3.2 Configure Chemicals

Figure 9 shows the CHEMICALS tab. The pane on the left side of the screen provides various options that operate on all the chemicals or the selected chemicals; these include buttons to change the sort order, select or deselect a batch of chemicals, add new chemicals, and compare chemical properties.

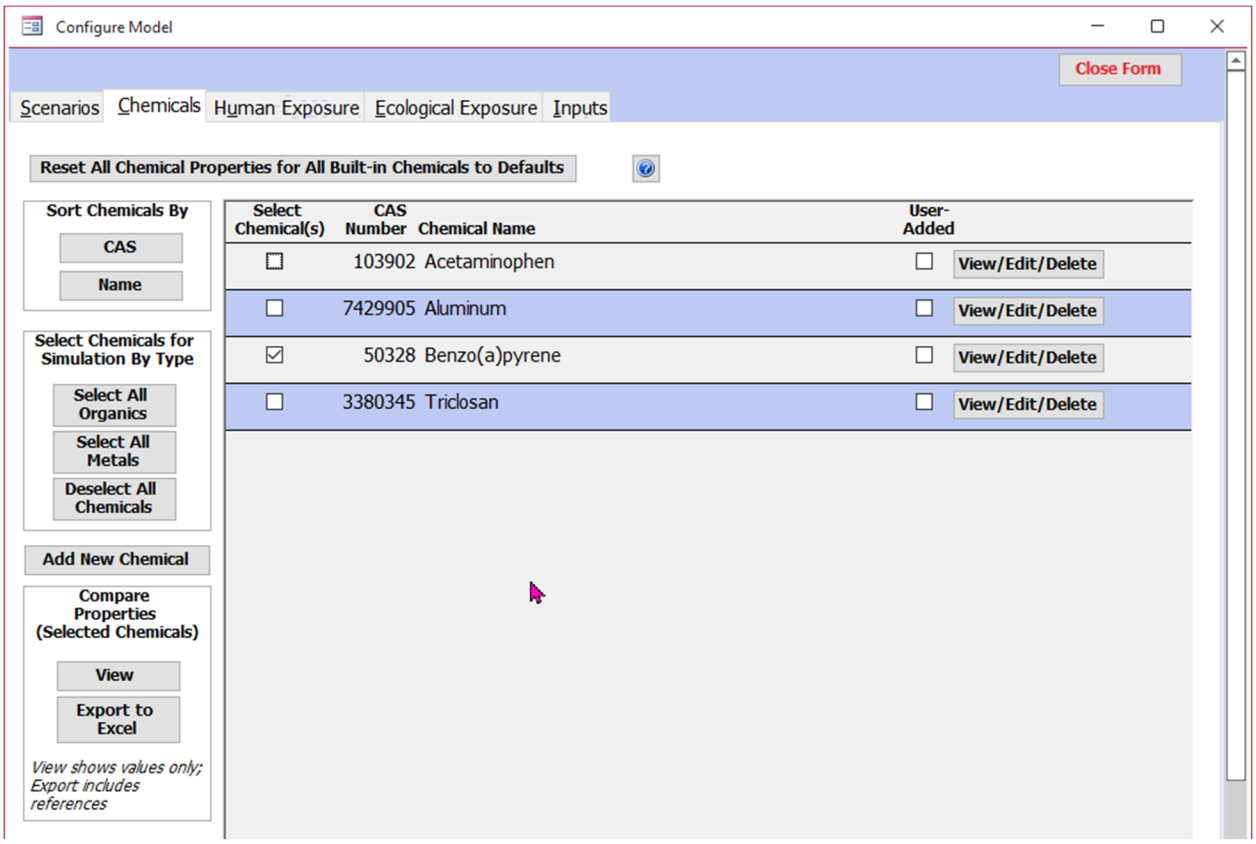


Figure 9. Chemicals tab: select chemicals, view and modify properties, add new chemicals, and compare properties.

The main part of the screen, at right, provides descriptive information on the available chemicals (CAS number, chemical name, and a 'user added' indicator) and two chemical-specific controls: a selection box (to the left of the CAS number) and a VIEW/EDIT/DELETE button (far right) that brings up the CHEMICAL PROPERTIES screen for that chemical, where you can view and edit the chemical-specific data (built-in and user-added chemicals), reset modified values to defaults (built-in chemicals only), and delete chemicals (user-added only). You can also reset any user-modified chemical properties for all built-in chemicals at once by clicking on the RESET ALL CHEMICAL PROPERTIES TO DEFAULT VALUES button at the top of the tab. Note this will have no

effect on user-added chemicals: those values will not be changed, nor will the user-added chemicals be deleted.

3.2.1 Select Chemicals to Include in a Simulation

To include a chemical in a simulation, use the scroll bar immediately to the right of the column of VIEW/EDIT/DELETE buttons to scroll through the list of chemicals and find the desired one. Click on the check box under "Select Chemical(s)" to the left of the CAS number. If the box is checked, the chemical has been selected. Click on the checkbox again to deselect it.

The chemical list can be sorted by CAS number or chemical name, as you prefer, using the CAS and NAME buttons at the top of the left pane. Chemical names that start with a number are sorted on the first letters, and the number prefix is shown at the end.

If you plan to include all or many of the chemicals available in your run, use the SELECT CHEMICALS FOR SIMULATION BY TYPE buttons in the middle of the left pane. Click on SELECT ALL ORGANICS to select all chemicals designated as organics (without deselecting anything first), and SELECT ALL METALS to select all inorganics (also without deselecting anything first). Used in succession, these two buttons will select all chemicals. From there, you can individually deselect any you do not wish to run. Conversely, if you want to run just a few chemicals, use the DESELECT ALL CHEMICALS button, and then select those you want to run individually.

3.2.2 Add New Chemicals

As mentioned in **Section 1.1**, the Tool is preloaded with data for some chemicals. You can add additional chemicals to the Tool to supplement the chemicals provided by clicking on the ADD NEW CHEMICAL button in the lower middle of the left pane of the CHEMICALS tab (Figure 8). To reduce the burden of entering new chemicals, the ADD NEW CHEMICAL forms include only the minimum set of chemical-specific parameters required, omitting others that can be calculated from these required properties (e.g., animal and plant bioconcentration factors from log K_{ow} for organics) or reasonably set to a conservative default (e.g., aquatic degradation rates). Once you have added a new chemical, you will have a chance later to edit any default values.

