Probabilistic Ambient Water Quality Criteria Calculator (PAWQCC)

ARCADIS
April 2, 2014 Negotiated Rulemaking,
Docket 58-0102-1201

Imagine the result

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Initialize

Start in the “Initialize” tab. Follow the step-by-step instructions in order to enable the macros and full functionality of PAWQCC.

Probabilistic Ambient Water Quality Criteria Calculator (PAWQCC)

Version Beta.4

Initialize This Workbook on First Use (Steps 1 through 5)

The Probabilistic Ambient Water Quality Criteria Calculator (PAWQCC) uses simple Visual Basic commands in Excel to format the desired output of the probablistic modeling for evaluating PAWQC. In order to enable this functionality, the workbook must be set up on your computer appropriately.

Please follow the instructions below, and THEN click the button in Step 4 below.

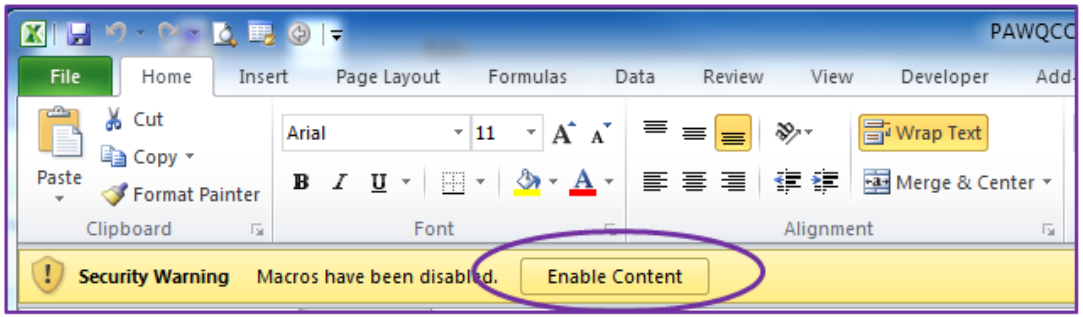
To Share This Workbook: UN-Initialize (Step 6)

The Probabilistic Ambient Water Quality Criteria Calculator (PAWQCC) uses simple Visual Basic commands in Excel to format the desired output of the probablistic modeling for evaluating PAWQC. In order to share this file and maintain this functionality, the workbook must be set up on the user's computer appropriately.

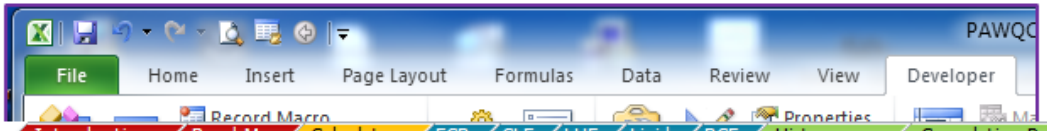
Please UN-Initialize this workbook before sharing with other users.

1 **Do NOT launch @RISK.**

2 **Place this workbook in a "Trusted Location" for Excel**, OR click on "Enable Content" along the yellow tab (example shown below).



3 **Allow Excel to Trust access to the VB project object model.** Click on the "Developer" Tab. In the "Code" Group, Click on "Macro Security"



If you do not have the Developer Tab:

1. Click the **File** tab and then click **Options**.

Initialize | Introduction | Read Me | Calculator | FCR | CLF | LHF | Lipid | BCF | Histograms | Cumulative Prob | Intercalcs | Bins | Toxicity | Bioconcentration | Input Results | Details

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Introduction

The “Introduction” tab provides a general overview of the purpose of PAWQCC. It also provides an inventory of all 18 tabs included within the workbook.

Probabilistic Ambient Water Quality Criteria Calculator (PAWQCC)

Version Beta.4

Summary

The Probabilistic Ambient Water Quality Criteria Calculator (PAWQCC) uses the fundamental equations employed by the United States Environmental Protection Agency (EPA) to derive ambient water quality criteria (AWQC). In addition to the parameters explicitly listed in the EPA equations, the PAWQCC software also includes implicit parameters that affect the outcome of the equations but are not listed specifically in the equations (e.g., exposure duration, loss of chemicals from fish tissue during cooking, fraction of fish consumed that are caught within the state, fraction of fish consumed that reside within the water body for their entire life cycle).

