White Paper

Development of Surface Water Screening Levels for PFOA and PFOS Based on the Protection of Human Health Using Probabilistic Risk Assessment

Prepared for the District and Business Support Program
Florida Department of Environmental Protection

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This white paper develops surface water screening levels for perfluorooctanoic acid (PFOA; CAS# 335-67-1) and perfluorooctane sulfonate (PFOS; CAS# 1763-23-1) protective of human health using probabilistic risk assessment (PRA). These screening levels are based on fish and shellfish ingestion pathways. PFOA and PFOS are manmade chemicals that belong to a group of thousands of chemicals known as perfluoroalkyl substances (PFAS). PFASs are water- and lipid-resistant. They are used as waterproofing and stain-resistant coatings for carpets, leather, textiles, furniture, and packaging materials. They are also used in fire-fighting foam and are added to aviation fluids to decrease flammability. PFOA and PFOS degrade slowly and are very persistent in the environment and the human body (USEPA, 2016a; USEPA, 2016b). The PFOA and PFOS present in surface water bioconcentrates and bioaccumulates into fish and shellfish that are consumed by local populations.

The following sections describe the technical basis for the proposed surface water screening levels.

<u>Equation and assumptions</u>

We calculated surface water screening levels protective of fish and shellfish consumption using a modified equation from the U.S. Environmental Protection Agency (USEPA) for the calculation of fish consumption limits based on concentrations of contaminants in fish tissue (USEPA, 2000a). The equation for non-carcinogens was used, modified by removing the drinking water intake component.

$$SWSL\ (\mu g/L) = \frac{RfD \times RSC \times BW \times CF}{\sum_{i=2}^{4}(FI_i \times BAF_i)}$$

Where:
SWSL = surface water screening level (μg/L)
RfD = oral reference dose (mg/kg-d)
RSC = relative source contribution
BW = body weight (kg)
CF = correction factor, 1000 μg/mg
FI_i = freshwater and estuarine finfish and shellfish consumption rate for aquatic trophic levels 2, 3, and 4 (kg/d)
BAF_i = bioaccumulation factor for aquatic trophic levels (TLs) 2, 3, and 4 (L/kg)
$\sum_{i=2}^{4} =$ summation of values for aquatic TLs, where the letter i stands for the TLs, starting with TL2 and continuing to TL4

For the PRA, body weight and freshwater and estuarine finfish and shellfish consumption rate (fish consumption rate) were chosen as distributions. Point values were selected for the other exposure parameters. This is identical to the PRA method proposed for the surface water standards in Chapter 62-302, F.A.C. (FDEP, 2016). The point value parameters are listed in Table 1 and the distributions for fish ingestion are provided in Table 2. Body weight was defined as a lognormal distribution with a mean of 79.96 kg and a standard deviation of 20.73 kg (USEPA, 2011). Figures showing the distributions for body weight and fish ingestion are included in Appendix A.

Table 1 – Point value parameters used in the derivation of surface water screening levels for PFOA and PFOS

Parameter	PFOA	PFOS	Source
Reference dose (mg/kg-d)	2E-05	2E-05	USEPA, 2016a USEPA, 2016b
Relative source contribution	0.6	0.6	CEHT, 2020
Bioaccumulation factor TL2 (L/kg)	35	937	See section on bioaccumulation factor
Bioaccumulation factor TL3 (L/kg)	71	2959	See section on bioaccumulation factor
Bioaccumulation factor TL4 (L/kg)	161	6304	See section on bioaccumulation factor

Table 2 – Fish ingestion lognormal distributions used in the PRA for the derivation of surface water screening levels for PFOA and PFOS

Trophic Level	Statistic	Atlantic (g/d)	Gulf (g/d)	Inland South (g/d)
2	Mean	4.9	4.2	3.1
	95^{th} Percentile	16.4	14.6	11.3
3	Mean	5.4	5.1	3.7
	95^{th} Percentile	16.6	16.4	11.9
4	Mean	2.6	2.5	2.8
	50^{th} Percentile	0.8	0.7	NA
	97^{th} Percentile	NA	NA	15.8

The fish ingestion distributions were derived from USEPA, 2014, Appendix E, Tables E-13, E-14, and E-15; NA – not applicable. This statistic was not used to define the distribution.

Reference Dose

The USEPA has developed reference doses for PFOA and PFOS in order to create drinking water Health Advisory Levels for these compounds. FDEP has used these reference doses for the calculation of alternative groundwater cleanup target levels (GCTLs) and soil cleanup target levels (SCTLs) for PFOA and PFOS (See letters to the FDEP dated April 16, 2018 and August 16, 2018 for details regarding the derivation of those screening levels). For consistency, the same RfD values are used in the surface water calculation, i.e., an oral reference dose (RfD) of 2E-05 mg/kg-d for both PFOA and PFOS.

We are aware that there is a lack of consistency among federal and state agencies in the derivation of safe limits for oral exposure to these substances. The Agency for Toxic Substances and Disease Registry (ATSDR) released a draft toxicity profile for PFAS, including PFOA and PFOS. The proposed Minimal Risk Levels (MRLs; analogous to RfDs) are an order of magnitude lower than the USEPA RfDs. This draft document received extensive public comment and has not yet been finalized. Additionally, North Carolina, Texas, Maine, Minnesota, and New Jersey have developed toxicity values for PFOA and PFOS based on differing endpoints and/or uncertainty factors. This results in different toxicity values than were proposed by the USEPA and ATSDR. California has also derived slope factors for PFOA and PFOS based on the development of pancreatic and liver tumors in male rats (CalEPA, 2019). The potential toxicity of PFOA and PFOS is a subject of active research, and the data available are rapidly evolving. Thus, while the USEPA RfD values are used for the surface water screening levels proposed here, we recommend re-visiting these screening levels as new information develops. Use of toxicity values developed based upon other endpoints, including cancer, instead of the USEPA RfDs will result in different screening level estimates that may be lower than those calculated here.

Body Weight

The Exposure Factors Handbook recommends using the body weight distributions calculated by Portier et al., (2007) for probabilistic risk assessment. For this analysis, body weight was defined as a lognormal distribution with a mean of 79.96 kg and a standard deviation of 20.73 kg (USEPA, 2011). This distribution represents the National Health and Nutrition Examination Survey (NHANES) IV estimated body weights for 18 to 65-year-old males and females. It was not truncated for the risk assessment. This body weight distribution was also used in the FDEP (2016) technical support document for the derivation of surface water standards.

