

User's guide for Human Health SQO Decision Support Tool (DST)

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1. Summary

The Decision Support Tool (DST) is an Excel workbook that performs the Tier 2 SQO site assessment. This guide describes the key steps needed to perform a Tier 2 standardized assessment with the DST. Before using the DST, the user should be advised that the DST does not perform all data steps needed to conduct the assessment. The DST performs the modeling and simulation analyses unique to the Tier 2 assessment. The DST also assigns categories for chemical exposure, site linkage, and overall site assessment, based on thresholds for these indicators. The user must compile and summarize the contamination and site data prior to using the DST. The distributed version of the DST includes sample data that can be used for demonstration purposes, without the user being required to add their own data. Section 2 describes the organization of the DST, and the remaining sections describe the steps for installing and using the DST. The appendix contains a list of key issues and their solutions that have been noted when using the DST.

Please note that while there is password protection of many of the cells in this version of the DST to prevent accidental modification of the tool, not all cells could be protected. Therefore, be very careful when looking at cells other than those designated for user input, as copy/paste actions or an inadvertent key stroke or deletion can unintentionally change critical values or formulas that will affect the function of the DST. Some of the output cells in the DST refer to hidden cells to the right or below the results section of the worksheet. Do not delete or modify any cells outside of the main portion of the worksheet, as you may modify the cell references or the contents of these cells and cause the DST to malfunction.

2. Organization of the Decision Support Tool

The DST contains five main worksheets for input and calculations (Figure 1), and additional worksheets that summarize and plot the results. After simulations are complete, the DST will contain additional worksheets that include simulation results (Figure 1, grey boxes).

- **Input.** The "Input" worksheet is where the user enters site specific data. Data entered into the "Input" sheet include the seafood species analyzed, each species' proportion within the consumer diet and lipid content, the total contaminant concentrations in seafood and sediment, site size, and water and sediment chemistry parameters.
- **Output Summary.** The "Output Summary" sheet is where all the output needed to determine the SQO categorization resides. This page is formatted so that it will print out on a single page. Information is also provided on the timing of the last macro run and the simulation run for which data is being shown. This page updates dynamically as simulations are run, or the output from a particular run can be selected by the user from the "Assessment Summary" page.
- **Contaminant Specific.** The "Contaminant Specific" sheet is where the user enters individual compound concentrations for the water column and porewater, if available, and for sediment. This sheet is where chemical partitioning calculations are performed based on compound-specific attributes.

- **Food Web Calculations.** The “Food Web Calculations” sheet employs the user input and default parameters to calculate the bioaccumulation factor for each contaminant class and food web component.
- **Assessment Summary.** The “Assessment Summary” is where all the calculations occur for SQO categorization. In addition, this sheet includes an echo of inputs and outputs of calculated BSAFs.
- **Equation Continuity Check.** The Equation Continuity Check page is designed to assure that none of the thousands of equations in the DST have been compromised. This sheet includes a dataset to be entered after which the Food Web macro and Simulation will be run. The output from this run will be compared to a standardized set of results to verify that the calculations are correct.
- **MCS.** Once the bioaccumulation factor has been calculated, Monte Carlo Simulation (MCS) is performed, based on equations in the “MCS” sheet. The data generated by the MCS is used to determine the SQO categorization.
- **Default Parameters.** The “Default Parameters” sheet contains various fixed parameters used in calculating chemical exposure, site linkage, and bioaccumulation modeling.

After the MCS is complete, three additional sheets are automatically created, containing the results of the MCS. These sheets consist of 1) “Iterations Output”, which lists the outcome of each iteration of the simulation, 2) “CFD Output”, which lists the results for each percentile of the iterations output, and 3) “Simulation Output”, which is a tabular summary of the MCS results that includes summary statistics and values for specific percentiles. Each time a new MCS is performed, an additional set of three worksheets is created.

Note: The DST was developed in Microsoft Excel 2003, with updates conducted using more recent versions. The tool has been tested to run successfully using Excel 2013-2016. Use of earlier versions of Excel are feasible, but not recommended. See following section for specific issues related to Excel.

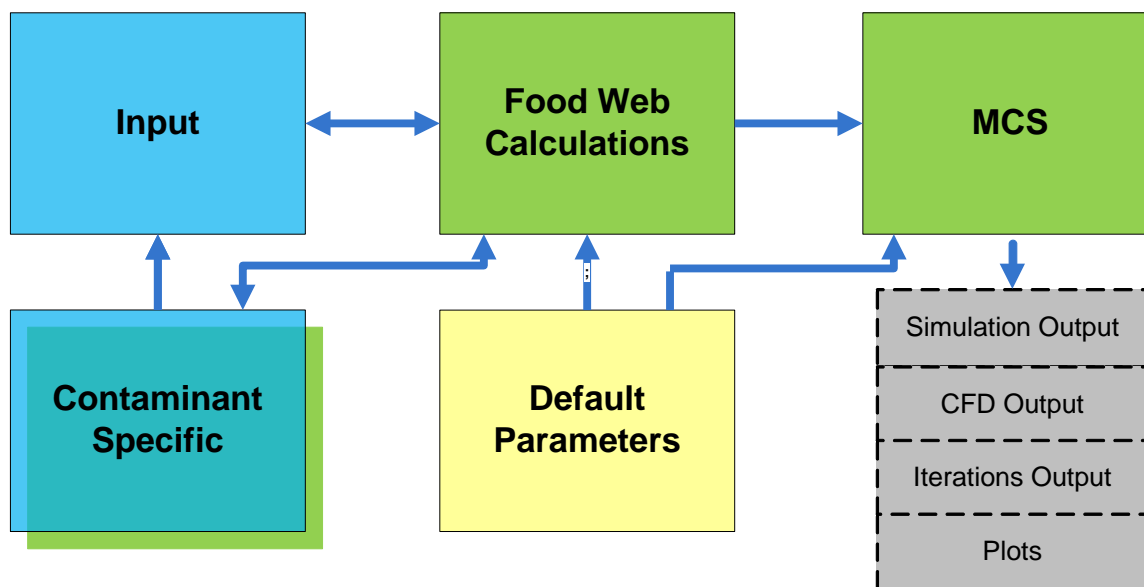


Figure 1. Organization of the Decision Support Tool (DST). Each colored box indicates a separate worksheet, and arrows indicate equations linking the worksheets. The grey boxes with dotted borders show the results worksheets that are produced upon completing the data input and analyses, as described in the text.

User Input Parameters to the Decision Support Tool

The DST allows user entry of multiple parameters based on local data. Some parameters should be locally obtained, while standardized or default values (based on analysis of statewide data) included in the tool may be used for other parameters. A sensitivity analysis was performed to determine which parameters most strongly influence the outcome of the SQO indicators. The sensitivity analysis, and information regarding the relative difficulty of estimating particular parameters, were used to determine which parameters should be determined locally in Tier 2 assessment. Table 1 lists which parameters should be obtained locally and which may use statewide values in the analysis.