The equation used in the probabilistic approach is a “forward” risk equation; that is, the equation estimates risk from a chemical concentration, exposure dose, and toxicity. This is the reverse of the more familiar "rearranged" equation used for the deterministic calculation of risk-based AWQC from a target risk level, exposure dose, and toxicity. The reasons for using the forward equation for probabilistic assessments are mathematically complex and are described in greater detail elsewhere (e.g., Burmaster et al. 1995, Ferson 1996). In essence, the forward equation will yield a distribution of risks dependent on several inputs that are also distributions. If the equation is “rearranged” to solve for one of the inputs, the resulting distribution and the original input distribution may have similar means, but the spread of the distributions will be different. Because it is the tails of a distribution that are typically of interest for calculating acceptable risk or acceptable media concentrations, this disparity has marked effects on the outcome of the calculation. Therefore, EPA recommends using forward equations when conducting probabilistic assessments to avoid the mathematical limitations associated with back-calculation (EPA 2001).

The PAWQCC software uses @Risk (Palisade Corporation), a probabilistic add-on program for Excel. The user must have @Risk installed on their computer and must be familiar with the basic functions of @Risk to define input parameters as distributions. With three exceptions, the user may enter any or all input parameters as either point estimates or distributions. The three exceptions, which may only be entered as point estimates, are the chemical concentration in water, the target risk level, and species-specific fish consumption rates, which are expressed as a proportion of the total fish consumption rate. The total fish consumption rate may be entered either as a point estimate or as a distribution.

When deriving AWQC using the probabilistic approach, point estimates or distributions for the input parameters will be combined to estimate potential risk. For probabilistic derivation, the process of estimating risk by selecting from the input point estimates or distributions will be repeated until the number of desired iterations (e.g., 10,000 iterations) is complete. One complete set of iterations is called a simulation. As long as one or more of the input parameters are distributions, the final output of a simulation will be a distribution of risks associated with a particular concentration of a chemical in water. The user will select the percentile of the distribution of risk (or statistical representation of the distribution) required to meet that State’s particular target allowable risk level and determine whether the estimate of risk at that percentile meets the State’s target risk requirements

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Read Me

The “Read Me” tab provides detailed, step-by-step instructions for using PAWQCC. It also provides definitions for all inputs and outputs within PAWQCC.

Follow the instructions below to calculate human health risk-based ambient water quality criteria (AWQC).

The Probabilistic Ambient Water Quality Criteria Calculator (PAWQCC) requires access to @RISK to derive probabilistic AWQC. PAWQCC will function without @RISK, but the user will only be able to derive AWQC using the deterministic approach.

All parameters may be defined as point estimates or distributions, with the following exceptions (which may only be defined as point estimates):

- Concentration in water (C_w)
- Target percentiles and risk thresholds
- Species consumption rate (FCR_s)

Please be sure you have **INITIALIZED this workbook** before using for the first time. Please **follow the intructions** in the Initialize tab of this workbook.

Return Links:

1

Define general exposure parameters

In section [1], define all general exposure parameters, including drinking water intake (DI), exposure duration (ED), bodyweight (BW), and carcinogenic averaging time (AT_c). By definition, non-carcinogenic averaging time (AT_{nc}) is equal to ED. This cell will automatically populate itself when the user defines ED.

Section 1 inputs

Drinking water intake (DI, L/day): The volume of water consumed each day that is assumed to have the same chemical concentration as the ambient surface water.

Exposure duration (ED, years): The length of time over which exposure occurs.

Body weight (BW, kg): Body weight of the exposed person.

Averaging time, non-carcinogenic (AT_{nc}, years): Used to calculate the average daily intake. For non-carcinogenic effects, intakes are calculated by averaging over the period of exposure. Therefore, for non-carcinogenic effects, AT_{nc} is by definition equal to ED, and the two parameters cancel out. Although ED and AT_{nc} could technically be dropped from the calculation of non-carcinogenic hazards for this reason, they are included in PAWQCC for the sake of completeness.

Averaging time, carcinogenic (AT_c, years): Used to calculate the average lifetime daily intake. For carcinogenic effects, intakes are calculated by averaging over a lifetime.

