in *TrophicTrace* are

developed on the basis of both NOAELs and LOAELs to provide perspective on the range of potential effects relative to measured or modeled exposures.

Differences in the feeding behavior of aquatic and terrestrial organisms determine the type of toxicity endpoints that are most easily measured and most useful in assessing risk. For example, the dose consumed in food is more easily measured for terrestrial animals than for aquatic organisms since uneaten food can be difficult to collect and quantify in an aqueous environment. Therefore, for aquatic organisms, toxicity endpoints are more often expressed as concentrations in external media (e.g., water) or as accumulated concentrations in the tissue of the exposed organism (also called a “body burden”). In some studies, doses are administered via gavage, intraperitoneal injection into an adult, or injection into a fish or bird egg. If appropriate studies are available, TRVs in *TrophicTrace* are selected on the basis of the most likely route of exposure, as described below:

- TRVs for fish are expressed as critical body residues (CBR) (e.g., mg/kg whole body weight and mg/kg lipid in eggs).
- TRVs for terrestrial receptors (e.g., birds and mammals) are expressed as daily dietary doses (e.g., mg/kg whole body wt/d).

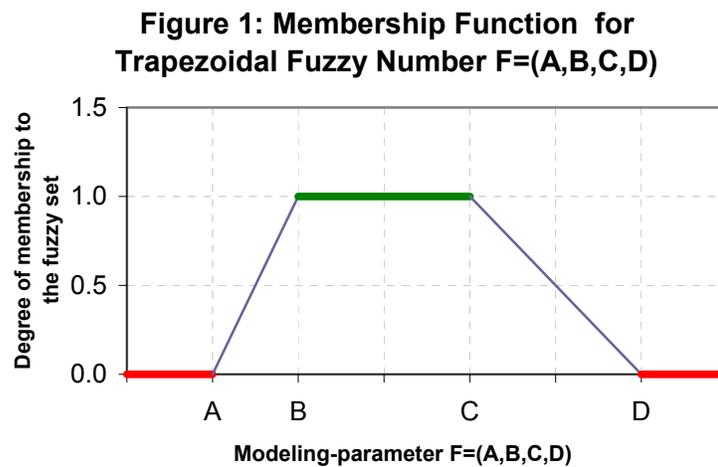
TRVs for birds are also expressed as concentrations in eggs (e.g. mg/kg wet wt egg).

## 6 Trapezoidal Fuzzy Numbers to Characterize Parameter Uncertainty

### 6.1 Trapezoidal fuzzy numbers

A trapezoidal fuzzy number is simply four numerical values (A, B, C, D) where A is less than or equal to B, B is less than or equal to C, and C is less than or equal to D. For the fuzzy parameter  $F=(A, B, C, D)$  the interval  $[A,D]$  represents the plausible range of the parameter. The number A is the minimum possible value of the parameter, and D is the maximum possible value of the parameter. The range  $[B,C]$  is the most likely range of the parameter F. So, fuzzy results yield both “worst case” and “best estimates” simultaneously.

Trapezoidal fuzzy numbers is an example of a fuzzy set and could be represented via its membership function showing the degree of membership for each value of the parameter (see Figure 1).

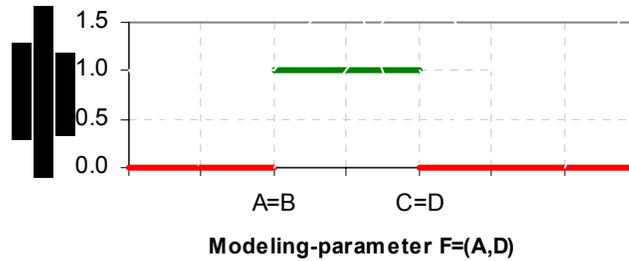


Degree of membership is a number between 0 and 1. The range of certain values of the parameter have a membership level equal to one (green line on Figure 1 corresponding to the interval  $[B,C]$ ). Restricted values with a degree of membership equal to zero are shown in red. All other values are more or less possible in proportion to their membership degree. This approach allows us to consider the fuzzy set as a measure for possibility (Zimmermann, 1991). Note that the y-axis does not represent a probability or likelihood. The degree of membership in the fuzzy set is proportional, however, such that if the degree of membership = 1 (B to C, also called the likeliest or probable range), then the parameter value, given the inputs, will definitely be within that range. The parameter may take on values from the sides of the trapezoid (A to B and C to D, also called the full or possible range), but these values are only “possibilities” with the degree of possibility reflected in the degree of membership. For example, a value that has a degree of membership of 0.8 is much more possible than a value with a degree of membership that is only 0.1.