Table1. Source of parameter values input into the DST. Statewide = standardized value provided with the DST. Local = site-specific value obtained using local data.

Parameter	Source of data	Statewide Default Values
Seafood contaminant concentration	Local *	
Seafood consumption rate	Statewide	32 g/day
Cooking reduction factor	Statewide	OEHHA
Exposure duration	Statewide	OEHHA
Body weight	Statewide	OEHHA
Sediment concentration	Local *	
Seafood lipid	Local	
Seafood foraging range	Statewide for each dietary guild *	
Sediment TOC	Local	
Proportion of fish species in diet	Statewide	Equal among species
Temperature	Statewide or optional local	17.36 °C
Suspended sediment concentration	Statewide or optional local	2.3E-05 kg/L
Particulate organic carbon	Statewide or optional local	1.57E-06 kg/L
Salinity	Statewide or optional local	25.44 PSU
Dissolved oxygen	Statewide or optional local	9.0 mg/L
Dissolved organic carbon	Statewide or optional local	2.15E-06 kg/L

* These parameters are varied as probability distributions in the Tier 2 assessment. All other parameters are treated as point estimates.

3. Install Monte Carlo Simulation (MCS) Add-In

The DST performs stochastic simulations using Monte Carlo Simulation. To make the DST fully functional, a free Excel Add-In (YASAIw) must be installed. The YASAIw Add-In was developed by Greg Pelletier, Washington Department of Ecology (gpel461@ecy.wa.gov), based on software originally developed by Jonathan Eckstein and Steven T. Riedmueller, Rutgers University.

A copy of the Add-In (YASAIw_SCCWRP.xla) is included in the zip file with the DST distribution. Only the Add-In provided with the DST should be used, as the code has been modified for use with the DST. The Add-In comes with a pdf document (Pelletier 2009) here referred to as the YASAIw User's Manual. Once the zip file is downloaded and opened, installation instructions, found on page 2 of the User's Manual, should be followed. The YASAIw User's Manual (Pelletier 2009) also contains helpful information about the Add-In. In particular, pages 13 through 17 contain additional information about running simulations, the charting tools, and troubleshooting.

The first time that the DST and YASAIw Add-In are installed on a new computer, a number of issues must be checked and resolved for the DST to function properly. Instructions are provided in the Appendix that should be followed for four issues:

1. Configure Excel Macro security (it is recommended that the DST be stored and run on a local computer as opposed to through a network. This allows the file to more easily be designated as “trusted” for Macro security).
2. Confirm YASAIw Add-In has been correctly installed.
3. Confirm macros are enabled.
4. Update links to YASAIw Add-In.

4. Set Up the Analysis

The DST is currently set up to perform a Tier 2 SQO assessment. The Tier 2 assessment is based on a combination of statewide and site-specific data and assumptions. After opening the DST, the user enters the site-specific data into the appropriate cells of the DST spreadsheet. The instructions in this document are intended to explain operation of the DST under typical applications. Specific decisions regarding which data and parameters to be used should follow the requirements of the relevant State and local regulatory agencies. The steps are as follows:

Open a new copy of the DST

The DST stores input data from a single site. To prevent overwriting and potential loss of data, it is recommended that each analysis be conducted using a separate copy of the DST. The spreadsheet cells are color coded as follows: **Blue cells** are areas for user data entry. **Green cells** are variables and calculations. **Purple cells** are headers for areas of input that maybe otherwise difficult to see.

Enter the data and select default parameters.

Select appropriate species from seafood species and guild menus in the “Input” worksheet.

The user should enter data for between one and eight species, each representing a different dietary guild. Species selection is organized using pull down menus contained within cells B4 and B11 on the “Input” worksheet (Figure 2). Appropriate species are selected from the corresponding guild. Table 2 contains a list of appropriate species, data entry cells, and the corresponding guilds. In most cases, data from the primary (indicator) species listed in Table 2 should be used for analysis. While the food web for the secondary species in each guild is similar, the forage range may be quite different and result in an inaccurate site linkage result. The forage range for the primary species is used for each guild, regardless of which species is selected for the analysis. For guilds that have no species monitored at the site, the user should leave the cells blank.

If a candidate species is not listed in Table 2, the user should first determine whether the species is appropriate for SQO evaluation and which dietary guild describes its feeding characteristics. If the species is appropriate for analysis, then the user may select the “Other” category in the appropriate guild for that species.

Table 2. Sportfish species for use in SQO assessment, and the corresponding guild and selection cell on the “Input” sheet. The preferred (primary) guild indicator species are shown in bold text and underlined.

Guild species	Dietary guild	Entry Cell
Barred sand bass	Benthic diet with piscivory	B5
Barred surfperch	Benthic diet without piscivory	B7
Bat ray	Benthic diet with piscivory	B5
Black perch	Benthic and pelagic diet without piscivory	B8
Black rockfish	Benthic and pelagic diet with piscivory	B6
Blue rockfish	Benthic and pelagic diet with piscivory	B6
Bonefish	Benthic diet with piscivory	B5
Brown rockfish	Benthic diet with piscivory	B5
Brown smoothhound	Benthic diet with piscivory	B5
Cabezon	Benthic diet with piscivory	B5
<u>California halibut</u>	<u>Piscivore</u>	<u>B4</u>
Channel catfish	Benthic diet with piscivory	B5
<u>Common carp</u>	<u>Benthic diet with herbivory</u>	<u>B9</u>
Dwarf perch	Benthic and pelagic diet without piscivory	B8
English sole	Benthic diet with piscivory	B5
Fantail sole	Benthic diet without piscivory	B7
Grass rockfish	Benthic diet with piscivory	B5
Kelp bass	Benthic and pelagic diet with piscivory	B6
Leopard shark	Benthic diet with piscivory	B5
Lingcod	Piscivore	B4
Monkeyface prickleback	Benthic diet with herbivory	B9
Other	Any	B4 - B11
Pacific angel shark	Piscivore	B4
Pacific sanddab	Benthic diet with piscivory	B5
Pile perch	Benthic diet without piscivory	B7
<u>Queenfish</u>	<u>Benthic and pelagic diet with piscivory</u>	<u>B6</u>
Redtail surfperch	Benthic diet with piscivory	B5
Rubberlip seaperch	Benthic diet without piscivory	B7
Sargo	Benthic diet without piscivory	B7
Señorita	Benthic diet with herbivory	B9
<u>Shiner perch</u>	<u>Benthic and pelagic diet without piscivory</u>	<u>B8</u>
Spotfin croaker	Benthic diet without piscivory	B7
<u>Spotted sand bass</u>	<u>Benthic diet with piscivory</u>	<u>B5</u>
Starry flounder	Benthic diet with piscivory	B5
<u>Striped mullet</u>	<u>Pelagic diet with benthic herbivory</u>	<u>B11</u>
Striped seaperch	Benthic diet without piscivory	B7
<u>Topsmelt</u>	<u>Benthic and pelagic diet with herbivory</u>	<u>B10</u>
Walleye surfperch	Benthic diet without piscivory	B7
<u>White catfish</u>	<u>Benthic diet with piscivory</u>	<u>B5</u>
<u>White croaker</u>	<u>Benthic diet without piscivory</u>	<u>B7</u>
White seabass	Benthic diet with piscivory	B5
White seaperch	Benthic diet without piscivory	B7
Yellowfin croaker	Benthic diet with piscivory	B5

Enter the proportion of the human seafood consumer diet for each guild.