Relative Source Contribution

This assessment uses the USEPA relative source contribution (RSC) values of 0.6 (60%) for both PFOA and PFOS. These chemical-specific RSCs for PFOA and PFOS were derived using the USEPA Exposure Decision Tree methodology (USEPA, 2000b), as explained in the companion white paper, "*Determination of Relative Source Contribution Values for Perfluorooctanoic Acid (PFOA) and Perfluorooctane Sulfonate (PFOS) in Support of Development of Florida Surface Water Screening Levels*" (CEHT, April 2020). As described in this document, there are several potential sources for PFOA and PFOS identified in the literature, of which drinking water, diet, consumer products, and indoor air and dust may be important. RSC values were derived using the percentage method, taking into account exposure from drinking water consistent with current FDEP screening levels, dietary exposure, and potential exposure to other sources combined. From this analysis, 60% of the intake corresponding to the RfDs for PFOA and PFOS were allocated to surface water exposure in the form of consumption of fish and shellfish.

Finfish and Shellfish Consumption Rate

No current Florida-specific fish consumption studies are available. The Degner et al. (1994) fish consumption study in Florida was used previously to develop fish consumption rates for Chapter 62-302, F.A.C. It also includes Florida-specific data on shellfish consumption for the general population. However, it is dated and may not represent current fish consumption rates. Therefore, we used NHANES 2003-2010 fish consumption data. The NHANES data are presented based on age, gender, and geographic region. The USEPA document summarizing the NHANES fish and shellfish consumption data presents several consumer categories that may be relevant to fish consumption in Florida (USEPA, 2014). However, none are specific to Florida. Based on the differences in fish and shellfish consumption rates for each geographic region in the U.S., these national data may not be appropriate for Florida. Regional data applicable to Florida include the South, Gulf of Mexico coastal counties, and Atlantic coastal counties. The FDEP determined that the combination of these regions provide the best estimate for a fish consumption rate for Floridians. They calculated that 44.8% of the Florida population resides within the Atlantic coastal counties, 31.6% reside in the Gulf of Mexico coastal counties, and 23.6% reside in the South geographic region (FDEP, 2016).

The USEPA document summarizing the NHANES fish consumption data also includes estimates of fish consumption by trophic level for each region. We used fit statistics to describe lognormal distributions for the consumption rates in Tables E-13, E-14, and E-15 of that document (Table 2). These statistics represent the total freshwater and estuarine finfish and shellfish consumption rates for adults.

Bioaccumulation Factor

Bioaccumulation factors (BAFs) for PFOA and PFOS from the literature are listed in Appendix Tables B1 and B2. Studies that included data on bioaccumulation in the muscle tissue (e.g., fillet) were utilized to calculate the freshwater BAFs. These studies include fish not present in Florida (e.g., rainbow trout) and fish not usually consumed (e.g., minnows, whitebait). The BAFs for these fish were used to calculate a freshwater BAF for PFOA and PFOS because bioaccumulation data in fish and shellfish are limited. By including all of the data available, it provides a better estimate of the BAF.

Bioaccumulation factors for the derivation of human health surface water criteria were calculated based on a modified version of the USEPA framework for deriving BAFs (USEPA, 2016c). Based on the USEPA proposed framework, we utilized field BAFs to calculate baseline BAFs for PFOA and PFOS. Field BAFs are the preferred source for calculating BAFs for nonionic organic chemicals. Typically, in this methodology, a baseline BAF is calculated based on the field BAF, the concentration of particulate organic carbon (POC) in the water, the concentration of dissolved organic carbon (DOC) in the water, the chemical-specific n-octanol-water partition coefficient (Kow), and the fraction of finfish and shellfish tissue that is lipid. However, for the purposes of this assessment, the field BAFs were used as the baseline BAFs. The reasoning for this includes:

1. The POC and DOC were not known for the majority of the BAF studies. Calculation of the fraction of chemical in water that is freely dissolved would require assumptions regarding the amount of dissolved and particulate carbon. Although national averages may be used as defaults, the majority of studies took place outside the United States and default POC and DOC values for these countries are unknown.

2. The K_{ow} has not been measured for PFOA and PFOS. Calculation of a baseline BAF would require a K_{ow} based on physical/chemical property estimation software (e.g., EPI Suite).

3. Unlike most non-ionic organics, PFAS are not distributed to the lipid. Therefore, use of a lipid adjustment to derive a baseline BAF is inappropriate for PFAS chemicals.

Bioaccumulation factors were derived for each trophic level (TL). To calculate a BAF, the fish and shellfish from the bioaccumulation studies were assigned to trophic levels (Table B3). A bioaccumulation factor was calculated for each trophic level for both PFOA and PFOS. Individual field BAFs were combined as the geometric mean for each species. The baseline TL-specific BAF was calculated as the geometric mean of all species geometric means (Table 3). These calculations are presented in Tables B4 though B9. The Minnesota study (MPCA, 2007b) combined bluegill and white bass in their river bioaccumulation study. Because the BAFs were listed as geometric means (MPCA, 2007b), they were retained in the assessment.

Table 3 – Trophic level 2, 3, and 4 geometric mean bioaccumulation factors for PFOA and PFOS

Chemical	Trophic Level	BAF
PFOA	2	35
	3	71
	4	161
PFOS	2	937
	3	2959
	4	6304

Method for the probabilistic risk assessment

PFOA and PFOS surface water screening levels were calculated using PRA. In this analysis, body weight and fish consumption were defined as distributions and the other parameters were entered as point values. The surface water screening levels were derived in using 100,000 iterations of a Monte Carlo analysis in Crystal Ball software (Version 11.1) with a seed of 123457. Each iteration represents a hypothetical person in the population. For each iteration, the software chose a body weight from the distribution. Then, a region was chosen based on the percentage of Floridians who live in each area. Once the region was identified, the software chose a region-specific fish consumption rate for trophic levels 2, 3, and 4 (Table 2). The fish consumption rates for each trophic level were multiplied by their respective BAFs (Table 3) before being summed. There was no correlation between the fish consumption rates for the three TLs. We could not locate any data suggesting that a high-end consumer of fish and shellfish in TL2 would also be a high-end consumer of fish and shellfish in the other TLs. Using the equation provided in this document, the software generated a distribution of surface water concentrations equivalent to a hazard index of 1 for each iteration. The PFOA and PFOS screening levels were set at the 10th percentile of this distribution. To check these values, the equation was rearranged and solved to ensure that the hazard index of 1 was not exceeded at the 90th percentile (Chapter 62-780, F.A.C.).