The inputs differ somewhat for organics and inorganics; therefore, you will be asked which type of chemical you want to enter (SELECT NEW CHEMICAL TYPE window). Click on the appropriate button (or CLOSE FORM to cancel and return to the CHEMICALS tab). **Figures 10** and **11** show the entry screens for organics and inorganics, respectively (note that the entire screen as shown in the figures does not all show at once in the Tool; use the vertical scroll bar to see all inputs).

A brief discussion of each of the inputs follows the figures; **Appendix C** provides a thorough explanation of the data required, sources for these data, and estimation methods for all chemical-specific parameters, both those on the ADD NEW CHEMICAL forms and those omitted from them.

Chemical Limitations of the Biosolids Tool

You should not add dioxin-like compounds (i.e., dioxins or PCBs) to the Biosolids Tool: the fate and transport algorithms contained in the Tool are not appropriate for these compounds. You should also not add mercury compounds. Although the Tool contains the appropriate algorithms for these, they must be combined in a somewhat different way that is beyond the scope of this User's Guide.

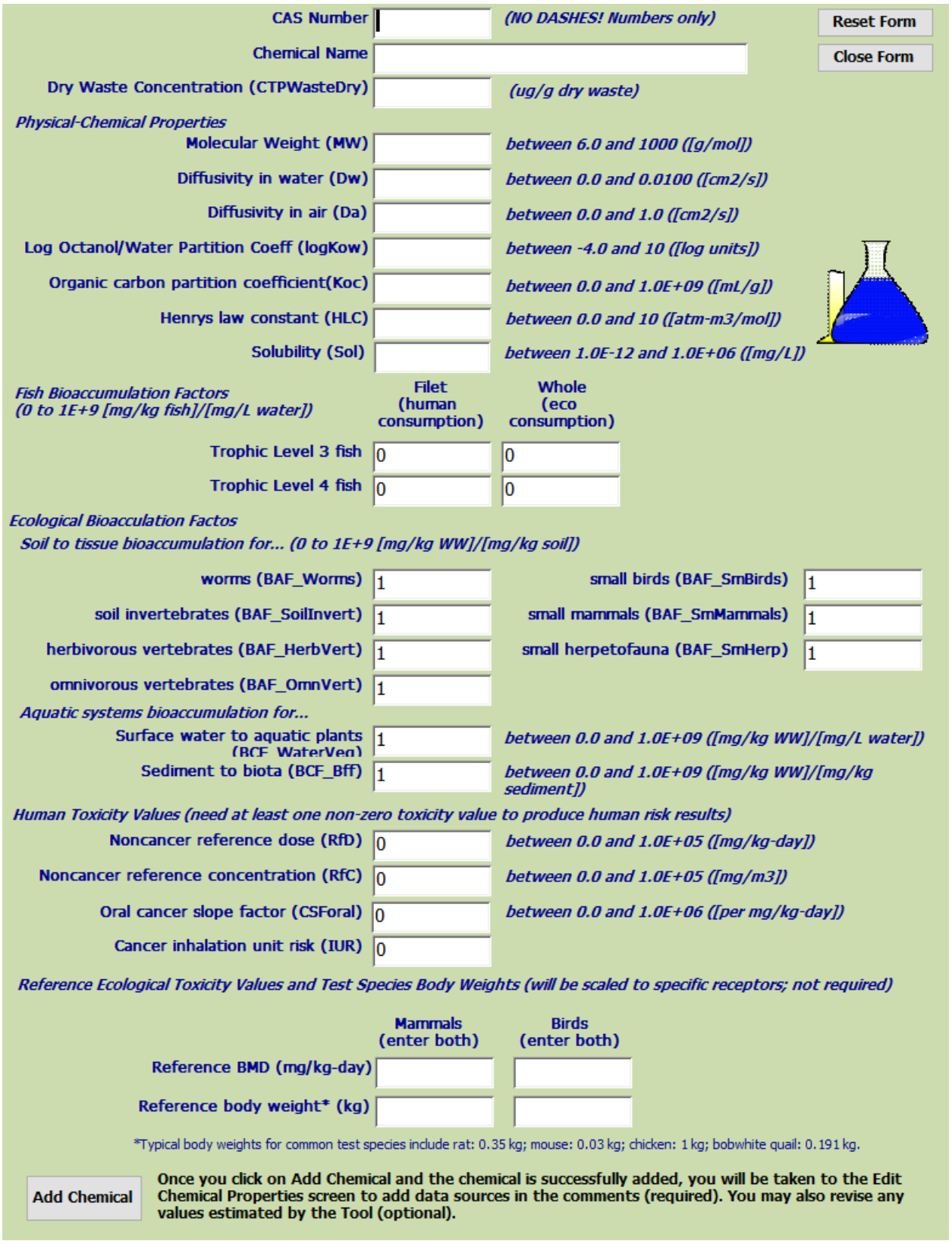


Figure 10. ADD NEW ORGANIC CHEMICAL window.