For each guild, the proportion of the human seafood consumer diet is entered. The proportion of the human seafood consumer diet should sum up to 1.0 (i.e., 100%). For guilds having no monitored species, enter 0. For Tier 2 analysis and cases where local dietary proportion data are not available, an assumption of equal proportions should be used (e.g., for three species, enter a value of 0.333 to represent equal proportions). In cases where consumer survey information on dietary proportions (by mass) is sufficient to determine relative proportion consumed among the different seafood species, varying proportions may be used. For example, if two species are chosen and one species constitutes 80% of the seafood consumer diet (by mass), enter 0.8 for that species and 0.2 for the other species.

Enter contamination data for summed compounds on “Input” worksheet

Summed contaminant data are key input parameters for both the chemical exposure and sediment contribution indicator. Summed contaminant concentrations in seafood are included in the equation to calculate chemical exposure. Similarly, summed contaminant concentrations in seafood and sediment are included in the equations that calculate site linkage.

For seafood contamination data, sum PCBs, sum DDTs, sum chlordanes, and dieldrin are entered on the “Input” worksheet. These sums are entered into appropriate cells for each guild and contaminant class, in the cell range F4 – M11 (**Figure 2**). The arithmetic average (mean) and standard error of the mean (SE), should be entered into the corresponding labeled columns. For species/guilds not included, the cells should be left blank. Concentration data should only be entered for the compounds for which there is data for all the guilds found at the site being studied. Uneven occurrence or missing data for a compound will result in an incorrect calculation of the weighted species average concentration and affect the accuracy of the chemical exposure and linkage calculations. A separate DST analysis will need to be conducted for the chemical class containing the missing data. For example, for the data shown in Figure 2, if dieldrin, DDT, and PCB concentrations were available for both species, but chlordane was missing for Shiner perch, chlordane data should not be included for any of the species. The DST analysis should be conducted using only Dieldrin, DDT, and PCB data. A separate DST analysis, using only the chlordane data for the specie(s) for which data are available should then be conducted to complete the assessment. The “portion of human consumption” would need to be adjusted appropriately to account for the reduced number of species. Because site assessment is performed for each contaminant class this will not impact the assessment results for other contaminants.

For sediment contamination data, contaminant totals are entered in the appropriate cells F15 – M15 of the “Input” worksheet (Figure 2). This includes concentrations (mean and SE) of sum chlordanes, dieldrin, sum DDTs, and sum PCBs found in site sediment. Sediment data are required for each contaminant class being assessed.

A		B		C	D	E	F	G	H	I	J	K	L	M
1	Inputs													
2	Analysis Descriptor	Mission Bay 2016						Chlordane Conc	Dieldrin Conc	DDTs Conc	PCBs Conc			
3	Dietary Guild	Seafood Species		Guid	Portion of human seafood	Lipid (%)	Mean (ng/g)	SE	Mean (ng/g)	SE	Mean (ng/g)	SE	Mean (ng/g)	SE
4	1			1Piscivore	0									
5	2	Spotted sand bass		2Benthic diet with piscivory	0.5	0.44%	2.04	0.91	0.25	0.00	2.41	1.30	71.08	36.31
6	3			3Benthic and pelagic with piscivory	0									
7	4			4Benthic without piscivory	0									
8	5	Shiner perch		5Benthic and pelagic without piscivory	0.5	1.25%	2.53	0.42	0.25	0.00	7.28	2.51	1.92	0.98
9		Black perch		6Benthic with herbivory	0									
10		Dwarf perch		7Benthic and pelagic with herbivory	0									
11		Other		8Pelagic with benthic herbivory	0									
12		Shiner perch												
13														
14								Chlordane Conc	Dieldrin Conc	DDTs Conc	PCBs Conc			
15								Mean (ng/g)	SE	Mean (ng/g)	SE	Mean (ng/g)	SE	Mean (ng/g)
16								0.50	0.00	0.50	0.00	1.19	0.77	1.33
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Figure 2. Input worksheet. The left-hand side of the figure illustrates selection of a species within appropriate guild.

Enter site-specific parameters on “Input” worksheet

Lipid content of target seafood species (percent of total wet weight) are entered into cells E4 – E11 for all species monitored. Lipid data should be checked carefully to make sure the data is entered into the cell on a percentage basis. It has been reported that MS Excel sometimes unexpectedly rescales percentage data (e.g., converting 0.15% to 15%). This rescale appears to occur when inputting a percentage less than 1 without typing the zero before the decimal place (i.e., .8 rather than 0.8).

Two parameters pertaining to site size are entered to calculate site use factor. Area of site (km²) is entered in cell D19. Length of site (km) along the longest axis is entered in cell D20.

Sediment organic carbon (%) is entered in cell D21 (Figure 2).

Optional water column parameters, if available, are entered into cells D22 – D27 of the “Input” sheet. If local values are not readily available, the statewide default values included in the sheet are used.

Optional parameters include:

- Dissolved organic carbon content of water (kg/L): 2.15E-06
- Particulate organic carbon content of water (kg/L): 1.57E-06
- Mean water temperature (°C): 17.36
- Salinity (PSU): 25.44
- Dissolved oxygen concentration (mg O²/L): 9.0
- Suspended solid concentration in water column (kg/L): 2.27E-0.5

Enter contamination data for individual compounds on “Contaminant Specific” worksheet

Individual sediment contaminant data (i.e., results for individual PCB congeners, DDT metabolites, and chlordanes compounds) are entered on the “Contaminant Specific” worksheet of the DST. These data influence the bioaccumulation factor because specific contaminants have different chemical properties. Individual data are always entered for the sediment (Figure 3, column C). Individual contaminant results are needed for sediment because the bioaccumulation factor varies and is calculated based on the physical properties of each separate compound. Because biota-sediment accumulation factor (BSAF) calculations are based on the mechanistic model in the tool and not empirical tissue data, individual compound results are not needed for tissue contamination.

If available, site-specific individual dissolved contaminant data may also be entered for the water column and for sediment porewater (Figure 3, columns D - F). Use of measured water column concentration data is required for Tier 2 assessment. However, for estimation purposes the DST calculates water column or porewater concentrations based on equilibrium partitioning from the sediment. This calculation currently assumes that the overlying water is in equilibrium with the sediment and will likely overestimate actual water column concentration.