Return Links: Section 1, DI, ED, BW, AT_{nc}, AT_c

2

Define fish intake parameters

In section [2], use the drop-down menu to select the fish consumption rate(s) [FCR(s)] available for input. User may choose to define either a single generic FCR or multiple species-specific FCRs.

a. If user chooses to define a generic FCR, all fish intake parameters must also be generic and will be defined within the 'Calculator' tab. Fish intake parameters include FCR, catch location factor (CLF), life history factor (LHF), proportion lipid, and bioconcentration factor (BCF).

b. If user chooses to define species-specific FCRs, all fish intake parameters will be defined within the subsequent blue tabs: 'FCR', 'CLF', 'LHF', 'Lipid', and 'BCF'.

i. Starting in the 'FCR' tab, first define the fish species and their trophic levels in section [A]. User must define the trophic level of each species only if trophic level-specific information is going to be used for any of the other fish intake parameters (i.e., CLF, LHF, proportion lipid, and BCF). Next, define the total fish consumption rate (FCR) and species-specific fish consumption rates (FCR_s), as a proportion of the total FCR, in section [B]. The sum of the individual FCR_s values may not exceed 1 (i.e., 100% of the total FCR). User may define FCR for up to ten species.

Return Links: Section 2, 'FCR' tab

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Calculator

The “Calculator” tab is where most, if not all, of the inputs are defined and also where results are displayed. It is broken up into seven sections.

Probabilistic Ambient Water Quality Criteria Calculator (PAWQCC)

To derive probabilistic AWQC, define inputs and click the 'Run Simulation to Calculate Risk' button at the bottom of this page.

PAWQCC requires access to @RISK to derive probabilistic AWQC.

PAWQCC will function without @RISK, but the user will only be able to derive AWQC using the deterministic approach.

Equations:

Noncarcinogenic effects	HI =	$C_w \times (((RBA_w \times DI) + (RBA_r \times \sum(FCR \times CLF \times LHF \times BCF_{lipid} \times Lipid) \times (1 - CL))) \times ED) / (BW \times AT_{nc} \times RSC \times RfD)$
Carcinogenic effects (non-linear)	ELCR =	$C_w \times (((RBA_w \times DI) + (RBA_r \times \sum(FCR \times CLF \times LHF \times BCF_{lipid} \times Lipid) \times (1 - CL))) \times ED) / (BW \times AT_c \times RSC \times (POD/UF))$
Carcinogenic effects (linear)	ELCR =	$C_w \times (((RBA_w \times DI) + (RBA_r \times \sum(FCR \times CLF \times LHF \times BCF_{lipid} \times Lipid) \times (1 - CL))) \times ED \times CSF) / (BW \times AT_c)$

Light blue shaded cells require input from the user.
Dark blue shaded cells contain @Risk functions defined by the user.
Gray shaded cells will automatically populate based on blue cell inputs.
Cells with underlined text, including section numbers, contain hyperlinks.

All parameters may be defined as point estimates or distributions, with the following exceptions (which may only be defined as point estimates):

- Concentration in water (C_w)
- Target percentiles and risk thresholds
- Species consumption rate (FCR_s)

1 General exposure parameters

Define parameters below.

DI	ED	BW	AT_{nc}	AT_c
drinking water intake L/day	exposure duration years	body weight kg	averaging time (non-cancer) years	averaging time (cancer) years

2 Fish intake parameters

Select the fish consumption rate (FCR) available for input.

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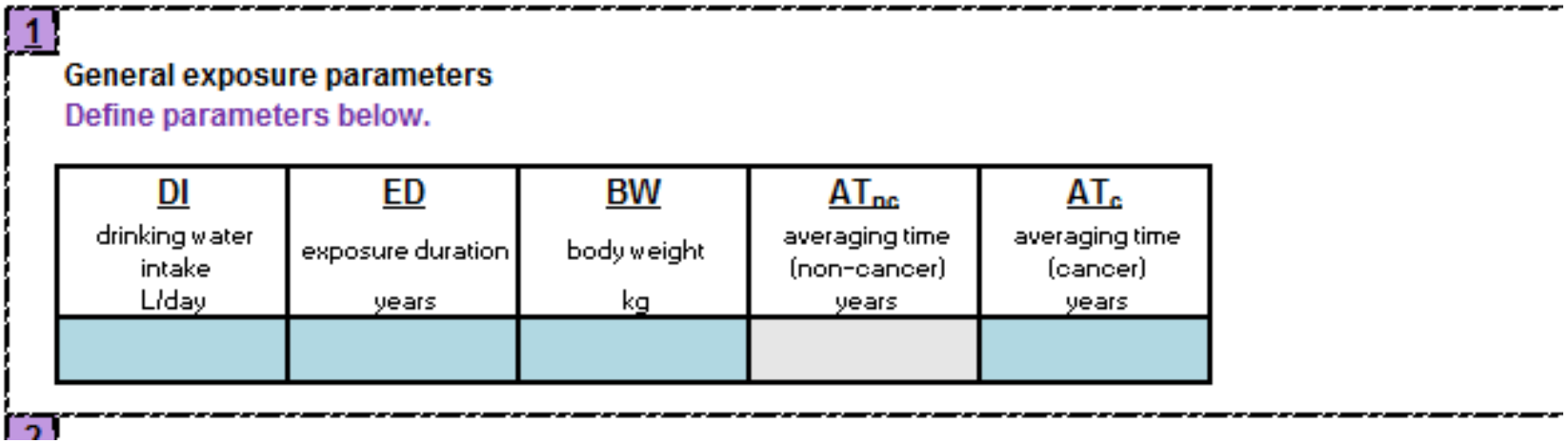
Section 1