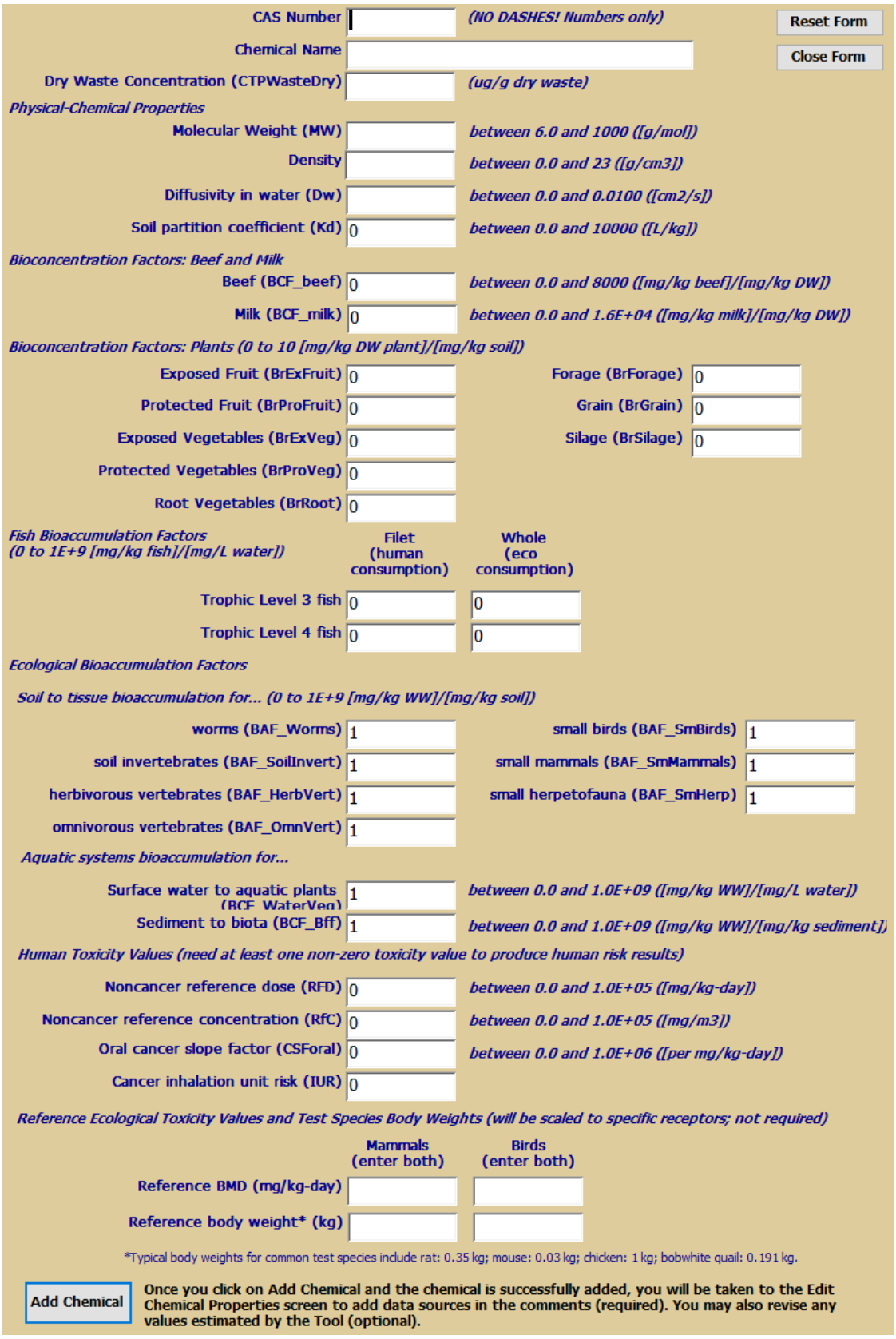
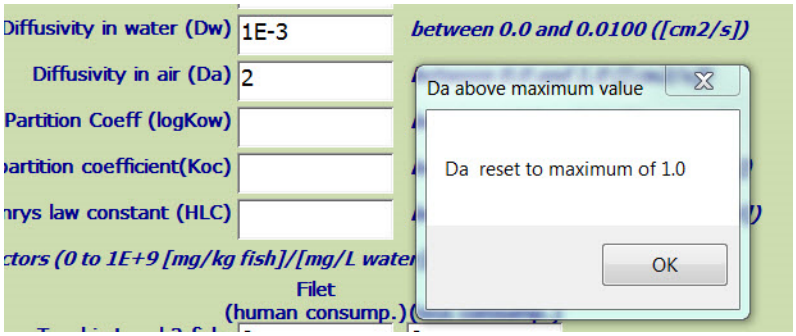


Figure 11. ADD NEW INORGANIC CHEMICAL window.

You can move through the fields on the ADD NEW CHEMICAL forms in order using the TAB key or you can skip around by clicking in the desired field. Once you are in a field, however, you must enter a value within the range specified to the right of the value field (or occasionally above, when it applies to multiple grouped entries). The ranges are inclusive (so below, diffusivity in water must be between 0 and 0.01, and can be exactly 0 or 0.01). If you enter a value outside the range, the Tool will reset it to the minimum or maximum when you leave the field, and you will see a warning that this has been done (shown at right). Click on the OK button to dismiss the warning. You can then either leave the value at the minimum or maximum or, if your entry was a typo and the minimum or maximum is not appropriate, you can correct it. For example, if you entered 2 instead of the actual value 0.2, the reset value of 1 is not appropriate and should be corrected to 0.2.



All of the inputs except chemical name are numeric and can be entered in either standard or scientific notation; scientific notation is not case sensitive (i.e., a value of 34 can be entered as 34, 3.4E+1, or 3.4e+1). Be sure to enter data in the units shown to the right of the allowable range; use of different units will produce erroneous risk results.

Click on the RESET FORM button (top right of ADD NEW CHEMICAL form) to clear your entries without saving and start over. Click on the CLOSE FORM button (also at top right) to cancel without saving and return to the SELECT NEW CHEMICAL TYPE form.

A few things to note:

General Chemical Information

- **CAS number** will be saved as all numbers whether you enter it that way or with hyphens.
- **Compound name** can be any text string, but it may be helpful for purposes of sorting the results by chemical name to move leading numeric prefixes to the end of the name, as follows: "Chlorophenol, 4-" instead of "4-Chlorophenol."
- **Dry waste concentration (CTPWasteDry)** must be a ***dry weight*** concentration and must be nonzero. If you have only a wet weight waste concentration, divide it by the fractional equivalent of the percent solids you entered on the SCENARIOS tab. So, for the default solids content of 40%, divide the wet weight by 0.4 to obtain a dry weight.

Physical-Chemical Properties

- **Molecular weight (MW)** can be derived from the chemical formula if you cannot locate it otherwise. However, these data are generally readily available.
- **Diffusivities in water (Dw) and air (Da)** reflect the molecular diffusion of chemicals through water or air. Data for diffusivity are not widely available, so they must typically

be estimated; see **Appendix C, Section C.4.1** for details on how to estimate. Diffusivity in air does not apply to non-volatile chemicals (i.e., most inorganics).

- **Log octanol-water coefficient (log K_{ow})** reflects how organic chemicals partition between octanol and water and is widely available. It applies to most organics, but for some chemicals that accumulate mainly to tissues besides fat, log K_{ow} is not appropriate. Some chemicals with surfactant properties may also not have meaningful log K_{ow} values as the chemical may mainly be present at the interface between the solvents. The Tool uses log K_{ow} only to calculate biotransfer factors for organics for terrestrial pathways. Thus, it can be left blank to indicate that it is not measurable or applicable for a new chemical. Note that setting log K_{ow} to zero is not the same as leaving it blank: zero is a valid value that indicates a K_{ow} of 1. The valid range shown in the form in Figure 10 applies to a non-blank value.
- **Organic carbon partition coefficient (K_{oc})** applies to organics only. If data cannot be located, it can be estimated using EPISuite (U.S. EPA, 2010).[1]
- **Henry's law constant (HLC)** applies to organics only. Compilations are widely available, or it can be estimated using EPISuite.[2] Regardless of whether you have measured data or an estimated Henry's law constant, if the value is less than 1×10^{-10}, you should set it to zero; otherwise, you will get unrealistically large values of the air-to-plant uptake factor, Bv.
- **Density** is used to estimate diffusivity in water for inorganics. Data are widely available.
- **Soil partition coefficient (K_d)** is an input for inorganics only; for organics, it is calculated from K_{oc} and fraction organic carbon (although you can change the calculated value later).
- **Solubility** is used only to generate a warning if the soil porewater concentration for the LAU exceeds the solubility value at any time during the simulation. It is not used directly in the LAU simulation or any other model computations, so different values will have no impact on the numeric results (but may affect whether the solubility warning is shown). See **Section 5.1** for more discussion of the solubility limit exceeded warning.