It is feasible to use the DST even when some contamination data are missing or below detection. Only available data should be entered; for missing data, cells should be left blank. If some individual compounds are missing, the BSAF will be calculated based on available compounds. In order for the BSAF to be calculated for a particular compound class (PCBs, DDTs, chlordanes, or dieldrin), individual results for at least one compound in that class must be included. Although concentrations are entered for each constituent, the average BSAF calculations for each class are influenced by the relative proportion of constituents in each compound class, so it is important that the data indicate the relative abundance of each constituent that is representative of the site.

Contaminant	Contaminant class	Observed Sediment Concentration	Observed Surface Water Concentration	Observed Dissolved Surface Water Concentration	Observed Porewater Concentration	Calculated Dissolved Surface Water Concentration	Freely Dissolved Surface Water Concentration	Porewater Concentration (Observed or Calculated)	Log Kow (Temp corrected to 25.0 C)	Metabolic Rate Constant	LeBas Molar Volume	Log Kow (Salinity corrected)	Log Koc	(Phi) proportion in water column freely dissolved
cis-Chlordane	Chlordanes	0.50				4.1	4.1E-06	3.31E-05	6.20	0	340.5	6.42	5.97	0.34
trans-Chlordane	Chlordanes	0.50				3.5	3.5E-06	2.82E-05	6.27	0	340.5	6.45	6.04	0.31
cis-Nonachlor	Chlordanes	0.49				12.4	1.2E-05	9.95E-05	5.70	0	361.4	5.94	5.48	0.62
trans-Nonachlor	Chlordanes	0.50				12.7	1.3E-05	1.02E-04	5.70	0	361.4	5.94	5.48	0.62
Oxychlordane	Chlordanes	0.23				8891.5	8.7E-03	6.95E-02	2.60	0	250	2.76	2.31	1.00
Dieldrin	Other pesticide	0.50				22.0	2.2E-05	1.76E-04	5.48	0	332.2	5.70	5.24	0.74
op-DDD	DDTs	1.09				68.1	6.8E-05	5.45E-04	5.34	0	312.6	5.54	5.09	0.80
pp-DDD	DDTs	1.09				35.3	3.5E-05	2.82E-04	5.83	0	305.2	5.83	5.37	0.67
op-DDT	DDTs	0.85				22.5	2.2E-05	1.80E-04	5.70	0	333.5	5.92	5.46	0.63
pp-DDT	DDTs	0.85				5.4	5.4E-06	4.36E-05	6.33	0	312.6	6.53	6.06	0.29
pp-DDT	DDTs	0.99				1.6	1.6E-06	1.28E-05	6.93	0	305.2	7.13	6.67	0.09
pp-DDT	DDTs	1.75				9.5	9.5E-06	7.57E-05	6.39	0	333.5	6.61	6.15	0.25
PCB 8	PCBs	0.50				46.5	4.7E-05	3.72E-04	5.22	0	226.4	5.37	4.92	0.85
PCB 11	PCBs	0.36				22.4	2.2E-05	1.79E-04	5.40	0	226.4	5.56	5.09	0.80
PCB 18	PCBs	0.50				29.1	2.9E-05	2.33E-04	5.41	0	247.3	5.58	5.12	0.79
PCB 27	PCBs	0.44				19.7	2.0E-05	1.57E-04	5.53	0	247.3	5.69	5.23	0.74
PCB 28	PCBs	0.50				12.5	1.3E-05	1.09E-04	5.78	0	247.3	5.94	5.49	0.61
PCB 29	PCBs	0.72				20.3	2.0E-05	1.63E-04	5.73	0	247.3	5.89	5.43	0.64
PCB 31	PCBs	0.43				8.2	8.2E-06	6.56E-05	5.90	0	247.3	6.06	5.60	0.55
PCB 33	PCBs	0.36				9.3	9.3E-06	7.40E-05	5.77	0	247.3	5.93	5.47	0.62
PCB 37	PCBs	0.42				7.8	7.8E-06	6.27E-05	5.91	0	247.3	6.07	5.61	0.54
PCB 44	PCBs	0.50				8.4	8.4E-06	6.73E-05	5.94	0	268.2	6.11	5.66	0.52
PCB 49	PCBs	0.50				6.2	6.2E-06	4.94E-05	6.07	0	268.2	6.25	5.79	0.44
PCB 52	PCBs	0.50				6.7	6.7E-06	5.40E-05	6.04	0	268.2	6.21	5.75	0.46
PCB 56	PCBs	0.54				5.5	5.5E-06	4.40E-05	6.16	0	268.2	6.33	5.88	0.39
PCB 60	PCBs	0.81				4.9	4.9E-06	3.95E-05	6.26	0	268.2	6.43	5.98	0.34
PCB 64	PCBs	0.38				6.7	6.7E-06	5.37E-05	5.92	0	268.2	6.05	5.64	0.53
PCB 66	PCBs	1.05				11.2	1.1E-05	8.94E-05	6.14	0	268.2	6.31	5.86	0.40
PCB 70	PCBs	1.35				11.7	1.2E-05	9.34E-05	6.23	0	268.2	6.40	5.95	0.35

Figure 3. Contaminant specific sediment data entry. For individual compounds, available contaminant data are entered into the blue cells (columns C, D, E, and F) of the “Contaminant Specific” sheet, here illustrated.

5. Run models

Once data are entered, the site-specific BSAF is calculated using a macro based on the food web model included in the DST. After the bioaccumulation factor is calculated, probability distributions are determined for site linkage, cancer risk, and noncancer hazard. This is achieved by Monte Carlo Simulation (MCS), which is performed using the YASAIw Add-In. **In order for the results to be correct, the bioaccumulation factor must be calculated prior to running the MCS. Therefore, the macro needs to be run before the simulation.**

Calculate biota-sediment accumulation factor

The BSAF is calculated using an Excel macro that runs a food web model sequentially for each contaminant compound, and records the results for each guild.

Type *Ctrl – R* to run the food web model macro. The macro then calculates BSAF for all compounds. The screen will rapidly flicker as it runs through the “Contaminant Specific” sheet. This is normal. The macro should take less than 20 seconds to complete. The resulting BSAFs for all summed compounds will be found in the “Assessment Summary” worksheet cells B165:E172.

Note: macros must be enabled for the macro to work. If typing Ctrl-R results in no change, most likely macros are disabled. Refer to the Appendix for instructions to reset macro security.

Perform Monte Carlo Simulation

Once the BSAFs have been calculated, a Monte Carlo Simulation (MCS) is performed to develop the data needed for an assessment outcome. To perform the simulation, click *Add-ins (Tools in Excel versions before 2007) -> YASAI simulation*. A simulation menu box should appear (Figure 4). In the simulation box, change Sample Size to 10,000. All other options may be kept as defaults. These values should be the same as shown in the grey box in Figure 4. Then, click the Simulate button, which will begin the MCS. Note that the sensitivity analysis option does not function in this version.