Screening levels

Surface water screening levels for PFOA and PFOS were calculated using the equations and assumptions described in this document. The surface water screening level for PFOA is 0.5 μg/L and for PFOS is 0.01 μg/L (Table 4). The distributions are presented in Figures 1 and 2. We also calculated the hazard index for the screening levels to insure it was below 1 at the 90th percentile. The hazard index for PFOA at a surface water screening level of 0.5 μg/L is 1 and the hazard index for PFOS at a screening level of 0.01 μg/L is 0.8 at the 90th percentile. The screening level for PFOS at a hazard index of 1 is 0.012 μg/L. This was rounded to 1 significant figure, which decreased the hazard index at the 90th percentile. The Crystal Ball output for the surface water screening level distributions and the distributions for the hazard index are presented in Appendix C.

Table 4 – Surface water screening levels for freshwater and estuarine finfish and shellfish for PFOA and PFOS

Surface Water Screening Levels (µg/L)	PFOA	PFOS
Freshwater and estuarine finfish and shellfish	0.5	0.01

Screening levels were rounded to one significant figure

Figure 1 – Surface water screening level distribution for PFOA

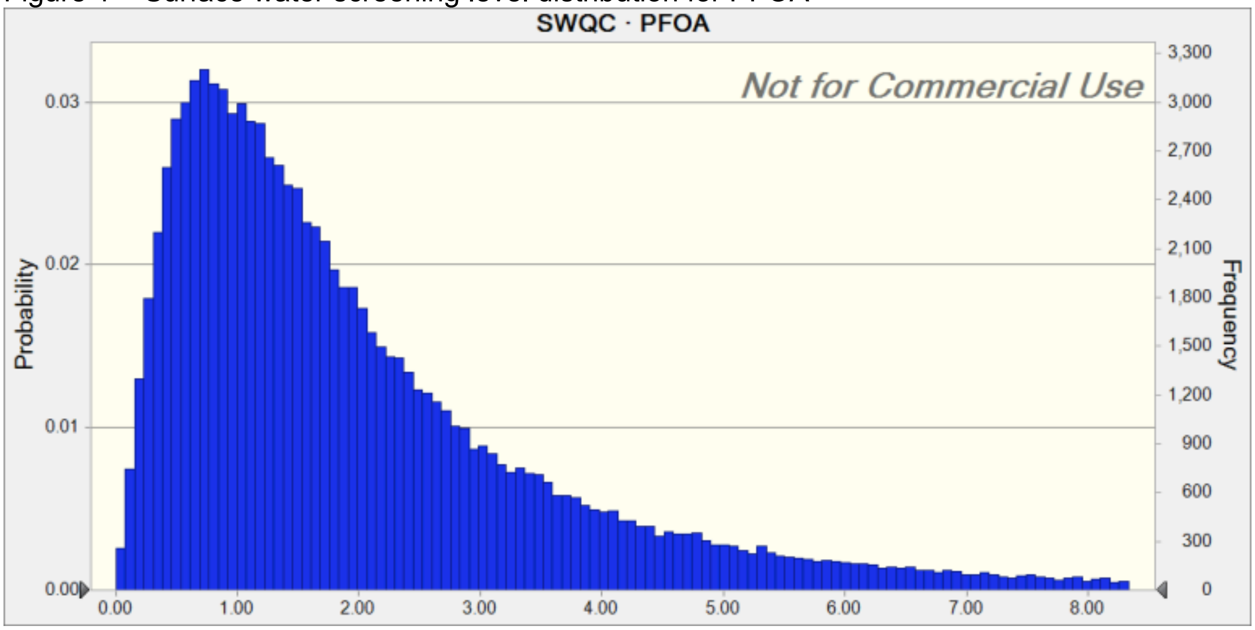
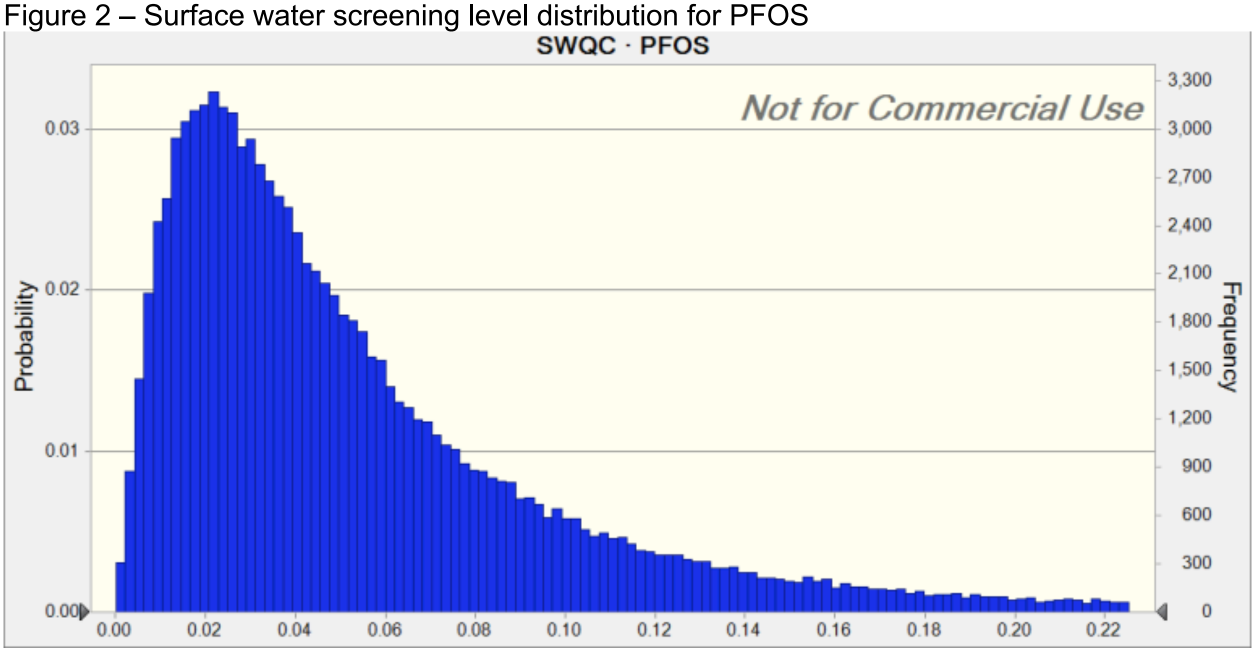


Figure 2 – Surface water screening level distribution for PFOS



The USEPA drinking water Health Advisory Levels (HALs) for PFOA and PFOS are each 0.07 µg/L. The USEPA recommends that the combined concentrations of PFOA and PFOS in drinking water be compared with this limit, based upon an assumption that their effects are additive. The rationale for this assumption is that their RfDs are derived for the same toxic endpoint (developmental effects) and that, although the mode of action for these effects has not been established, it is likely to be the same for these closely related chemicals. The fact that their individual Health Advisory Levels are identical makes it relatively straightforward to implement this recommendation. While the same argument could be made that the surface water screening levels for PFOA and PFOS should also address combined effects, this is more difficult because of the large difference in their values, approximately an order of magnitude. Picking the lower, higher, or average of these values for comparison with combined PFOA and PFOS concentrations could result in gross over- or underestimation of risk, depending on the individual PFOA and PFOS concentrations. As a practical matter, comparison of PFOA and PFOS concentrations in surface water with the screening levels should be made individually.