Bioconcentration and Bioaccumulation Factors

- **Terrestrial bioconcentration factors for beef, milk, produce, and grains** are inputs for inorganics; for organics the BST will estimate from log K_{ow} (although you can change those calculated values later). You should be aware if the chemical is part of a category that is not appropriate for using K_{ow} to estimate bioaccumulation in organisms.
- **Fish and other aquatic BAFs** are available from a variety of literature sources, or they can be estimated using EPISuite for organics (such BAFs will be flagged as "BAF estimated" in the results; see **Section 5.1**).[2] Four BAFs can be entered: trophic level 3 (TL 3) whole fish; TL4 whole fish; TL3 filet; and TL4 filet. Filet BAFs are used to estimate tissue concentrations in fish consumed by human receptors, while whole fish BAFs are used to estimate tissue concentrations in fish consumed by ecological receptors. Human receptors are assumed to eat both trophic level 3 and 4 fish; specific ecological receptors may eat one, both, or neither, depending on the receptor.

[1] When using EPISuite to estimate parameter values, be sure to enter any properties data you do have so that the estimated property value will be consistent with the data you have, and always select the "Full Results" option.

If you are using literature data, select the longest study time available. If values are not available for both filet and whole for both trophic levels, you can substitute the values you do have for the others (such BCFs/BAFs will be flagged as "BCF/BAF is surrogate" in the results; see **Section 5.1**).

If you estimate BCFs/BAFs using EPISuite, select values from the Arnot-Gobas method, and use "mid-trophic level" for TL 3 and "upper trophic level" for TL 4. Be careful to select the actual BCF/BAF value in parentheses, not the log BCF/BAF value that is listed first. The EPISuite estimates do not distinguish between whole fish and filet, but can be used for both; these are flagged only as "BCF/BAF estimated"; any estimated BCF/BAF is also inherently a surrogate.

Fish BCFs/BAFs can be used as a surrogate for BCFs/BAFs for aquatic plants and benthic filter feeders if data are not available.

If no BCFs/BAFs are available for inorganics (which cannot be estimated using EPISuite), the risks for human receptors and any fish-eating ecological receptors will be zero for the fish pathway and reduced for the total ingestion or (for ecological receptors) total diet. If ingestion is a concern for a chemical, further information will be required to evaluate transfer effects.

- **Terrestrial BAFs** are sometimes available in literature for metals, but these BAFs for organic chemicals are generally lacking. If a BAF or BCF is missing or set to zero, then the concentration in the particular food item will be zero and that part of an ecological receptor's diet will not contribute to risk. So, if the BAF_SmMammals is 0, then any ecological receptor that consumes small mammals as part of their diet will not receive any dose from small mammals. Alternatively, BAFs with missing data can be set to a default of 1.

Toxicity Values

- **Human toxicity values** must be chronic (not acute) cancer or noncancer values, preferably from EPA's Integrated Risk Information System (IRIS), available at http://www.epa.gov/iris/, or the Office of Pesticide Programs (for pesticides). If no toxicity value is available from IRIS or OPP, use the hierarchy of sources shown in **Appendix D, Section D.1.** Set any for which you do not have data to zero. However, if you do not enter at least one nonzero human toxicity value, the Tool will not generate human risk results for the new chemical. A warning will advise you of this and give you the option to add values or leave them all zero. Human toxicity values can be added later in the Edit Chemicals screen.
- **Ecological toxicity values for mammals and birds** are typically scaled from a reference benchmark and the body weight of the test species it was based on. The reference benchmark doses and body weights for mammals and birds can be entered if available or left blank if not. Once you enter a benchmark dose, you must enter an associated benchmark body weight. Ecological toxicity values for direct contact receptors must be added later by editing chemical properties.

Zero Toxicity Values

A toxicity value of zero is not an indication that the chemical is not hazardous, only that hazard data have not yet been found or developed for that chemical in that organism or route of exposure (inhalation, ingestion, direct contact). Therefore, the lack of risk results for a receptor or pathway in the summary output table resulting from a zero toxicity value indicate an absence of toxicity data, not an absence of risk.

Click on the ADD CHEMICAL button at the bottom of the form to add the chemical and its properties to the database. If you have left log K_{ow} blank (not zero, which is a valid value), you will see a warning; you can click on OK to continue with log K_{ow} null or CANCEL to go back and add a value if the omission was inadvertent. A window will then pop up confirming that your data have been saved; click OK. A second window will then appear with information about adding references and ecological toxicity values (which are not included on the ADD NEW CHEMICAL forms). Click OK to continue. The Tool will open the EDIT CHEMICAL PROPERTIES screen for the new chemical, where you can enter references for the properties you just entered (required), revise any defaults or calculated values if you have data or can estimate them (optional), add aquatic degradation rates if data are available, and add receptor-specific ecological toxicity values (optional, but some must be added to obtain non-zero ecological risk results). The EDIT CHEMICAL PROPERTIES screen is described in the next section.

3.2.3 View, Edit, and Delete Chemicals

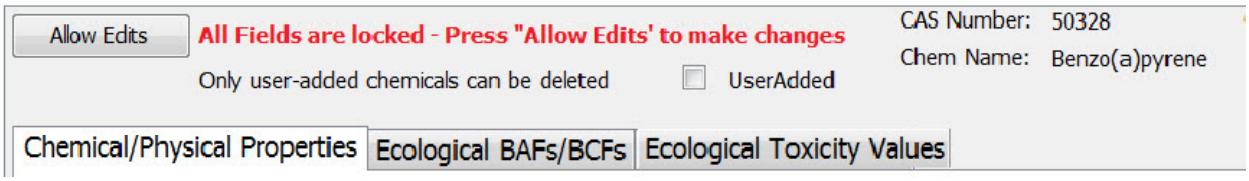
Click on the VIEW/EDIT/DELETE button next to a chemical name on the CHEMICALS tab (see Figure 8) to display the CHEMICAL PROPERTIES screen, the top of which is shown in **Figure 12**. Here you can

- View and edit the chemical-specific data (built-in and user-added chemicals)
- Reset modified values to defaults (built-in chemicals only)
- Delete chemicals entirely (user-added only).