This simulation will take a couple of minutes to complete on typical computers using the settings described above. For slower computers, if multiple other processes are running, or settings have been changed, it may take longer to run. During the time the simulation is running, the statistical distributions in the cancer risk, noncancer hazard, and sediment contribution equations are resampled 10,000 times, and the key results are stored and summarized. Note that the distributions of cancer risk and noncancer hazard are provided for informational purposes; they are not used in the final SQO site assessment.

After the MCS is completed, three new worksheets are produced. “Simulation Output 1” summarizes the simulation, including the mean, standard deviation, and percentiles of the results for cancer risk, noncancer hazard, and site linkage. All information needed to perform the assessment may be found on this page. “CFD Output 1” presents the entire cumulative frequency distribution (i.e., the percentiles) for each result. It can be examined to determine what portion of the population exceeds various values. “Iterations Output 1” contains the results of each MCS iteration. This is essentially the raw data that the MCS produces, which is then summarized in the other worksheets. If additional simulations are performed, additional worksheet pages with sequential numeric labels are added (e.g., “Simulation

Output 2”, etc.). Further information on the simulation output pages may be found in the YASAIw User’s Manual (Pelletier 2009).

On the output pages, results are presented under abbreviated headers. The header, “CancerRiskX” indicates the probability of additional cancer cases to seafood consumers from exposure to compound X, where X is chlordanes, DDTs, dieldrin, or PCBs. “NoncanHazardX” indicates the noncancer hazard to seafood consumers from exposure to compound X. “SedLinkX” indicates the site linkage to seafood tissue concentrations of compound X. The chemical exposure evaluation is based on the average tissue concentration data and does not use MCS to determine the result.

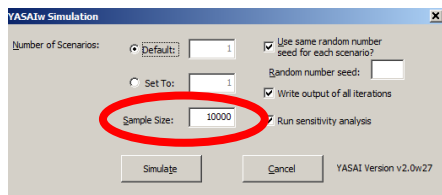


Figure 4. Set up window for Monte Carlo Simulation.

6. Interpret results

The SQO assessment is based on the percentile results of the MCS. This is achieved by obtaining key results from the “Simulation Output” worksheet, and comparing these results to thresholds, as described in this section. The “Assessment Summary” worksheet automates this process.

Using the “Assessment Summary” worksheet

The “Assessment Summary” worksheet is designed to calculate and summarize key SQO assessment results from the MCS. Rows 1 to 28 of this sheet contains a summary of user input parameters, and thresholds for the chemical exposure and sediment contribution. The lower portion of the sheet (**Model results**) contains summary information from the MCS results and generates a site assessment outcome.

The “Assessment Summary” will automatically update with the most current results. The results from the most recent simulation run is automatically displayed on the page (Note: this feature does not work in Excel 2010 and earlier). To generate summary information for analyses other than the current MCS analysis (or any analysis including the most recent in Excel 2010 or earlier), simply enter the name of the Simulation Output worksheet from the most recent simulation into cell A32 and the name of the corresponding CFD Output into cell B32 of the worksheet (Figure 5). For each compound, the simulation results for the key threshold percentiles are listed, along with the indicator category outcome, and final site category.

- **Chemical exposure categories:** 1 = Very Low, 2 = Low, 3 = Moderate, and 4 = High, 5 = Very High.
- **Site linkage categories:** 1 = Very Low, 2 = Low, 3 = Moderate, and 4 = High.
- **Site assessment categories:** 1=Unimpacted, 2 = Likely Unimpacted, 3 = Possibly Impacted, 4 = Likely Impacted, 5 = Clearly Impacted.

A1												
Input Data												
Seafood Data			Chlordane Conc		Dieldrin Conc		DDT ₂ Conc		PCB ₂ Conc			
Species	Guild	of human seafood	Lipid (%)	Mean (ng/g)	SE	Mean (ng/g)	SE	Mean (ng/g)	SE	Mean (ng/g)	SE	
Spotted sand bass	1Piscivore	0	0.44%	2.04	0.91	0.25	0.00	2.41	1.30	71.08		
Shiner perch	2Benthic diet with piscivory	0.5										
	3Benthic and pelagic with piscivory	0										
	4Benthic without piscivory	0										
	5Benthic and pelagic without piscivory	0.5	1.25%	2.53	0.42	0.25	0.00	7.28	2.51	1.92		
	6Benthic with herbivory	0										
	7Benthic and pelagic with herbivory	0										
	8Pelagic with benthic herbivory	0										
Sediment Contaminant Concentration			Chlordane Conc		Dieldrin Conc		DDT ₂ Conc		PCB ₂ Conc			
			Mean (ng/g)	SE	Mean (ng/g)	SE	Mean (ng/g)	SE	Mean (ng/g)	SE		
			0.50	0.00	0.50	0.00	1.19	0.77	1.33	1.60		
Other Site Data			Risk Thresholds				Categories					
Daily seafood consumption rate (CR) (kg/d)	Mean	0.032	Cancer Risk Threshold				9.5E-06					
Area of Site (SA) (km ²)	8.056833		Noncancer Hazard Threshold				0.35					
Length of site (km)	6		Site Linkage Threshold				0.45					
Sediment Total Organic Carbon (TOC) (%)	1.63%		Tissue Chem Thresholds									
Dissolved Organic Carbon Content of water (DOCw) (kg/L)	2.15E-06		FCG	ATL3	ATL2	ATL1						
Particulate Organic Carbon Content of water (POCw) (kg/L)	1.57E-06		Chlordane	5.6	190	280	560					
Mean Water Temp (T) (Dea. C)	17.4		DDT ₂	21	520	1000	2100					
Salinity (Sal) (PSU)	25.4		Dieldrin	0.46	15	23	46					
Dissolved Oxygen Concentration (DO) (mg/L)	3		PCB ₂	3.6	21	42	120					
Suspended solid concentration in water column (SSC) (kg/L)	2.27E-05											
Model Results (Note: Make Sure That Simulation Output Sheet Corresponds to the CFD Output Sheet #)												
Simulation Output Worksheet Name	CFD Output Worksheet Name	12	Last Output Sheet Name				Last CFD Sheet #		Last CFD Sheet Name			
Example Simulation Output	Example CFD Output		Example Simulation Output				13		Example CFD Output			
Note: Yellow coloring indicates exceeding the threshold												
Compound	Indicator	25%	50% or mean	75%	95%	Category Outcome						
Chlordane ₂	Weighted observed tissue conc. (ng/g)	2.3				1						
Chlordane ₂	Cancer Risk	2.9E-07	5.1E-07	1.2E-06								
Chlordane ₂	Non Cancer Hazard Quotient	1.6E-02	2.8E-02	6.4E-02								
Chlordane ₂	Site Linkage	1.3E-01	1.9E-01	2.8E-01		1						
Chlordane ₂	Site Assessment Outcome					1						
DDT ₂	Weighted observed tissue conc. (ng/g)	4.8				1						
DDT ₂	Cancer Risk	1.6E-07	2.8E-07	6.7E-07								
DDT ₂	Non Cancer Hazard Quotient	2.1E-03	3.9E-03	9.2E-03								
DDT ₂	Site Linkage	6.4E-01	1.1E+00	1.8E+00		4						
DDT ₂	Site Assessment Outcome					1						
Dieldrin	Weighted observed tissue conc. (ng/g)	0.3				1						
Dieldrin	Cancer Risk	3.9E-07	6.3E-07	1.5E-06								
Dieldrin	Non Cancer Hazard Quotient	1.1E-03	2.0E-03	4.5E-03								
Dieldrin	Site Linkage	3.5E-01	5.0E-01	7.1E-01		3						
Dieldrin	Site Assessment Outcome					1						
PCB ₂	Weighted observed tissue conc. (ng/g)	36.5				3						
PCB ₂	Cancer Risk	6.4E-06	1.2E-05	3.2E-05								
PCB ₂	Non Cancer Hazard Quotient	3.7E-01	7.2E-01	1.8E+00								
PCB ₂	Site Linkage	6.5E-02	1.3E-01	2.5E-01		1						
PCB ₂	Site Assessment Outcome					2						
Chlordane ₂	Chlordane ₂ Conc (ng/g)	4.0	11									
Dieldrin	Dieldrin Conc (ng/g)	0.0	0.2	0.2	0.2							
DDT ₂	DDT ₂ Conc (ng/g)	226.1	404.3	128.3	68.7							
PCB ₂	PCB ₂ Conc (ng/g)	120.7	214.8	63.0	115.5							
Chlordane ₂	Chlordane ₂ Conc (ng/g)	63.5	36.7	20.9	18.6							
Dieldrin	Dieldrin Conc (ng/g)	30.0	30.0	30.0	30.0							