## 6.2 Example: Interval

In the case when all possible values of the parameter are equally plausible (e.g., equivalent to a uniform distribution), then the range of the parameter can be described by an interval and interval analysis is used to analyze a model with such parameters. The membership function for an interval is a stepped function (see Figure 2).

**Figure 2: Membership Function for Interval  $F=(A,D)$**

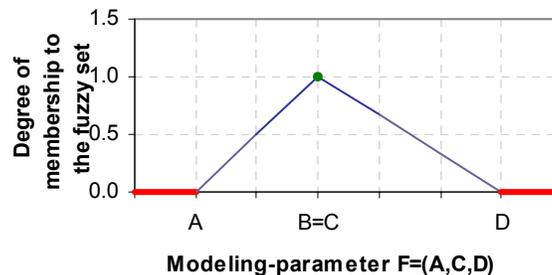


This approach also provides the possibility to consider the interval  $(A,D)$  as a trapezoidal fuzzy number  $(A,B,C,D)$  with  $B=A$  and  $C=D$ , i.e. as the fuzzy number  $(A,A,D,D)$ , and to use such parameters in modeling.

## 6.3 Triangular Fuzzy Numbers as a Particular Case of Trapezoidal Fuzzy Numbers

Trapezoidal fuzzy numbers also include fuzzy numbers with a triangular shape for the membership function. A triangular fuzzy number is evaluated as a trapezoidal fuzzy number  $(A,B,C,D)$  with  $B=C$ , i.e.  $(A,B,B,D)$ . Such a fuzzy number could be used for a quantitative description of a parameter for which a possible range is known together with a single most likely value. This is shown graphically in Figure 3.

**Figure 3: Triangular Fuzzy Number  $F=(A,C,D)$**



## 6.4 Exact Parameter Value

It might be possible to know or only have information for one value for some parameters in the model. The approach to treat them as a trapezoidal fuzzy number (A,B,C,D) with A=B=C=D allows the model to include such parameters simultaneously with other parameters that are more uncertain. Zadeh (1965) provides an implementation for processing of fuzzy numbers by the extension principle.

*TrophicTrace* performs the extension principle for the model equation process, but approximates results by trapezoidal shapes, too. The approximation approach uses the vertex method (Dong and Shah, 1987) for computing a function of fuzzy variables.

## 6.5 Arithmetic of Trapezoidal Fuzzy Numbers

### 6.5.1 Addition

According to the extension principle, the sum of two trapezoidal fuzzy numbers is also a trapezoidal number. The following formula provides the exact value used by *TrophicTrace*.

$$(A_1, B_1, C_1, D_1) + (A_2, B_2, C_2, D_2) = (A_1 + A_2, B_1 + B_2, C_1 + C_2, D_1 + D_2) \quad (10)$$

### 6.5.2 Subtraction

As for addition, the extension principle provides an exact solution for this operation, as shown in the following formula.

$$(A_1, B_1, C_1, D_1) - (A_2, B_2, C_2, D_2) = (A_1 - A_2, B_1 - B_2, C_1 - C_2, D_1 - D_2) \quad (11)$$

### 6.5.3 Multiplication

*TrophicTrace* uses the following approximate formula for multiplication of fuzzy numbers.

$$(A_1, B_1, C_1, D_1) * (A_2, B_2, C_2, D_2) \sim (A_1 * A_2, B_1 * B_2, C_1 * C_2, D_1 * D_2) \quad (12)$$

The vertex method is based on  $\alpha$ -cut conception and interval analysis. It can be shown that the exact solution of multiplying trapezoidal fuzzy numbers has a curvilinear trapezium shape. The vertexes of this curvilinear are calculated by the formula above.

### 6.5.4 Division

$\alpha$ -cut conception and interval analysis provides the following formula used in the *TrophicTrace* model for operation of division of positive trapezoidal fuzzy numbers.

$$(A_1, B_1, C_1, D_1) / (A_2, B_2, C_2, D_2) \sim (A_1 / D_2, B_1 / C_2, C_1 / B_2, D_1 / A_2) \quad (13)$$

As in interval analysis, the multiplication and division of fuzzy numbers are inverse to each other only for the case when all fuzzy parameters are exact values (all four components are equal). If parameter F has plausible range  $[A_1, D_1]$  and the plausible range for parameter Y is  $[A_2, D_2]$ , then to obtain the minimum value for the parameter F/Y one needs to divide minimum value of the parameter F by maximum value of the parameter Y. The maximum value of F/Y is obtained by dividing maximum F by minimum Y.