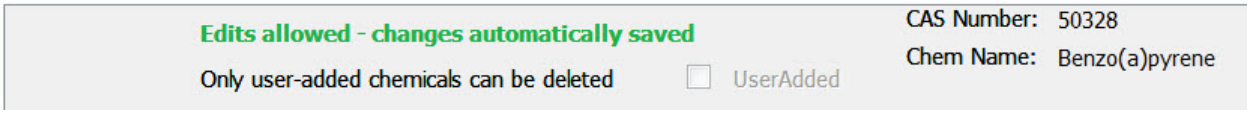
IMPORTANT! Any modifications you make to the chemical data are automatically saved in the underlying database and will be used until you change them again or choose explicitly to reset them to the original, default values.

See **Section 5.3** for a discussion of how to save a version of the Tool with such changes while retaining an original version; you will need to prepare to do this BEFORE you change any configuration values.

(A) VIEW mode, built-in chemical



(B) EDIT mode, built-in chemical



(C) VIEW mode, user-added chemical (DELETE CHEMICAL button visible)

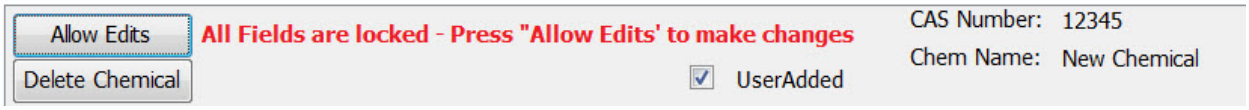


Figure 12. CHEMICAL PROPERTIES screen header: in (A) VIEW mode for a built-in chemical, (B) EDIT mode for a built-in chemical, and (C) VIEW mode for a user-added chemical (DELETE CHEMICAL button visible).

When you first open this screen, it will be in VIEW mode (top of Figure 12): the data fields are locked to prevent accidental changes and cannot be edited. When the fields are locked, there will be an ALLOW EDITS button and a red warning that the fields are locked in the upper left corner of the screen. If you just want to view the data, leave it in view mode. If you want to edit or add data, click on the ALLOW EDITS button. This will place you in EDIT mode (center of Figure 12);

the ALLOW EDITS button will no longer be displayed, and the red "All fields are locked" warning will be replaced with "Edits allowed – changes automatically saved" in green. The individual tabs showing the data you can edit are described below. All changes are saved immediately and automatically in EDIT mode.

If the chemical you have chosen to view is a user-added chemical (bottom of Figure 12), the USERADDED checkbox below the locked message will be checked, and the DELETE CHEMICAL button will be displayed below the ALLOW EDITS button. (For built-in chemicals, the DELETE CHEMICAL button is not displayed, and a message notes that only user-added chemicals can be deleted, as shown in the top and center panes of Figure 12). Click on the DELETE CHEMICAL button to delete the chemical completely from the database. The Tool will ask for confirmation; click YES to delete (this cannot be undone) and close the CHEMICAL PROPERTIES screen, NO to keep the chemical and close the CHEMICAL PROPERTIES screen, and CANCEL to keep the chemical and remain on the CHEMICAL PROPERTIES screen,

The chemical-specific data are organized into three tabs: CHEMICAL/PHYSICAL PROPERTIES, ECOLOGICAL BAFS, and ECOLOGICAL TOXICITY VALUES. Each tab shows a list of properties, the current value, the units and allowable range, a comment, a checkbox indicating whether you have modified the value, and a reference. The references are a short citation; **Section 7** contains a list of full citations for all references used in the database, sorted by this short citation. Note that human health toxicity values and reference ecological benchmark doses are found on the CHEMICAL/PHYSICAL PROPERTIES tab, while concentration-based ecological toxicity values as well as receptor-specific benchmark doses for various mammal and bird species (for which there may be multiple receptors with different toxicity values) are found on the ECOLOGICAL TOXICITY VALUES tab. The benchmark doses for mammal and bird receptors are scaled from the reference benchmarks in the CHEMICAL/PHYSICAL PROPERTIES tab; see **Appendix D** for more details on ecological benchmark scaling.

Use the inner scroll bar on the right to scroll through the list of properties on a tab. Click in a box to change the value or comment. You can also tab through the entry fields. For each property, you can change the value (which may be entered in either standard or scientific notation) and add a comment. The comment is required and should note the source and any assumptions or surrogates of values for chemicals you have added or values you have changed. The User Modified check box under the range for each property will be checked if you change a value, for both built-in and user-added chemicals. This way, you can see if you have changed a value on a user-added chemical after adding it (e.g., if you change a calculated or default value). In addition, the reference will be changed to "User supplied."

On all tabs, be sure to enter new values in the units shown—the units cannot be modified. If your source does not report values in the same units, you will need to convert the reported value to the units required by the Tool. Entering data that are not in the units shown will produce erroneous risk results. You must also enter a value within the range specified in the entry screen to the right of the value field. If you enter a value outside that range, it will be reset to the minimum or maximum and you will see a warning that this has been done. You can either leave the reset value or, if your entry was a typo and the minimum or maximum is not appropriate, you can correct it after clicking on OK to dismiss the warning.

If you have just added a new chemical and been brought to this screen, you will need to enter references (in the comments field) on the CHEMICAL/PHYSICAL PROPERTIES and ECOLOGICAL BAFS/BCFS tabs, and values and references on the ECOLOGICAL TOXICITY VALUES tab.

CHEMICAL/PHYSICAL PROPERTIES tab: This tab (**Figure 13**) shows chemical/physical properties (including aquatic degradation rates), BCFs/BAFs for human pathways, and human toxicity values in alphabetical order by the MODEL CODE, which is a short property name (e.g., Henry's law constant is alphabetized by HLC, its MODEL CODE).

If you change chemical/physical property values and then change your mind, click on the RESET CHEMICAL PROPERTIES TO DEFAULTS button above the parameter list. This only resets values shown on this tab; the other tabs have their own reset buttons.

Uptake Factors

Please note that this User's Guide is written for a varied audience and that the terminology used by environmental toxicologists continues to evolve. For these reasons this Guide uses BCF/BAF to include the multitude of approaches and computations used to quantify the movement of chemicals from a surrounding medium (air, soil, sediment, water) into living organisms. These may include bioaccumulation, bioconcentration, biomagnification, and biotransfer factors. A tiered approach is considered when using measured or modeled bioaccumulation, bioconcentration, biomagnification, and biotransfer factors.