Figure 5. Model results on the Assessment Summary worksheet. The model results correspond to the name of a Simulation Output worksheet which is entered into purple cell A32 and the name of the CFD Output sheet entered into cell B32. In this example, the results for Simulation 2 are summarized.

Using the “Output Summary” worksheet

The Output Summary worksheet pulls information mainly from the Assessment Summary page, but also from the other output pages to build a summary of the key information needed for a site assessment.

The most important outputs are the chemical exposure categories, the site linkages, and the site assessment categories. The health indicators are provided as ancillary information, but are not used in the site assessment. The data displayed on this page is controlled by which output summaries are selected on the Assessment Summary worksheet. The Output Summary worksheet is formatted to be printed on a single page.

Using “Simulation Output” worksheet

It is also possible to examine detailed results of the MCS on the “Simulation Output” worksheet, and manually compare results to the thresholds. The “Simulation Output” sheet contains more detailed information on the results at a range of distribution percentiles. However, the numerical results shown on the “Simulation Output” worksheet are not initially formatted in a useful way. Because some output values are much lower than 1, they should be displayed in scientific notation. In most versions of Excel, this is achieved in the following six steps: 1. Select appropriate cells on the sheet; 2. Click the *Format* pulldown menu; 3. Select *Cells*; 4. Select the *Number* tab; 5. Select *Scientific*; 6. Click *OK*.

Categorical results on the summary worksheets are derived by comparisons to a series of thresholds. For the chemical exposure indicator, the mean observed tissue concentration weighted by consumption of each species is compared to the thresholds in Table 3:

- If the tissue concentration is \leq the Fish Contaminant Goal, the chemical exposure is “1 – Very Low”
- Otherwise, if the tissue concentration is \leq the ATL3, the chemical exposure is “2 – Low”
- Otherwise, if the tissue concentration is \leq the ATL2, the chemical exposure is “3 – Moderate”
- Otherwise, if the tissue concentration is \leq the ATL1, the chemical exposure is “4 – High”
- Otherwise, if the tissue concentration is $>$ the ATL1, the chemical exposure is “5 – Very High”

For the site linkage outcome, the following comparisons are performed:

- If linkage $<$ 0.5 at 75% Percentile, the sediment contribution outcome is “1 – Very Low”
- Otherwise, if linkage $<$ 0.5 at 50% Percentile, the sediment contribution outcome is “2 – Low”
- Otherwise, if linkage $<$ 0.50 at 25% Percentile, the sediment contribution outcome is “3 – Moderate”
- Otherwise, if percent contribution \geq 50% at 25% percentile, the sediment contribution outcome is “4 – High”

Table 3. Tier 2 Tissue contaminant thresholds. Values for ATLs represent the maximum of the concentration range established by OEHHA.

Parameter	Tier 2 Contaminant Threshold			
	FCG ¹ (ng/g ww)	ATL3 ² (ng/g ww)	ATL2 ³ (ng/g ww)	ATL1 ⁴ (ng/g ww)
Chlordane	5.6	190	280	560
DDTs	21	520	1,000	2100
Dieldrin	0.46	15	23	46
PCBs	3.6	21	42	120

1. FCG - Fish Contaminant Goal based on 1 meal per week
2. ATL3 - Tissue Advisory Level based on consumption of 3 meals per week
3. ATL2 - Tissue Advisory Level based on 2 meals per week
4. ATL1 - Tissue Advisory Level based on 1 meal per week

7. Plot and Graphically Evaluate Results

In some cases, the user may wish to plot the cancer risk and site linkage results to examine the distributions. Examination of plots aids in judging the amount of variability of the results and the possibility of exceeding the threshold, which could aid in management decisions. For the convenience of the user, two sheets are included that contain pre-formatted plots of cancer risk and site linkage (Figures 6 and 7). These plots have been designed so that they can be easily updated with the results of the most recent analysis in a manner like the “Assessment Summary”.

Plotting Cancer Risk

The “Cancer Risk Plot” worksheet contains a cumulative distribution plot of cancer risk. Enter the name of the current CFD Output sheet in cell B3 and the plot will be automatically updated (Figure 6). Results for each contaminant class are shown in a different color, along with the reference value of 1×10^{-5} probability of additional cases of cancer. Columns N-R show the individual percentile values for reference (same values as on the specified output worksheet).