Section 1 is where the user enters general exposure parameters. These include drinking water intake, exposure duration, body weight, and averaging time.



1

General exposure parameters

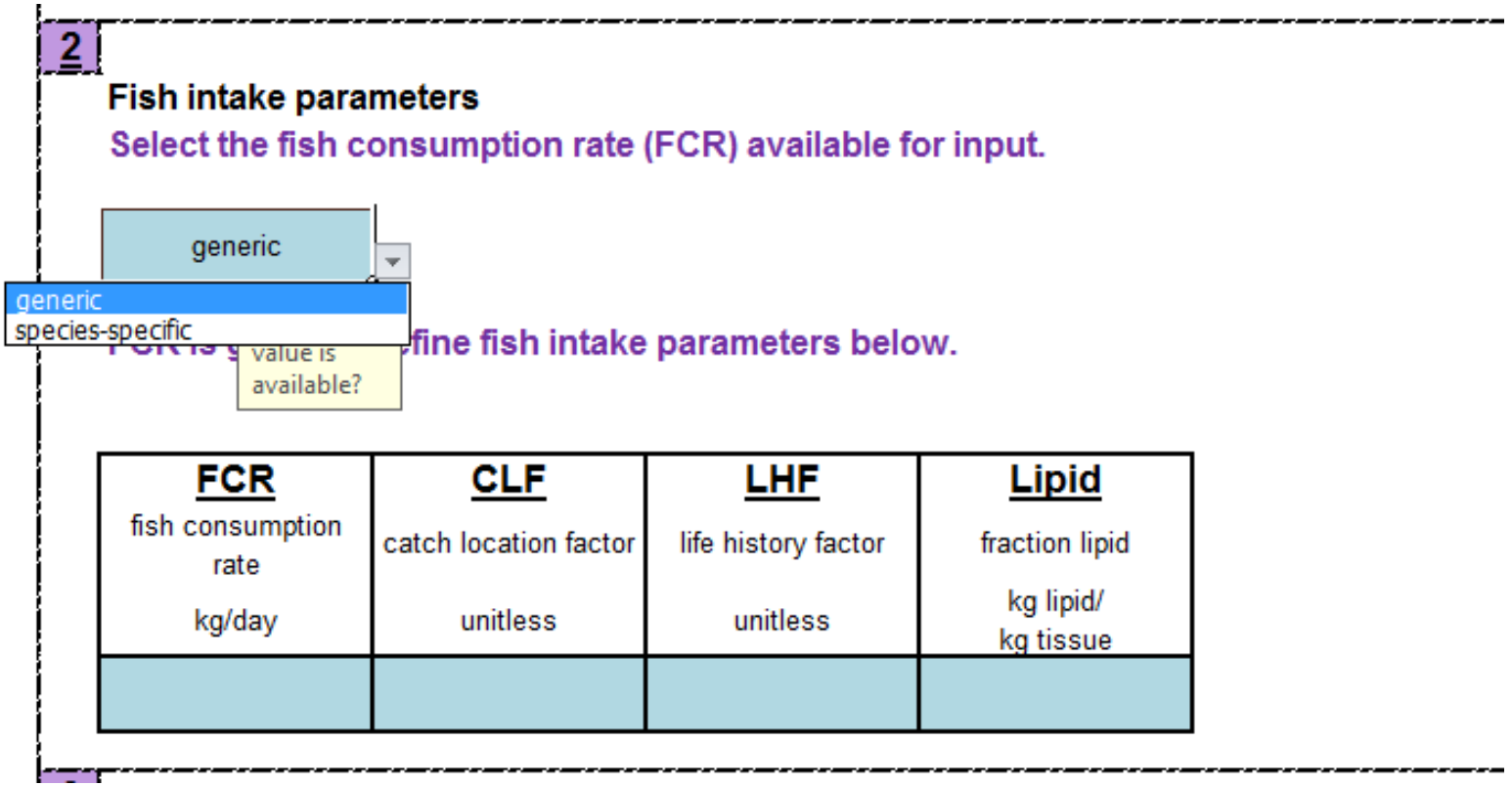
Define parameters below.