Terrestrial BCFs/BAFs (i.e., for plants and animal products) for organic chemicals are calculated based on the log K_{ow} (and HLC in the case of B_v, vapor air-to-plant uptake) if a value is available for log K_{ow} (and HLC for B_v). These BCFs/BAFs are denoted with an asterisk at the end of the parameter description, and a reminder of this appears next to the RESET CHEMICAL PROPERTIES TO DEFAULTS button. If you change the values for either log K_{ow} or HLC, the Tool will ask if you want to recalculate these BCFs/BAFs. Click on YES to recalculate them (this will overwrite any values you changed for the affected BCFs/BAFs), or NO to skip recalculating if you feel this is not appropriate for the chemical in question or you have entered values from another source and do not want them overwritten. You will need to enter terrestrial BCFs/BAFs for any new chemical which does not have a log K_{ow}. If you change an existing log K_{ow} to a blank (or null) value (not zero, which is a valid value), the Tool will reset the terrestrial BCFs/BAFs for that chemical to zero, unless you have entered or modified the terrestrial BCF/BAFs values (in which case, the values you entered will not be overwritten).

Human toxicity values include cancer and noncancer toxicity values for oral and inhalation exposures, so a total of four possible toxicity parameters. However, a few chemicals (e.g., cadmium, manganese) have multiple oral noncancer toxicity values, or pathway-specific RfDs, instead of the typical single RfD used for all oral exposures. These pathway-specific RfDs are for water, soil, fish, food, or some subset of these. The Tool supports the use of either a general or pathway-specific RfDs for all chemicals. Near the top of this tab is a checkbox, which is enabled in Edit mode, that allows you to choose whether to display and use the single RfD for all ingestion pathways (checkbox unchecked) or the four pathway-specific RfDs (checkbox unchecked).

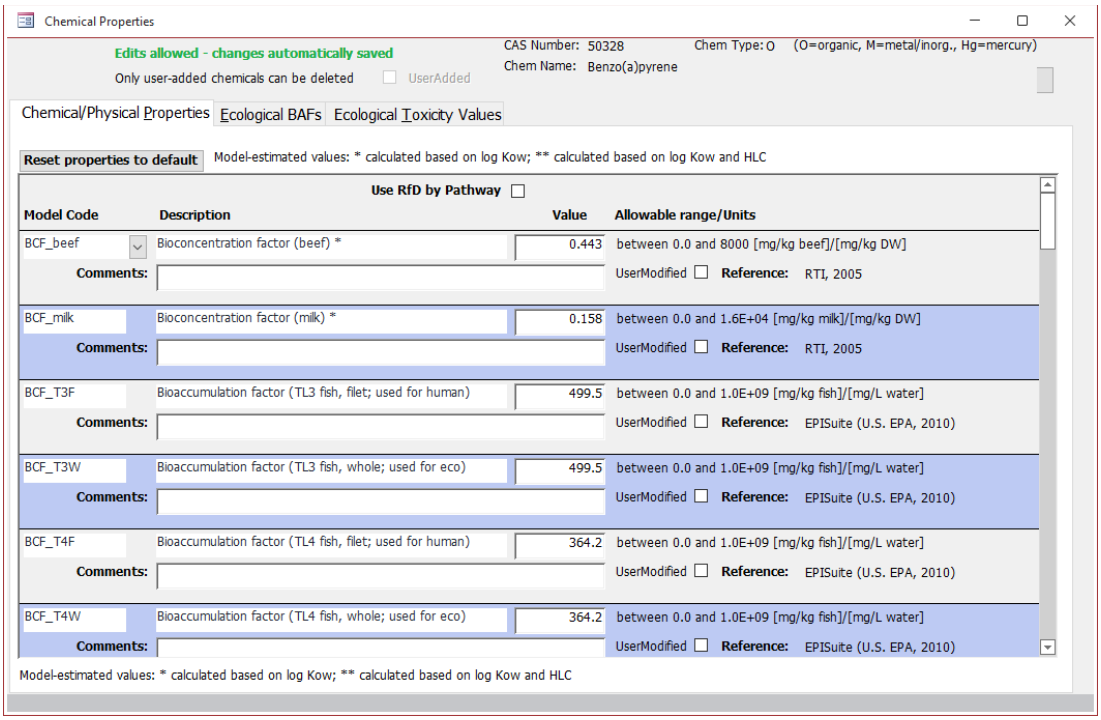


Figure 13. Chemical/Physical Properties tab.

Section 3.2.2, **Add New Chemicals**, has more information about many of the values shown on this tab. Additional information for all parameters shown in this tab except toxicity values, including the equations for calculating BCFs/BAFs for animal products, produce, and grains, may be found in **Appendix C**; more information on human toxicity values may be found in **Appendix D**.

ECOLOGICAL BAFS TAB: On this screen (**Figure 14**), you can edit existing ecological terrestrial and aquatic BAFs, as well as add new ones. The existing BAFs and BCFs are listed in alphabetical order by parameter name; to edit one, simply click in the value field and change the value. Enter the source in the comment field. To add a new one, use the inner scroll bar to get to the bottom of the list and select a type of BAF or BCF from the dropdown box under MODEL CODE. Then enter the value in the value field and the source in the comment field. **Section 3.2.2**, **Add New Chemicals**, has more information about BCF/BAF values. Additional information may be found in **Appendix C**, **Section C.5**.

If you change BCF/BAF values and then change your mind, click on the RESET PROPERTIES TO DEFAULT button above the parameter list. This only resets values shown on this tab; the other tabs have their own reset buttons. It does not delete or reset new BCFs/BAFs that you added.