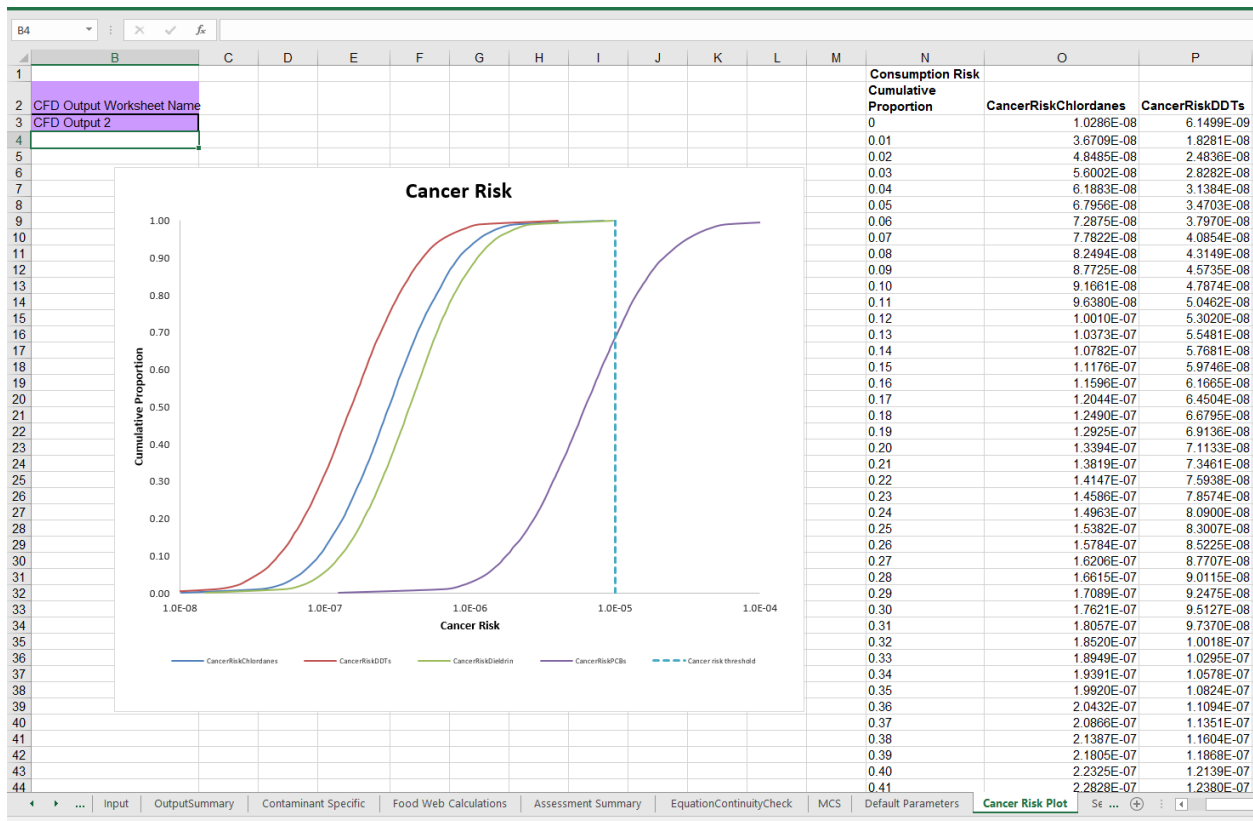


Figure 6. Plot of cancer risk distribution.

Plotting Site linkage

The “Site linkage Plot” worksheet contains a cumulative distribution plot of the site linkage factor (Figure 7). Like the chemical exposure plot, enter the name of the current CFD Output sheet in cell B3 and the plot will be automatically updated. Results for each contaminant class are shown in a different color, along with the provisional threshold of 0.5. The site linkage indicator category is determined by the percentile at which the linkage factor equals or exceeds 0.5, which is represented by the colored box where the plot line crosses the vertical dashed threshold line. Columns N-R show the individual percentile values for reference (same values as on the specified output worksheet).

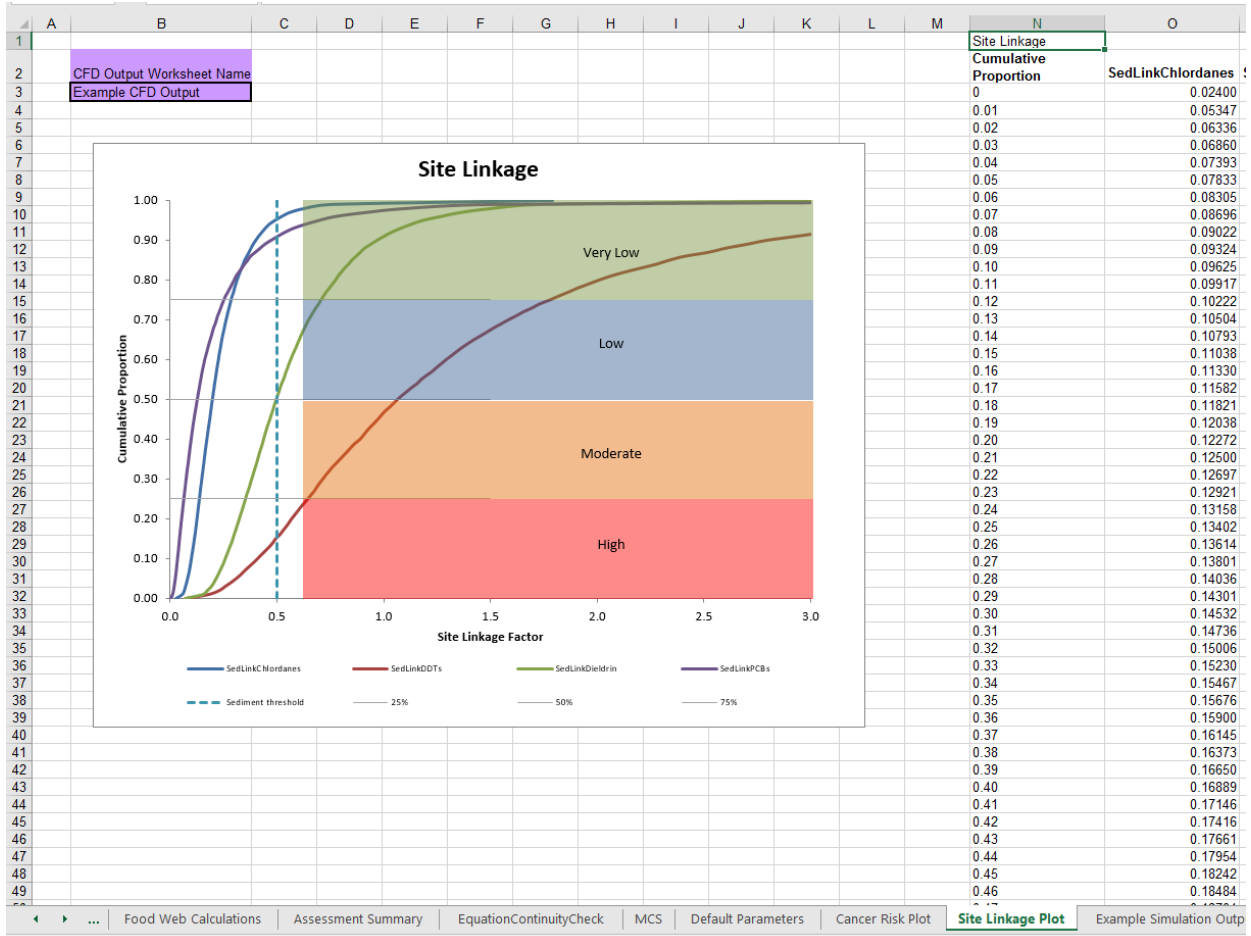


Figure 7. Plot of site linkage distribution.