#### 6.5.5 Power operations

The extension principle provides an exact solution for extending the exponent function for fuzzy numbers.

$$\text{EXP}(A_1, B_1, C_1, D_1) = (\text{EXP}(A_1), \text{EXP}(B_1), \text{EXP}(C_1), \text{EXP}(D_1)) \quad (14)$$

This function is the particular case of a power function for which the extension principle also provides the exact solution, as shown below.

$$(A_1, B_1, C_1, D_1)^{(A_2, B_2, C_2, D_2)} = (A_1^{A_2}, B_1^{B_2}, C_1^{C_2}, D_1^{D_2}) \quad (15)$$

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## APPENDIX B ACRONYMS

ADDAMS	USACE fate and transport modeling system
BCF	Bioconcentration Factor
BSAF	Biota Sediment Accumulation Factor (here used only as a benthic sediment accumulation factor)
CSF	Cancer Slope Factor (mg/kg-day) <sup>-1</sup>
DOC	Dissolved Organic Carbon
ITM	Inland Testing Manual
K <sub>oc</sub>	Log
K <sub>ow</sub>	Log-octanol water partitioning coefficient
LOAEL	Lowest Observed Adverse Effect Level for ecological receptors
NJDA	New Jersey Department of Agriculture
NOAEL	No Observed Adverse Effect Level for ecological receptors
NY/NJ	New York/New Jersey
OTM	Ocean Testing Manual
PCBs	Polychlorinated Biphenyls
POC	Particulate Organic Carbon
RfD	Reference Dose (mg/kg-day)
TBP	Theoretical Bioaccumulation Potential
TTF	Trophic Transfer Factor (from invertebrates to fish)
TRV	Toxicity Reference Value for ecological receptors
USACE	United States Army Corps of Engineers
USEPA	United States Environmental Protection Agency

## APPENDIX C

**THE VALUES PROVIDED IN APPENDIX C ARE FOR DEMONSTRATION PURPOSES ONLY. A SITE-SPECIFIC ASSESSMENT SHOULD USE APPROPRIATE SITE-SPECIFIC OR REGION-SPECIFIC DATA. PLEASE CONSULT THE REFERENCES PROVIDED TO DETERMINE WHETHER THESE VALUES ARE APPROPRIATE FOR YOUR APPLICATION.**

**C1: ENVIRONMENTAL AND GOBAS MODEL PARAMETERS SPECIFIED IN *TROPICTRACE***

<b>Parameter</b>	<b>Units</b>	<b>Value</b>	<b>Reference</b>
Total organic carbon (TOC)	percent	site-specific	site-specific
Sediment concentration	mg/kg bulk dry weight	site-specific	site-specific
Whole water concentration	ng/L whole water	site-specific or equilibrium partitioning	
Freely dissolved water concentration	ng/L freely dissolved	site-specific or subroutine	
Temperature	degrees Celsius	15	assumed
Particulate organic carbon (POC)	mg/L	0.059	Parsons et al., 1984
Dissolved organic carbon (DOC)	mg/L	1.2	Parsons et al., 1984
Sandworm lipid content	percent	1.2	Wilson and Ruff, 1988
Mummichog lipid content	percent	1.75	Abraham, 1985
Mummichog weight	grams	3	Abraham, 1985
Summer flounder lipid content	percent	1.5	Grimes et al., 1989
Summer flounder weight	grams	574	Grimes et al., 1989

**C2: CONTAMINANT-SPECIFIC PARAMETERS**

<b>Abbreviation--&gt;&gt; Parameter--&gt;&gt;</b>		<b>BCF</b>	<b>Reference</b>	<b>TTF</b>	<b>Reference</b>	<b>Log K<sub>ow</sub></b>	<b>Reference</b>	<b>CSF</b>	<b>RfD</b>
<b>Chemical</b>	<b>Category</b>	<b>Bioconcentration Factor</b>		<b>Trophic Transfer Factor</b>		<b>Octanol Water Partition Coefficient</b>		<b>Cancer Slope Factor (mg/kg- day)<sup>-1</sup></b>	<b>Reference Dose mg/kg- day</b>
Arsenic	inorganic	3.5	USEPA, 1999c	0.25	USEPA, 2000	3.9 (Kd – sed/water)	USEPA, 1999b	1.5	0.003
Polychlorinated biphenyls (PCB)	organic					6.301	Mackay et al., 1992	2.0	0.00002
DDT	organic					6.0	ATSDR, 2000	0.34	0.0005
DDE	organic					6.51	ATSDR, 2000	0.34	0.0005
DDD	organic					6.2	ATSDR, 2000	0.24	0.0005