DI drinking water intake L/day	ED exposure duration years	BW body weight kg	AT_{nc} averaging time (non-cancer) years	AT_c averaging time (cancer) years

2

Section 2

Section 2 is where the user enters fish intake parameters. PAWQCC gives the user the option of defining either generic or species-specific fish consumption rates.



Section 3

Section 3 is where the user enters chemical-specific parameters. The user may use drop-down menus to select from a list of chemicals for which default bioconcentration and toxicity factors are available within PAWQCC.

3

Chemical-specific parameters

Define chemicals and associated parameters below.

Use buttons to look up default bioconcentration and toxicity factors.

chemical name	noncarcinogenic health endpoint	carcinogenic health endpoint	$RBA_{w,nc}$ relative bioavailability of water, noncarcinogenic unitless	$RBA_{w,c}$ relative bioavailability of water, carcinogenic unitless	$RBA_{f,nc}$ relative bioavailability of fish, noncarcinogenic unitless	$RBA_{f,c}$ relative bioavailability of fish, carcinogenic unitless	CL cooking loss unitless	RSC relative source contribution unitless		BCF_{lipid} lipid-based bioconcentration factor L/kg lipid	BCF_{tissue} tissue-base bioconcentrat factor L/kg tissue
									Look Up EPA BCF →		
									Look Up EPA BCF →		
									Look Up EPA BCF →		
									Look Up EPA BCF →		
									Look Up EPA BCF →		
									Look Up EPA BCF →		
									Look Up EPA BCF →		
									Look Up EPA BCF →		
									Look Up EPA BCF →		
									Look Up EPA BCF →		

1,1,1-Trichloroethane
1,1,2,2-Tetrachloroethane
1,1,2-Trichloroethane
1,1-Dichloroethene
1,2,4,5-Tetrachlorobenzene
1,2,4-Trichlorobenzene
1,2-Dichlorobenzene
1,2-Dichloroethane

Note:

Green font = the user has ent

Red font = text has been ente

4

Risk thresholds

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Section 4

Section 4 is where the user defines risk management thresholds. The user may select target risk thresholds for the mean of the population as well as up to three percentiles. The user may also define deterministic risk thresholds in order to derive deterministic criteria in Section 5.

4

Risk thresholds

Define up to three target percentiles between 0 and 100 below. Targets must be point estimates.

percentile 1	percentile 2	percentile 3
90		

Define target risk thresholds below. Thresholds must be point estimates.

	HI_{target} target hazard index unitless	$ELCR_{target}$ target excess lifetime cancer risk unitless
deterministic		
arithmetic mean		
90th percentile		

5

Section 5

Section 5 calculates AWQC using the traditional deterministic approach. If the user has entered point estimates for all inputs and defined deterministic risk thresholds in Section 4, deterministic AWQC will be calculated automatically in Section 5.

5

Deterministic approach: solve for water concentration to derive AWQC

Water concentration is calculated below.

chemical name	$C_{w,nc}$ concentration in water, noncarcinogenic endpoint mg/L	$C_{w,c}$ concentration in water, carcinogenic endpoint mg/L

Section 6

Section 6 is where the user will calculate AWQC using the probabilistic approach. This approach uses the “forward” risk equation, meaning the user will enter a water concentration and the result will be a distribution of potential risk.

6

Probabilistic approach: solve for target risk to derive AWQC

Define water concentration below.
Concentration must be a point estimate.

Deterministic hazard and/or risk is calculated below.

Probabilistic hazard is calculated below.