Appendix

Set up instructions and troubleshooting for Decision Support Tool and Add-In

The first time that the Decision Support Tool (DST) and YASAIw Monte Carlo Simulation Add-In are installed on a new computer, four issues must be checked and resolved for the DST to function properly. These are each described in this Appendix.

Note: The DST spreadsheet was developed in Microsoft Excel 2003 and modified using later versions of Excel. Although menu commands (here designated in *Italics*) will differ among Excel versions, the spreadsheet should be fully functional in the newer versions. The DST has been used successfully in versions through Excel 2016. However, the MCS Add-In will not function in Excel 2000, or earlier versions of Excel.

Configure Microsoft Excel security

For the DST to work properly, it is necessary to establish a lower macro security setting.

In Excel 2010: *Developer* ->*Macros Security*; select "Enable all macros"; click OK.

Note: Upon opening the workbook, a warning message may appear indicating that the sheet contains macros. Select *Enable macros* to achieve full functionality.

In Excel 2016: *Developer* ->*Macros Security*; select "Disable all macros with notification". A warning button will appear when the file is opened stating that the file contains macros. Click to enable the content.

Confirm YASAIw Add-In has been correctly installed

The YASAIw Add-In must have been installed in the right windows location. In Excel 2010 and later, this can be assessed by selecting >*Add-Ins* (In earlier versions *Tools* > *Add-Ins*. YASAIw should be on the list, and checked. Check it if it is on the list but not checked; then click OK).

When YASAIw is correctly installed, "YASAI Simulation..." and "YASAI Charts..." will appear in the *Add-Ins* menu. Additionally, cells C176 to F179 in the "Input" worksheet will contain numeric values, rather than "#NAME?" or other error messages.

For additional troubleshooting options (if needed) refer to the YASAIw User's Manual (Pelletier 2009) that is provided with the YASAIw Add-In installation.

Confirm macros are enabled

Upon opening the workbook, a warning message may appear indicating that the sheet contains macros. Select *Enable macros* to achieve full functionality.

Update links to YASAIw Add-In

For functionality of the Monte Carlo Simulations, Excel must recognize and update the links to the YASAIw Add-In. This should be done automatically in Excel versions 2010 and newer, however links have often been lost when the DST was transferred between computers.

Link updating is generally required when a YASAI-based spreadsheet is moved between two computers having YASAIw installed in different locations in the file system. Upon opening the workbook, Excel may display the message that it contains "automatic links to another workbook", and may ask if the user wants to update the links. YASAI should automatically repair the links regardless of the user's choice.

If linking is unsuccessful, some spreadsheet formulas may contain strings like "'!C:Documents and Settings\USER\...\YASAI.xla!:". E.g., cells C30 to F32 of the Input worksheet. If this occurs, try the following method to fix these strings.

It is possible to manually delete these strings with Excel's "Replace" function, for YASAIw to start working normally again. In Excel 2010 and newer, this method is not recommended because a much simpler method exists (see #5 in the Known Excel Issues section below). If it is necessary to manually delete the strings, the following steps should be performed to accomplish this:

1. Begin by opening a fresh copy of the DST.
2. For cell C32 (and all other MCS cells), something like the following will be displayed in the formula toolbar:

```
='C:\Users\Ben\AppData\Roaming\Microsoft\AddIns\YASAIw.xla!simoutput(MCS!D29,  
"SedLinkChlordanes")
```

3. Select the contents of the string up to (and including) the portion **YASAIw.xla!** Note that in the example above, this is all **bold**.
4. *Edit -> Replace* (or type ctrl+h). Copy the string (in bold), and place it in the "Find what" cell. Keep the "Replace with" cell blank.
5. Click the "Options" button and change the "within" option from "sheet" to "workbook".
6. Click the "Replace all" button.
7. Manually check all cells and make sure that they have been successfully replaced. The following cells should be checked
 - a. Input sheet: C30:F32
 - b. MCS sheet: D4:G8 and B19:G26
8. This should have fixed all YASAIw functionality. If there are still problems, review troubleshooting sections above.

Known Excel Issues (and Solutions) Affecting DST Performance

1. In Excel versions 2010 and newer. The *Add-Ins* choice on the toolbar may not appear when Excel is first opened, even though the YASAIw is properly installed. Click *File > Options > Add-Ins*. At the bottom of the window, click *Go* next to Excel Add-Ins. A window with a table of all installed Add-Ins will open and YASAIw should be listed and checked. Uncheck the box and click OK. Again, go through the process described and re-check the YASAIw box and click OK. The *Add-Ins* choice should now appear on the toolbar and YASAIw will be present there. This will remain until Excel is closed. Unfortunately, this process may need to be repeated each time Excel is opened. Microsoft is aware of the problem, but so far has not fixed it.

2. In Excel versions 2010 and newer. If the DST and another Excel file are opened at the same time and the user switches to the other open file, upon returning to the DST many of the cells may show the #Value error. Simply press F9 (the recalculation key) and the cells will return to their numeric values.
3. In Excel versions earlier than 2013. The function to automatically select data from the last Simulation Output sheets does not work. The Simulation Output can be manually selected by entering the name of the correct worksheets in cells A and B 32 on the “Assessment Summary” worksheet (e.g. Simulation Output 6 in A32 and CFD Output 6 in B32).
4. In all versions of Excel. The Macro and MCS will run extremely slowly if one or both of the plotting worksheets point to an output sheet that does not exist. This issue usually occurs if output sheets from earlier runs are deleted in the DST file in use. Check cell B3 on both the Cancer Risk and Site linkage Plot worksheets and verify that they contain reference to a sheet name that is valid within the DST file.
5. In Excel versions 2010 and newer. Incorrect link to YASAIw Add-In. Depending upon several factors, some of the key equations involved in the simulation may not have the correct reference path. If this occurs and the simulation is run, an “Error 9—subscript out of range” message will display at the end of the run. Another way to verify this problem is to check the equations on the MCS worksheet. Most of the equations in the gridded box should begin with “=GenLognormal(Input”. If they instead begin with a file path (e.g. “=C\AshleysDesktop”), then the link is incorrect. Follow the instructions below to fix the link.

In Excel versions 2010 and newer, click “Data” on the toolbar. In the “Connections” group click “Edit Links”. A new window will pop-up and there should only be one link listed. You can click “Check Status” to verify the link is incorrect. If after clicking, the status in the window shows an error, the link will need to be changed. If this is the case, click “Change Source”, then navigate to the folder location of the YASAIw file and click on the file. Click “Close”. Save the file. The simulation should now run without error.