<u>Surface water screening levels in Florida and other states</u>

Table 5 – State surface water screening levels

State	PFOA (µg/L)	PFOS (µg/L)
Florida	0.5	0.01
Minnesota (lakes)	1.6	0.006
Minnesota (rivers)	2.7	0.007
Michigan	12	0.012
Alaska	0.07*	0.07*

* - Concentrations of PFOA and PFOS are summed before being compared to the criterion.

Minnesota has also developed freshwater surface water criteria based on fish consumption for the protection of human health. These criteria are based on site-specific bioaccumulation factors. For PFOA, the Minnesota surface water criteria include 1.6 µg/L for lakes and 2.7 µg/L for rivers (MPCA, 2017; Table 5). These criteria are higher than our proposed screening level of 0.5 µg/L. The difference in values is due to the use of a higher oral reference dose (1.4E-04 mg/kg-d) and slightly lower bioaccumulation factor (40 L/kg for lakes and 24 L/kg for rivers). Recently, the Minnesota Department of Health (MDOH) updated their reference doses for PFOA and PFOS (MDOH, 2019a; MDOH, 2019b). The updated reference dose for PFOA is 1.8E-05 mg/kg-d (MDOH, 2019a). Using this reference dose in their surface water equation would decrease the Minnesota criterion by approximately one order of magnitude. These updated values would be slightly lower than our proposed screening level of 0.5 µg/L.

The screening level for PFOS is lower than PFOA due to the large bioaccumulation factor for PFOS. For PFOS, the Minnesota surface water criteria include 0.006 µg/L for lakes 0.007 µg/L for rivers (MPCA, 2017). Our proposed PFOS screening level of 0.01 µg/L is similar to these two criteria. This is due to the use of a similar reference dose (8E-05 mg/kg-d) and bioaccumulation factors (6,087 L/kg for lakes and 3,877 for rivers) (MPCA, 2010a; MPCA, 2010b). The MDOH updated reference dose for PFOS is 3.1E-06 mg/kg-d (MDOH, 2019b). Use of this reference dose would lower the PFOS criteria to less than 0.001 µg/L, which is an order of magnitude below our proposed screening level.

The Michigan Department of Environmental Quality (MDEQ) criteria for PFOA and PFOS are human health-based non-cancer values for non-drinking surface water sources.

They were derived based on Michigan Rule 57 for toxic substances (MDEQ, 2020; Table 5). Their surface water screening level for PFOA is an order of magnitude greater than the screening level of 0.5 μg/L proposed in this document. The Michigan surface water screening level for PFOS is equivalent to our proposed PFOS surface water value of 0.01 μg/L. The Alaska Department of Environmental Conservation uses a criterion of 0.07 μg/L for PFAS in surface water used as drinking water (ADEC, 2019; Table 5). The criterion includes the sum of PFOA and PFOS concentrations. It is based on the USEPA drinking water HAL.

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Appendix A

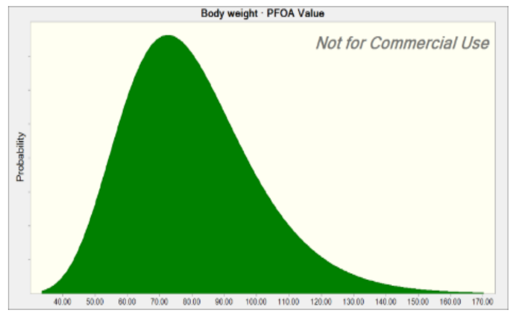
Crystal Ball Report - Assumptions

Assumptions

Assumption: Body weight · PFOA Value

Lognormal distribution with parameters:

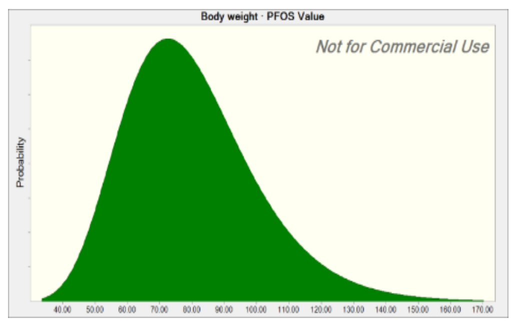
Location	0.00
Mean	79.96
Std. Dev.	20.73



Assumption: Body weight · PFOS Value

Lognormal distribution with parameters:

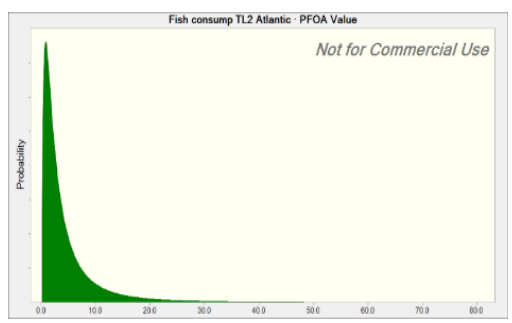
Location	0.00
Mean	79.96
Std. Dev.	20.73



Assumption: Fish consump TL2 Atlantic · PFOA Value

Lognormal distribution with parameters:

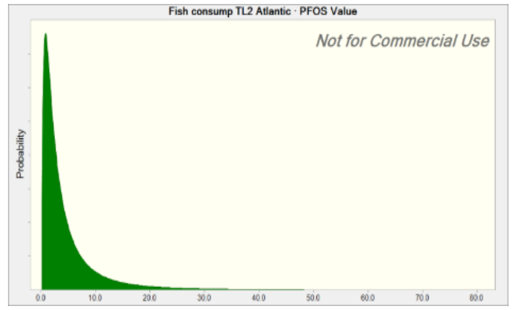
Location	0.0
Mean	4.9
95%	16.4



Assumption: Fish consump TL2 Atlantic · PFOS Value

Lognormal distribution with parameters:

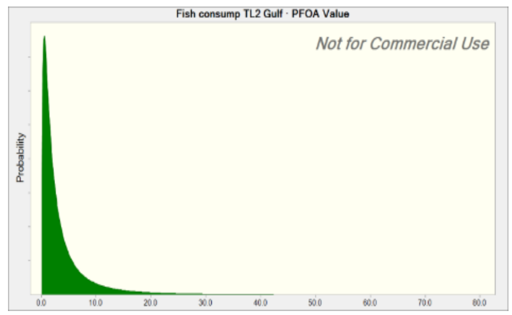
Location	0.0
Mean	4.9
95%	16.4



Assumption: Fish consump TL2 Gulf · PFOA Value

Lognormal distribution with parameters:

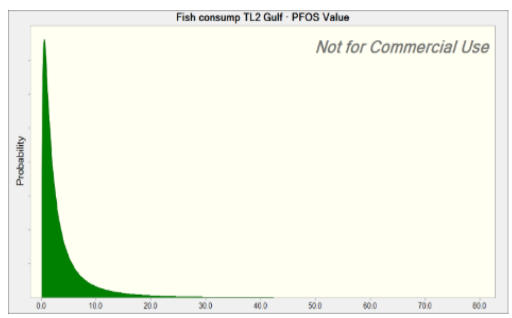
Location	0.0
Mean	4.2
95%	14.6



Assumption: Fish consump TL2 Gulf · PFOS Value

Lognormal distribution with parameters:

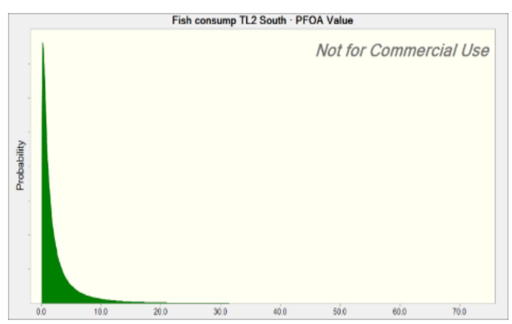
Location	0.0
Mean	4.2
95%	14.6



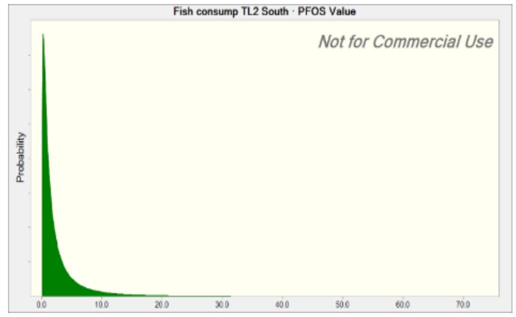
Assumption: Fish consump TL2 South · PFOA Value

Lognormal distribution with parameters:

Location	0.0
Mean	3.1
95%	11.3



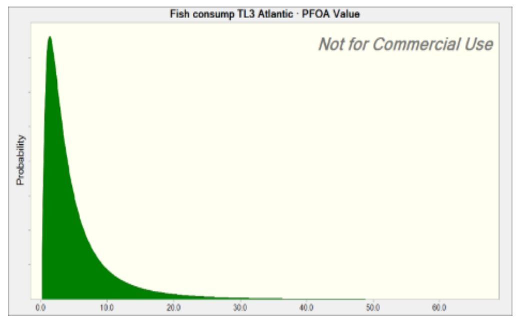
Assumption: Fish consump TL2 South · PFOS Value



Lognormal distribution with parameters:

Location	0.0
Mean	3.1
95%	11.3

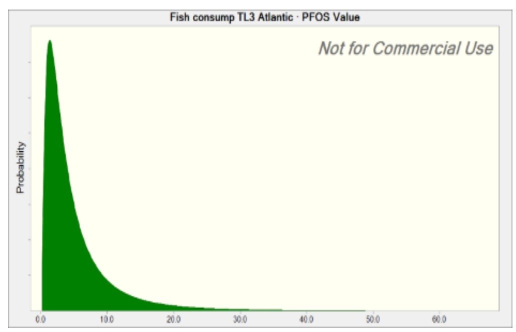
Assumption: Fish consump TL3 Atlantic · PFOA Value



Lognormal distribution with parameters:

Location	0.0
Mean	5.4
95%	16.6

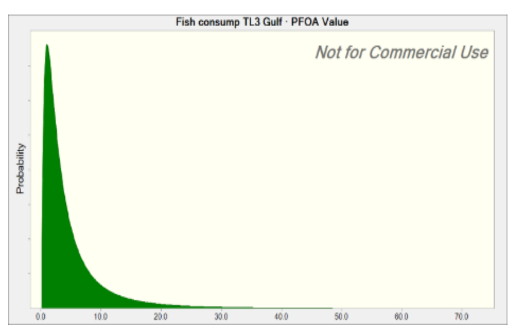
Assumption: Fish consump TL3 Atlantic · PFOS Value



Lognormal distribution with parameters:

Location	0.0
Mean	5.4
95%	16.6

Assumption: Fish consump TL3 Gulf · PFOA Value



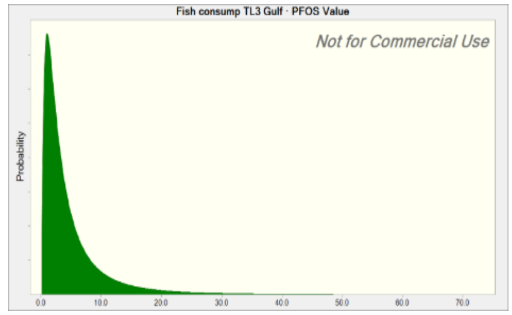
Lognormal distribution with parameters:

Location	0.0
Mean	5.1
95%	16.4

Assumption: Fish consump TL3 Gulf · PFOS Value

Lognormal distribution with parameters:

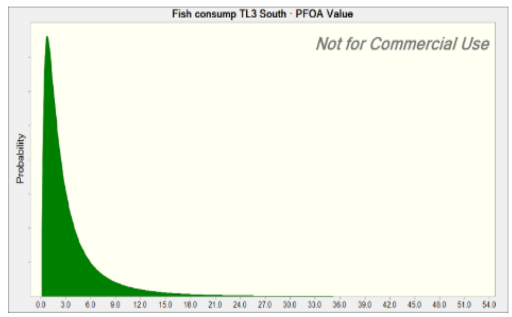
Location	0.0
Mean	5.1
95%	16.4



Assumption: Fish consump TL3 South · PFOA Value

Lognormal distribution with parameters:

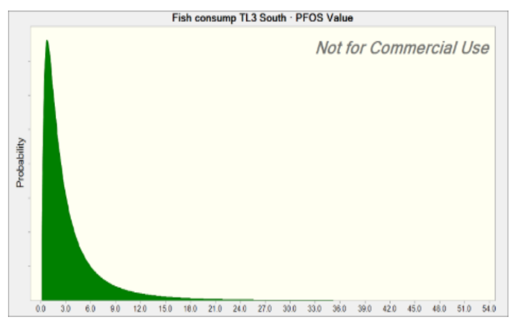
Location	0.0
Mean	3.7
95%	11.9



Assumption: Fish consump TL3 South · PFOS Value

Lognormal distribution with parameters:

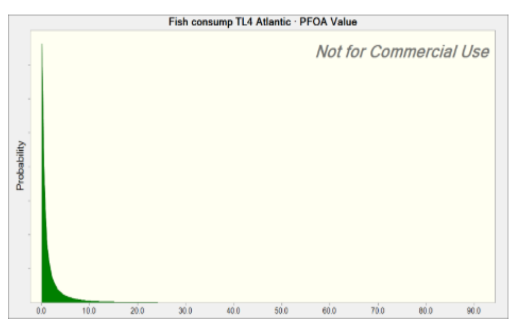
Location	0.0
Mean	3.7
95%	11.9



Assumption: Fish consump TL4 Atlantic · PFOA Value

Lognormal distribution with parameters:

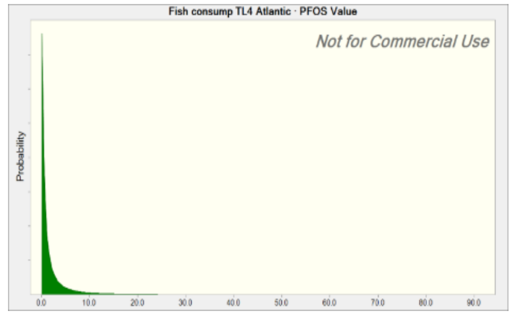
Location	0.0
Mean	2.6
50%	0.8



Assumption: Fish consump TL4 Atlantic · PFOS Value

Lognormal distribution with parameters:

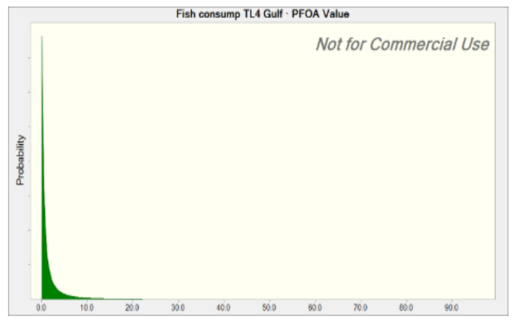
Location	0.0
Mean	2.6
50%	0.8



Assumption: Fish consump TL4 Gulf · PFOA Value

Lognormal distribution with parameters:

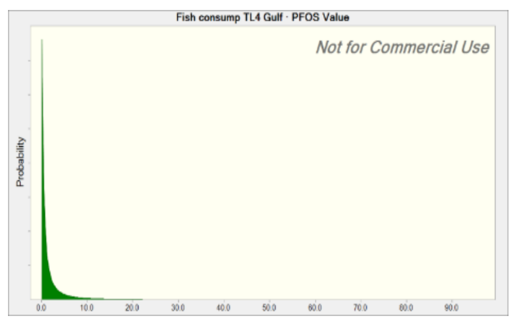
Location	0.0
Mean	2.5
50%	0.7



Assumption: Fish consump TL4 Gulf · PFOS Value

Lognormal distribution with parameters:

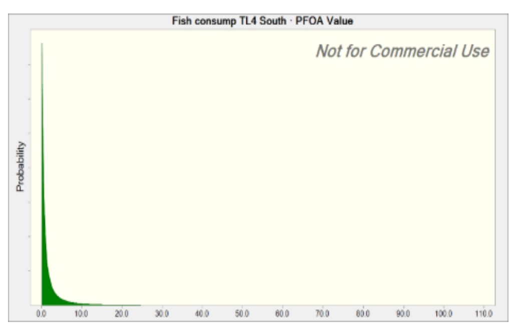
Location	0.0
Mean	2.5
50%	0.7



Assumption: Fish consump TL4 South · PFOA Value

Lognormal distribution with parameters:

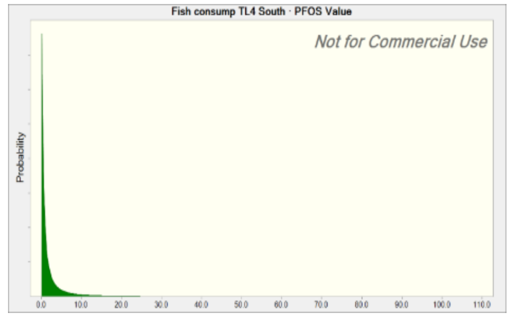
Location	0.0
Mean	2.8
97%	15.8



Assumption: Fish consump TL4 South · PFOS Value

Lognormal distribution with parameters:

Location	0.0
Mean	2.8
97%	15.8



Appendix B

Table B1 – Bioaccumulation factors for PFOA in fish fillets and shellfish tissue

Species	Place	Fresh or Marine	Exposure	Tissue	BAF	Study
Common carp	laboratory	Fresh	static 28d, 28d flow through depuration	muscle	3.85	Fang et al, 2016
Minnow	Taihu Lake, China	Fresh	wild caught	muscle	112.5	Fang et al., 2014
Silver carp	Taihu Lake, China	Fresh	wild caught	muscle	11.8	Fang et al., 2014
Whitebait	Taihu Lake, China	Fresh	wild caught	muscle	147	Fang et al., 2014
Crucian carp	Taihu Lake, China	Fresh	wild caught	muscle	81	Fang et al., 2014
Lake saury	Taihu Lake, China	Fresh	wild caught	muscle	284	Fang et al., 2014
Common carp	Taihu Lake, China	Fresh	wild caught	muscle	177	Fang et al., 2014
Mongolian culter	Taihu Lake, China	Fresh	wild caught	muscle	161	Fang et al., 2014
Mud fish	Taihu Lake, China	Fresh	wild caught	muscle	163	Fang et al., 2014
Chinese bitterling	Taihu Lake, China	Fresh	wild caught	muscle	87.9	Fang et al., 2014
Goby	Taihu Lake, China	Fresh	wild caught	muscle	37.7	Fang et al., 2014
Common carp	China	Fresh	wild caught	muscle	182	Zhou et al., 2012
White shrimp	Taihu Lake, China	Fresh	wild caught	soft part	12.5	Fang et al., 2014
Pearl mussel	Taihu Lake, China	Fresh	wild caught	soft part	39.7	Fang et al., 2014