Probabilistic risk is calculated below.

chemical name	C_w concentration in water mg/L	HI_{det} deterministic hazard index unitless	$ELCR_{det}$ deterministic excess lifetime cancer risk unitless	HI_{mean} arithmetic mean hazard index unitless	HI_{p1} 90th percentile hazard index unitless	HI_{p2} unitless	HI_{p3} unitless Target HI:	$ELCR_{mean}$ arithmetic mean excess lifetime cancer risk unitless	$ELCR_{p1}$ 90th percentile excess lifetime cancer risk unitless	$ELCR_{p2}$ unitless	$ELCR_{p3}$ unitless Target ELCR:

Note:
Green shading = calculated hazard or risk does not exceed user-defined target level.
Yellow shading = calculated hazard or risk exceeds user-defined target level.
All calculated hazards and risks are rounded to two significant figures before comparison to target levels.

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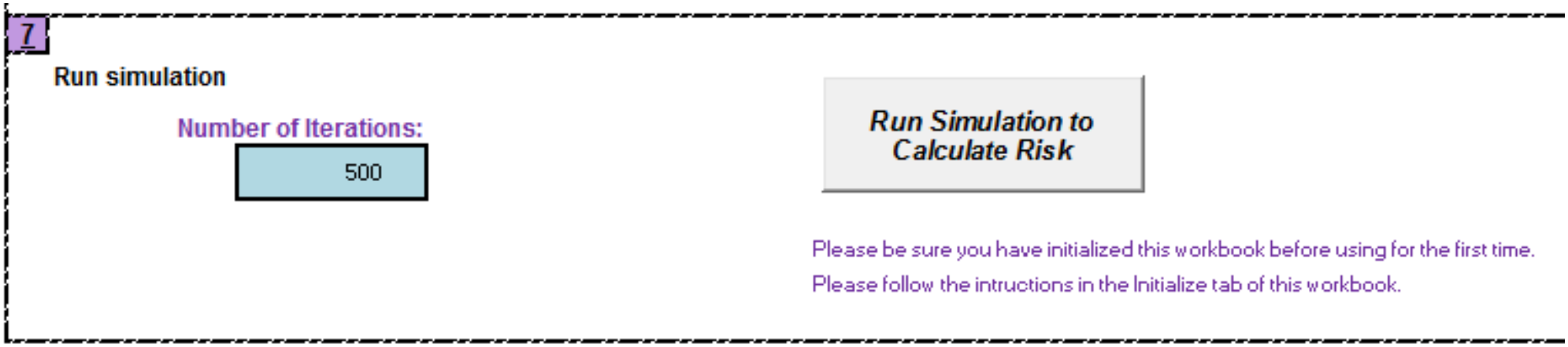
Section 7

Section 7 is where the user will choose the number of Monte Carlo iterations to run and then click the “Run Simulation” button.



Section 6: Evaluate Results

After the simulation is complete, evaluate the results in Section 6. If the resulting risk distribution meets the risk management criteria, the water concentration may be used as the AWQC. If not, iteratively adjust the water concentration until the resulting risk distribution meets the risk management criteria.

6

Probabilistic approach: solve for target risk to derive AWQC

Define water concentration below.
Concentration must be a point estimate.

Deterministic hazard and/or risk is calculated below.

Probabilistic hazard is calculated below.

Probabilistic risk is calculated below.

chemical name	C_w concentration in water mg/L	HI_{det} deterministic hazard index unitless Target HI: 1	$ELCR_{det}$ deterministic excess lifetime cancer risk unitless Target ELCR: 1.0E-06	HI_{mean} arithmetic mean hazard index unitless Target HI: 1	HI_{p1} 90th percentile hazard index unitless Target HI: 1	HI_{p2} unitless	HI_{p3} unitless Target HI:	$ELCR_{mean}$ arithmetic mean excess lifetime cancer risk unitless Target ELCR: 1.0E-06	$ELCR_{p1}$ 90th percentile excess lifetime cancer risk unitless Target ELCR: 1.0E-05	$ELCR_{p2}$ unitless	$ELCR_{p3}$ unitless Target ELCR:
PCBs	8.976E-08		1.4E-06					1.0E-06	2.3E-06		
Heptachlor	1.103E-07		1.4E-06					1.0E-06	2.3E-06		
Butylbenzyl phthalate	0.2069	0.683139464		0.502109334	0.997346871						

Note:
Green shading = calculated hazard or risk does not exceed user-defined target level.
Yellow shading = calculated hazard or risk exceeds user-defined target level.
All calculated hazards and risks are rounded to two significant figures before comparison to target levels.