**C3: HUMAN EXPOSURE PARAMETERS**

Parameter	Units	General Public Child Under 6	General Public Adult	Recreational Angler under 6	Recreational Angler - Adult	Reference
Body weight	kg	14.5	70	14.5	70	USEPA, 1997a
Fish ingestion rate	g/day	8	8	29.42	46	USEPA, 1997b; NJDA, 1994
Percent of fish obtained from site	percent	50	50	80	80	USEPA, 1997b; NJDA, 1994
Exposure frequency	days/yr	365	365	365	365	USEPA, 1997a
Exposure duration	years	6	30	6	30	USEPA, 1997a
Averaging time (carcinogens)	days	27375	27375	27375	27375	USEPA, 1989
Averaging time (noncarcinogens)	days	2190	10950	2190	10950	USEPA, 1989
Type of fish in diet	NA	summer flounder	summer flounder	summer flounder	summer flounder	
<i>Fish Ingestion Summary</i>						
Lifetime fish consumption	gr/lifetime	17520	87600	64430	503700	
Lifetime fish consumption	oz/lifetim	626	3129	2301	17989	
	e					
10 oz adult; 5 oz child	# of meals	125	313	460	1799	
Number of meals from site	# of meals	63	156	368	1439	

#### C4: ECOLOGICAL RECEPTOR EXPOSURE PARAMETERS

Species	Foraging Rate (kg/d)	Body Weight (kg)	Foraging/Migration Factor (unitless)	Dietary Composition (%)
Osprey	0.3	1.568	1.0	100% mummichog
Eagle	0.65	5.1	1.0	100% flounder
Mink	0.132	0.83	1.0	35% mummichog; 16.5% sandworm
Otter	0.9	7.32	1.0	100% flounder

References:

Body weight and foraging rates taken from USEPA, 1993

**C5: FISH TOXICITY REFERENCE VALUES**

Species	Contaminant	NOAEL based CBR (mg/kg wet weight)	LOAEL based CBR (mg/kg wet weight)	NOAEL based egg (mg/kg lipid normalized)	LOAEL based egg (mg/kg lipid normalized)
Mummichog	DDT, DDE, DDD	2.4	24	NA	NA
Mummichog	PCB	1.9	9.3		
Mummichog	Arsenic	0.47	4.7		
Summer Flounder	PCB	1.9	9.3		
Summer Flounder	DDT, DDE, DDD	2.4	24	NA	NA
Summer Flounder	Arsenic	0.47	4.7	NA	NA

References:

PCBs: Hansen et al., 1974

DDX: Hamelink et al., 1971

Arsenic: Dixon and Sprague, 1981

**C6: AVIAN TOXICITY REFERENCE VALUES**

Species	Contaminant	NOAEL based dietary dose (mg/kg-day)	LOAEL based dietary dose (mg/kg-day)	Egg biomagnification factor (unitless)	NOAEL based egg (mg/kg wet weight)	LOAEL based egg (mg/kg wet weight)
Osprey	PCB	1.8	7.1	28	4.7	7.6
Osprey	DDT, DDE, DDD	0.11	1.1	28	NA	NA
Osprey	Arsenic	5.14	12.84	NA	NA	NA
Eagle	PCB	1.8	7.1	28	5.5	8.7
Eagle	DDT, DDE, DDD	0.11	1.1	28	NA	NA
Eagle	Arsenic	5.14	12.84	NA	NA	NA

References:

PCB dietary dose: Dahlgren et al., 1972

PCB egg: Hoffman et al., 1993 (osprey); Wiemeyer, 1984; 1993 (eagle)

DDT, DDE, DDD: Lincer, 1972

Arsenic: Sample et al., 1996

Egg biomagnification factor: Giesy et al., 1995

### C7: MAMMALIAN TOXICITY REFERENCE VALUES

Species	Contaminant	NOAEL based dietary dose (mg/kg-day)	LOAEL based dietary dose (mg/kg-day)
Mink	PCB	0.004	0.04
Mink	DDT, DDE, DDD	0.8	4.0
Mink	Arsenic	1.1	NA
Otter	PCB	0.004	0.04
Otter	DDT, DDE, DDD	0.8	4.0
Otter	Arsenic	1.1	NA

#### References:

PCB: Restum et al., 1998

DDT, DDE, DDD: Fitzhugh, 1948

Arsenic: Byron et al., 1967