BAF – bioaccumulation factor

Table B2 – Bioaccumulation factors for PFOS in fish fillets and shellfish tissue

Species	Place	Fresh or Marine	Exposure	Tissue	BAF (L/kg)	Study
Bluegill	Lake Calhoun, MN	Fresh	wild caught	fillet	2802	MPCA, 2007b
Bluegill and white bass	Mississippi River, MN	Fresh	wild caught	fillet	5737	MPCA, 2007b
Common carp	laboratory	Fresh	static 28d, 28d flow through depuration	muscle	9500	Fang et al, 2016
Minnow	Taihu Lake, China	Fresh	wild caught	muscle	3212	Fang et al., 2014
Silver carp	Taihu Lake, China	Fresh	wild caught	muscle	832	Fang et al., 2014
Whitebait	Taihu Lake, China	Fresh	wild caught	muscle	1350	Fang et al., 2014
Crucian carp	Taihu Lake, China	Fresh	wild caught	muscle	6898	Fang et al., 2014
Lake saury	Taihu Lake, China	Fresh	wild caught	muscle	4401	Fang et al., 2014
Common carp	Taihu Lake, China	Fresh	wild caught	muscle	3679	Fang et al., 2014
Mongolian culter	Taihu Lake, China	Fresh	wild caught	muscle	6927	Fang et al., 2014
Mud fish	Taihu Lake, China	Fresh	wild caught	muscle	4854	Fang et al., 2014
Chinese bitterling	Taihu Lake, China	Fresh	wild caught	muscle	2861	Fang et al., 2014
Goby	Taihu Lake, China	Fresh	wild caught	muscle	2876	Fang et al., 2014
Common carp	China	Fresh	wild caught	muscle	11749	Zhou et al., 2012
Taihu Lake shrimp	Taihu Lake, China	Fresh	wild caught	soft part	2161	Fang et al., 2014
White shrimp	Taihu Lake, China	Fresh	wild caught	soft part	978	Fang et al., 2014
Freshwater mussel	Taihu Lake, China	Fresh	wild caught	soft part	256	Fang et al., 2014
Pearl mussel	Taihu Lake, China	Fresh	wild caught	soft part	466	Fang et al., 2014

BAF – bioaccumulation factor

Table B3 – Trophic level weighting for fish and shellfish in the PFOA and PFOS bioaccumulation studies

Fish and shellfish	Scientific Name	Trophic Level 2 Weighting	Trophic Level 3 Weighting	Trophic Level 4 Weighting	Reference
Minnow	*Hemiculter leucisculus*	0	1	0	FishBase.org
Silver carp	*Hypophthalmichthys molitrix*	0	1	0	USEPA 2014
Whitebait	*Reganisalanx brachyrostralis*	0	1	0	FishBase.org
Crucian carp	*Carassius cuvieri*	0	1	0	USEPA 2014
Lake saury	*Coilia mystus*	0	1	0	FishBase.org
Common carp	*Cyprinus carpio*	0	1	0	USEPA 2014
Mongolian culter	*Culter mongolicus*	0	0.5	0.5	FishBase.org
Mud fish	*Misgurnus anguillicaudatus*	0	1	0	FishBase.org
Chinese bitterling	*Rhodeus sinensis*	0.5	0.5	0	FishBase.org
Goby	*Ctenogobius giurinus*	0	1	0	FishBase.org
White shrimp	*Exopalaemon sp.*	0.5	0.5	0	USEPA 2014
Pearl mussel	*Lamellibranchia sp.*	1	0	0	USEPA 2014
Bluegill	*Lepomis macrochirus*	0	1	0	FishBase.org
White bass[a]	*Morone chrysops*	0	0	1	USEPA 2014
Taihu Lake shrimp	*Macrobrachium nipponense*	0.5	0.5	0	USEPA 2014
Freshwater mussel	*Lamellibranchia sp.*	1	0	0	USEPA 2014

[a] – The white bass value is the geometric mean concentration of *Lepomis macrochirus* and *Morone chrysops*

Table B4 – Species-specific TL2 BAFs and geometric mean TL2 BAF for PFOA

Species	Scientific name	TL2 BAF
Chinese bitterling	*Rhodeus sinensis*	87.9
White shrimp	*Exopalaemon sp.*	12.5
Pearl mussel	*Lamellibranchia sp.*	39.7
	Geometric mean TL2 BAF	35

TL – trophic level
BAF – bioaccumulation factor

Table B5 – Species-specific TL3 BAFs and geometric mean TL3 BAF for PFOA

Species	Scientific name	TL3 BAF
Minnow	*Hemiculter leucisculus*	112.5
Silver carp	*Hypophthalmichthys molitrix*	11.8
Whitebait	*Reganisalanx brachyrostralis*	147
Crucian carp	*Carassius cuvieri*	81
Lake saury	*Coilia mystus*	284
Common carp	*Cyprinus carpio*	50
Mongolian culter	*Culter mongolicus*	161
Mud fish	*Misgurnus anguillicaudatus*	163
Chinese bitterling	*Rhodeus sinensis*	87.9
Goby	*Ctenogobius giurinus*	37.7
White shrimp	*Exopalaemon sp.*	12.5
	Geometric mean TL3 BAF	71

TL – trophic level
BAF – bioaccumulation factor

Table B6 – Species-specific TL4 BAFs and geometric mean TL4 BAF for PFOA

Species	Scientific name	TL4 BAF
Mongolian culter	*Culter mongolicus*	161
	Geometric mean TL4 BAF	161

TL – trophic level
BAF – bioaccumulation factor

Table B7 – Species-specific TL2 BAFs and geometric mean TL2 BAF for PFOS

Species	Scientific name	TL2 BAF
Chinese bitterling	*Rhodeus sinensis*	2861
White shrimp	*Exopalaemon sp.*	978
Pearl mussel	*Lamellibranchia sp.*	466
Taihu Lake shrimp	*Macrobrachium nipponense*	2161
Freshwater mussel	*Lamellibranchia sp.*	256
	Geometric mean TL2 BAF	937