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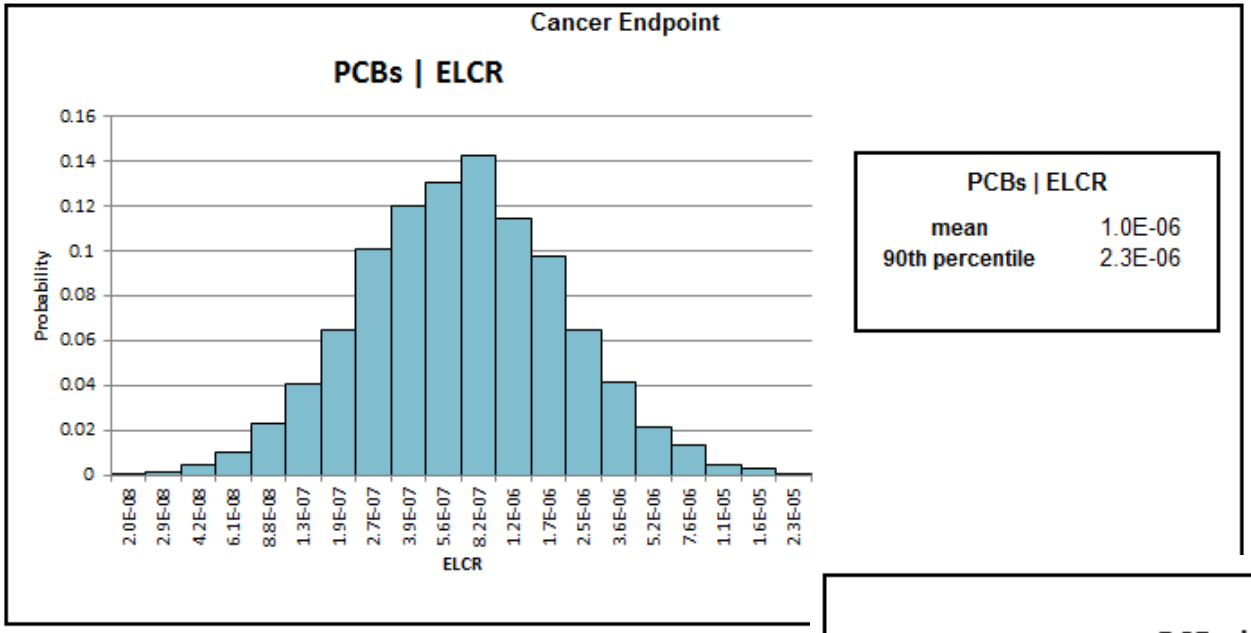
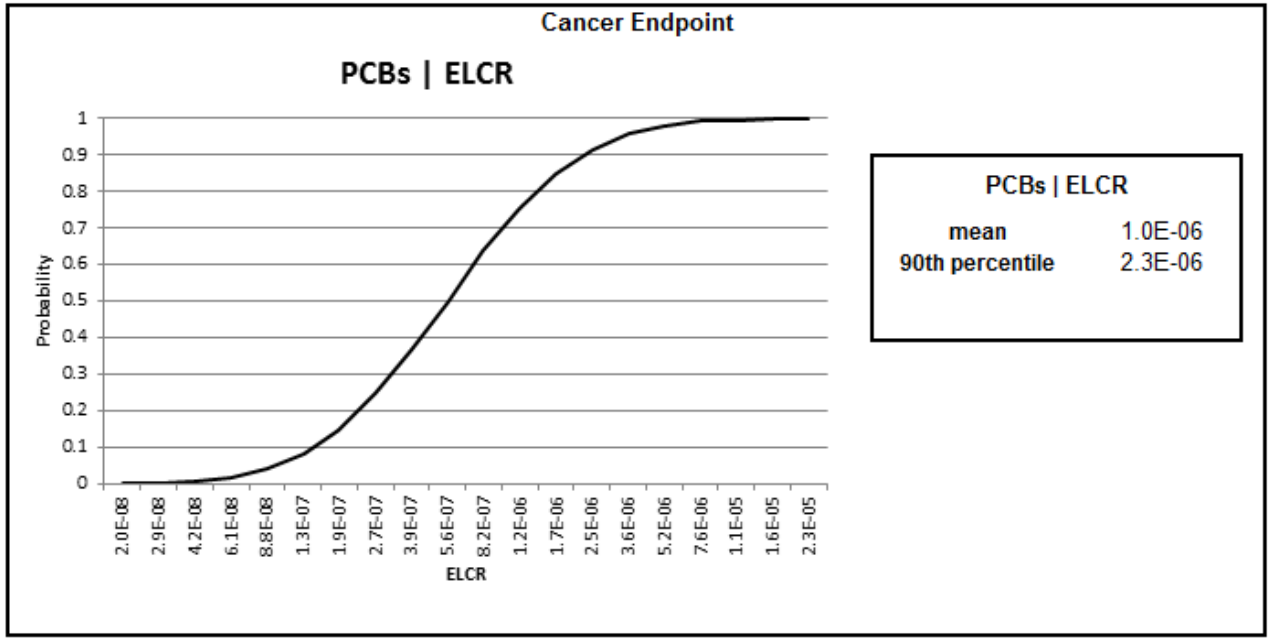
Plots