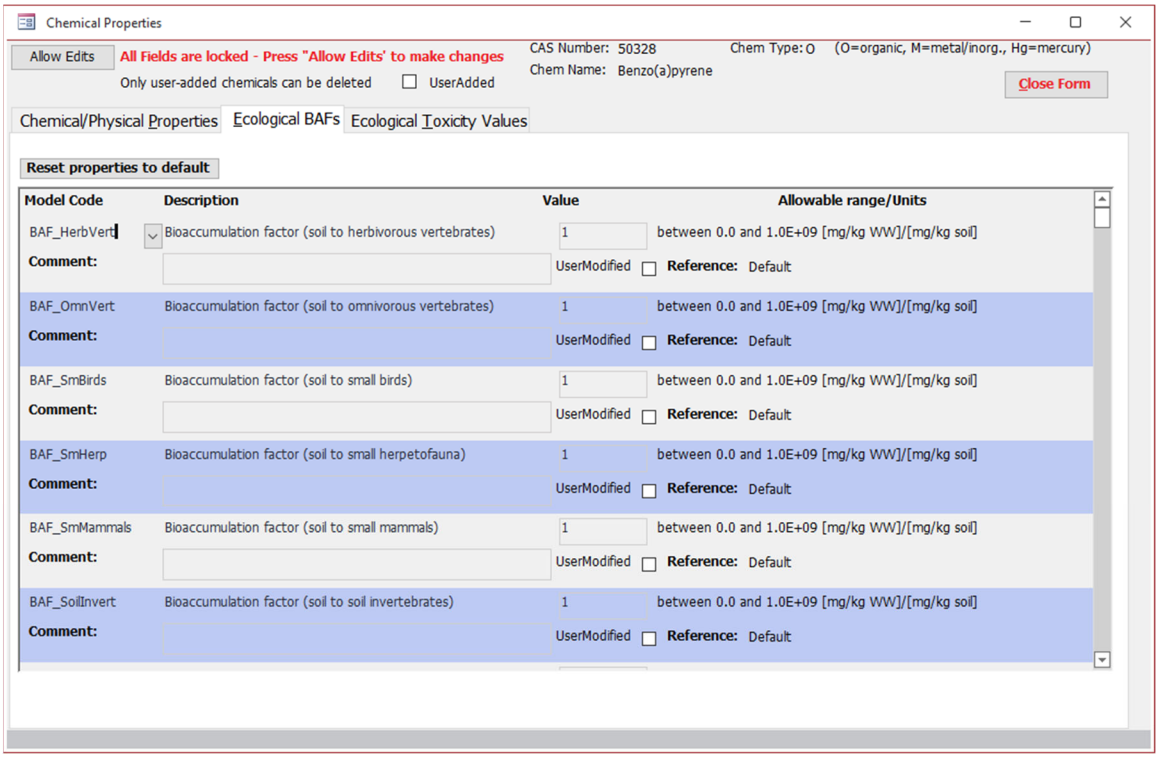


Figure 14. CHEMICAL PROPERTIES window: view or edit ecological BAFs/BCFs.

ECOLOGICAL TOXICITY VALUES tab: On this screen (**Figure 15**), you can edit existing ecological toxicity values and add additional receptors that do not currently have ecological toxicity values. Each type of receptor has an associated type of toxicity value:

- **Birds and mammals** have a benchmark dose (BMD); these are typically based on two reference BMDs and associated test species body weights, one for birds and one for mammals. The reference data may be added or edited on the CHEMICAL/PHYSICAL PROPERTIES tab described above. If you add or change the reference data, the Tool will ask if you want to calculate new scaled species-specific values. You will need to have entered both the reference BMD and reference body weight, so you may want to select No after you change one if you are about to change the other. If you are entering data where there was none before, it will be able to calculate until you enter both values. However, the computation is very fast. The resulting scaled values for individual bird and mammal receptors are shown in this tab. However, you can override those scaled values in this tab by entering a different value.
- **Soil community receptors** have a benchmark concentration in soil (BMC_soil); these must be entered or edited here.
- **Aquatic receptors** (including amphibians) have a benchmark concentration in water (BMC_water); these must be entered or edited here. This benchmark also requires an exposure duration (ED_Eco), which is a separate record, to enable the Tool to use a water concentration averaged over the same time period. ED values are restricted to 1 day, 4 days, or 365 days, as these are the available averaging times for water concentrations in the Tool and the most common values associated with available BMC_Water values.

- **Sediment community receptors** have a benchmark concentration in sediment (BMC_sed); these must be entered or edited here.

To edit an existing toxicity values, simply click in the value field and change the value. When you leave the field, you will be prompted to enter a reference or other text documenting the source of the value; this will be saved in the comment field. If you do not enter something, the Tool will enter "No reference supplied" in the comments field. If you edit a BMC_Water, be sure to check (and edit if necessary) the associated ED_Eco value (this should be the record immediately below the BMC_Water record for the same receptor). Currently, the Tool can only accommodate one BMC_water/ED_Eco pair for a particular chemical and receptor at a time. If you want to do runs for different pairs for the same chemical and receptor, you will need to do separate runs, and edit the values in between.