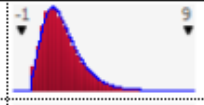
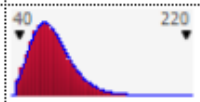
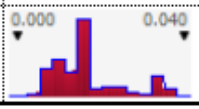
The “Histograms” and “Cumulative Prob” tabs provide histograms and cumulative probability plots of the resulting risk distributions.





Input Results

The “Input Results” tab provides snapshots of input distributions as well as summary statistics.

Name	Cell	Graph	Min	Mean	Max	5%	95%	Errors
drinking water intake	C29		0.002447818	1.729691	8.970859	0.3512815	3.789966	0
fish consumption rate	C43		0.000556064	0.02404868	0.5353408	0.003156312	0.07441738	0
body weight	E29		44.02193	80.49844	200.8354	52.3589	117.8904	0
fraction lipid	F43		0.004043383	0.01714495	0.03698238	0.007663916	0.03363821	0

Details, Data

The “Details” tab provides additional detailed statistics for all resulting risk distributions. The “Data” tab provides all individual risk results calculated for each iteration of the simulation.

Name	PCBs | HI	PCBs | ELCR	Heptachlor | HI	Heptachlor | ELCR	Butylbenzyl phthalate | HI	E
Description	Output	Output	Output	Output	Output	C
Cell	Calculator!F132	Calculator!G132	Calculator!F134	Calculator!G134	Calculator!F136	C
Minimum	n/a	1.4E-08	n/a	1.4E-08	0.008329991	n
Maximum	n/a	2.3E-05	n/a	2.3E-05	8.856514	n
Mean	n/a	1.0E-06	n/a	1.0E-06	0.5021093	n
Std Deviation	n/a	1.4E-06	n/a	1.4E-06	0.5595345	n
Variance	n/a	2.07334E-12	n/a	2.04305E-12	0.3130789	n
Skewness	n/a	4.999529	n/a	4.996923	4.755264	n
Kurtosis	n/a	43.45884	n/a	43.42631	40.59643	n
Errors	5000	0	5000	0	0	5
Mode	n/a	2.0E-07	n/a	2.7E-07	0.2610868	n
5% Perc	n/a	9.8E-08	n/a	1.0E-07	0.105301	n
10% Perc	n/a	1.5E-07	n/a	1.5E-07	0.1396006	n
15% Perc	n/a	1.9E-07	n/a	1.9E-07	0.1640425	n
20% Perc	n/a	2.3E-07	n/a	2.4E-07	0.1897781	n
25% Perc	n/a	2.7E-07	n/a	2.8E-07	0.2118796	n
30% Perc	n/a	3.2E-07	n/a	3.3E-07	0.2348182	n
35% Perc	n/a	3.7E-07	n/a	3.8E-07	0.2591672	n
40% Perc	n/a	4.3E-07	n/a	4.3E-07	0.283195	n
45% Perc	n/a	5.0E-07	n/a	5.0E-07	0.3101472	n
50% Perc	n/a	5.7E-07	n/a	5.7E-07	0.339001	n

Additional Supporting Tabs

- **Intercalcs**: Intermediate calculations supporting the "Calculator" tab. Used for species-specific fish intake calculations.
- **Bins**: Intermediate calculations used to build histograms and cumulative probability plots.
- **Toxicity**: Default toxicity factors that are retrieved by look-up buttons.
- **Bioconcentration**: Default USEPA bioconcentration factors that are retrieved by look-up buttons.

Imagine the result