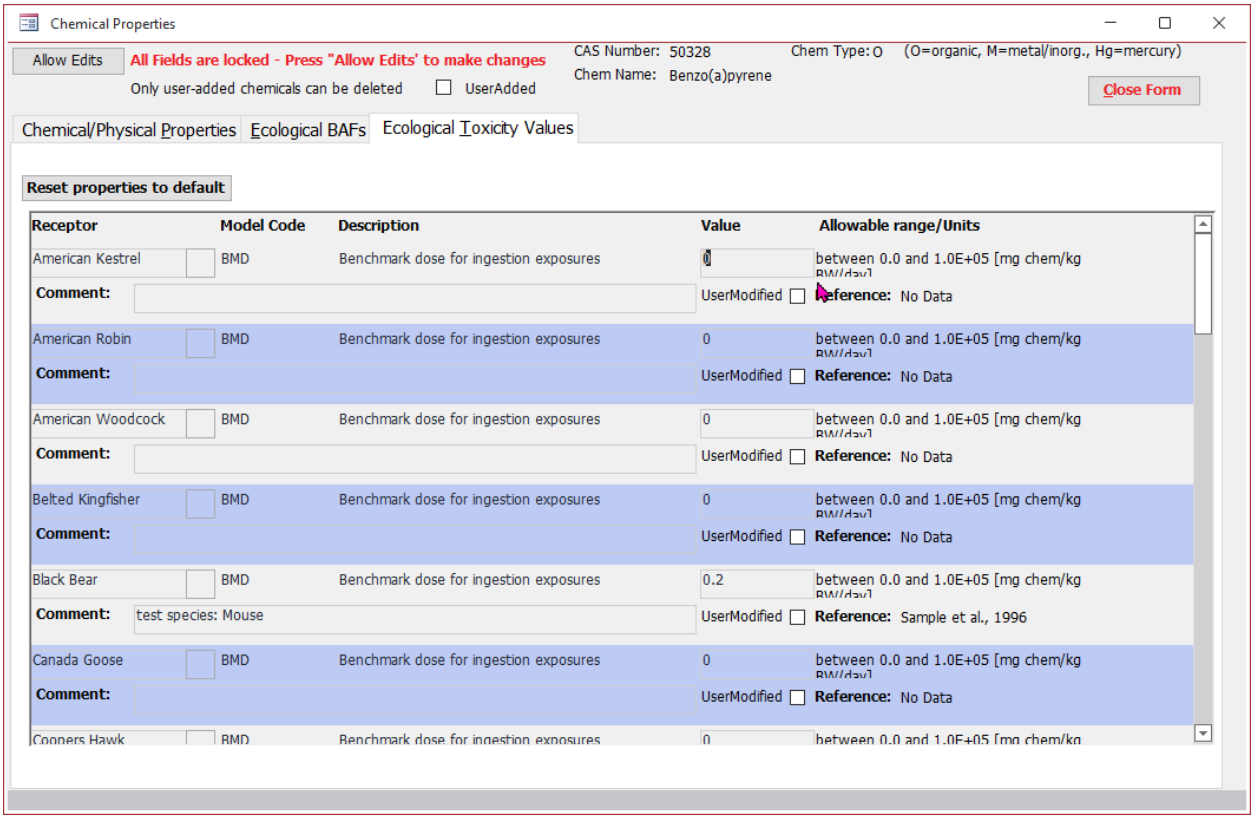


Figure 15. CHEMICAL Properties window: view or edit ecological toxicity values.

To add a toxicity value for a receptor not already listed, click on the ADD RECEPTOR(S) FOR THIS CHEMICAL button at the top of the form. This will open a dialog box with a dropdown from which you can select any receptor for which this chemical does not already have a toxicity value. Click on the ADD RECEPTOR button to add the receptor. The dialog box will remain visible, so you can add another receptor if desired. When you are done adding receptors, click on the CLOSE button. You should now have one or two new records per new receptor, at the bottom of the list of receptors shown in Figure 15; receptors that use a BMC_Water will have two new records, one for the benchmark and one for the exposure duration and all others will have one new record, for the benchmark. These records are pre-populated with the receptor name, the toxicity value

type, and a default value of 1 for the benchmark and, if applicable, 365 days for the exposure duration. You can then edit these default values to the desired values. Additional information on ecotoxicity values may be found in **Appendix D**.

If you change ecological toxicity values and then change your mind, click on the RESET PROPERTIES TO DEFAULT button above the parameter list. This only resets values shown on this tab; the other tabs have their own reset buttons. It does not delete or reset new receptor-toxicity value combinations that you added. You can delete records for receptors you have added (but not records for receptors included with the Tool) by clicking on the red Delete button at the right edge of the tab by the record you wish to delete.

When you are done editing chemical data, click on the × in the upper right corner of the CHEMICAL PROPERTIES form to close it; this will return you to the CHEMICALS tab of the CONFIGURE MODEL screen (Figure 9). Additional information may be found in **Appendix C** for physical-chemical properties and ecological BAFs/BCFs, and in **Appendix D** for toxicity values (both human and ecological).

3.2.4 Compare Non-default Properties for Selected Chemicals

You can compare the non-default (user-entered) chemical properties for the set of chemicals you have selected to include in a simulation. On the CHEMICALS tab, click on the VIEW button under COMPARE PROPERTIES OF SELECTED CHEMICALS (to the left of the list of chemicals; see Figure 8). **Figure 16** shows an example of the CHEMICAL PROPERTY COMPARISON window. In this example, only two chemicals were selected, but if more are selected, the display includes additional columns to the right for each chemical. While not all columns will show on the screen at once if you have more than a few chemicals selected, you can scroll over to view the data. You may find it easier to export comparisons for many chemicals to Excel; you can do that by clicking on the EXPORT TO EXCEL button under the VIEW button. You will be prompted for a file name and location. The Excel file is structured the same way as the window shown in Figure 16, but also includes a second tab with the references for each property for each chemical where the value is shown in Figure 16.

Chemical Property Comparison

Model_Code	Units	Description	Aluminum	Benzo(a)pyr
BCF_beef	[mg/kg beef]/[mg/kg DW]	Bioconcentration factor (beef)	0.0184	0.443
BCF_milk	[mg/kg milk]/[mg/kg DW]	Bioconcentration factor (milk)	0.00414	0.158
BCF_T3F	[mg/kg fish]/[mg/L water]	Bioaccumulation factor (TL3 fish, filet; used for human)	36	980
BCF_T3W	[mg/kg fish]/[mg/L water]	Bioaccumulation factor (TL3 fish, whole; used for eco)	36	980
BCF_T4F	[mg/kg fish]/[mg/L water]	Bioaccumulation factor (TL4 fish, filet; used for human)	36	400
BCF_T4W	[mg/kg fish]/[mg/L water]	Bioaccumulation factor (TL4 fish, whole; used for eco)	36	400
BrExfruit	[mg/kg DW plant]/[mg/kg soil]	Biotransfer (soil to exposed fruit)	0.00065	0.00348
BrExveg	[mg/kg DW plant]/[mg/kg soil]	Biotransfer factor (soil to exposed vegetables)	0.004	0.00348
BrForage	[mg/kg DW plant]/[mg/kg soil]	Biotransfer factor (soil to forage)	0.004	0.00348
BrGrain	[mg/kg DW plant]/[mg/kg soil]	Biotransfer factor (soil to grain)	0.00065	0.00348
BrProfruit	[mg/kg DW plant]/[mg/kg soil]	Biotransfer factor (soil to protected fruit)	0.00065	0.00348
BrProveg	[mg/kg DW plant]/[mg/kg soil]	Biotransfer factor (soil to protected vegetables)	0.00065	0.00348
BrRoot	[mg/kg DW plant]/[mg/kg soil]	Biotransfer factor (soil to roots; inorganics only)	0.004	
BrSilage	[mg/kg DW plant]/[mg/kg soil]	Biotransfer factor (soil to silage)	0.004	0.00348
Bv	[ug/g DW plant]/[ug/g air]	Biotransfer factor (vapor phase air to all plants; organics only)		3490000
CSFOral	[per mg/kg-day]	Oral cancer slope factor (human toxicity)	0	1
CTPWasteDry	[ug/g DW]	Dry biosolids concentration	34300	2.19
Da	[cm2/s]	Diffusivity in air		0.0405
Density	[g/cm3]	Density (chemical)	2.7	
Dw	[cm2/s]	Diffusion coefficient in water	0.0000381	5.74E-6
Heat_of_Henry	[J/mol]	Enthalpy of phase transformation from aqueous solution to air solu	0	17000
HLC	[atm-m3/mol]	Henry's law constant		4.57E-7

Figure 16. Chemical Property Comparison window.