TL – trophic level
BAF – bioaccumulation factor

Table B8 – Species-specific TL3 BAFs and geometric mean TL3 BAF for PFOS

Species	Scientific name	TL3 BAF
Minnow	*Hemiculter leucisculus*	3212
Silver carp	*Hypophthalmichthys molitrix*	832
Whitebait	*Reganisalanx brachyrostralis*	1350
Crucian carp	*Carassius cuvieri*	6898
Lake saury	*Coilia mystus*	4401
Common carp	*Cyprinus carpio*	7433
Mongolian culter	*Culter mongolicus*	6927
Mud fish	*Misgurnus anguillicaudatus*	4854
Chinese bitterling	*Rhodeus sinensis*	2861
Goby	*Ctenogobius giurinus*	2876
White shrimp	*Exopalaemon sp.*	978
Bluegill	*Lepomis macrochirus*	2802
Taihu Lake shrimp	*Macrobrachium nipponense*	2161
	Geometric mean TL3 BAF	2959

TL – trophic level
BAF – bioaccumulation factor

Table B9 – Species-specific TL4 BAFs and geometric mean TL4 BAF for PFOS

Species	Scientific name	TL4 BAF
Mongolian culter	*Culter mongolicus*	6927
White bass	*Morone chrysops*	5737
	Geometric mean TL4 BAF	6304

TL – trophic level
BAF – bioaccumulation factor

Appendix C

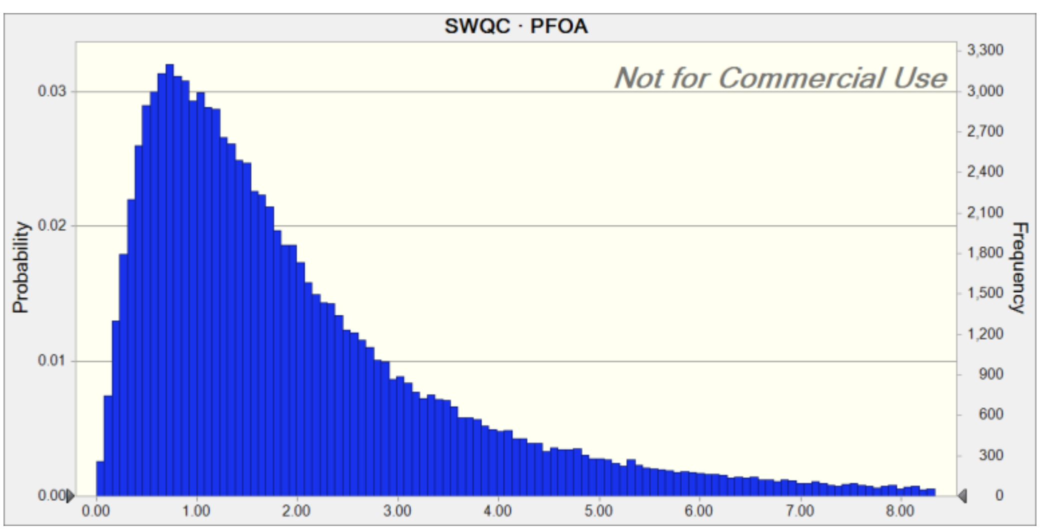
Crystal Ball Report - Forecasts

Run preferences:	
Number of trials run	100,000
Monte Carlo	
Seed	123457
Precision control on	
Confidence level	95.00%
Run statistics:	
Total running time (sec)	57.11
Trials/second (average)	1,751
Random numbers per sec	38,525
Crystal Ball data:	
Assumptions	22
Correlations	0
Correlation matrices	0
Decision variables	0
Forecasts	12

Forecasts

Forecast: SWQC · PFOA

Summary:
Entire range is from 0.00 to 55.36
Base case is 1.16
After 100,000 trials, the std. error of the mean is 0.01



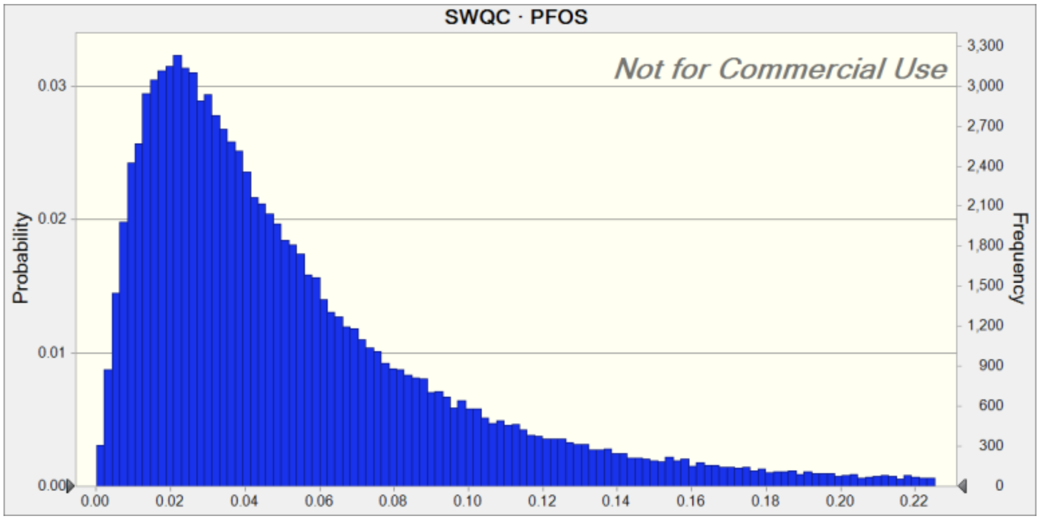
Statistics:	Forecast values
Trials	100,000
Base Case	1.16
Mean	2.19
Median	1.56
Mode	---
Standard Deviation	2.20
Variance	4.82
Skewness	3.91
Kurtosis	36.47
Coeff. of Variation	1.00
Minimum	0.00
Maximum	55.36
Range Width	55.36
Mean Std. Error	0.01

Forecast: SWQC · PFOA (cont'd)

Percentiles:	Forecast values
0%	0.00
10%	0.49
20%	0.74
30%	0.99
40%	1.26
50%	1.56
60%	1.93
70%	2.42
80%	3.15
90%	4.53
100%	55.36

Forecast: SWQC · PFOS

Summary:
Entire range is from 0.00 to 1.30
Base case is 0.03
After 100,000 trials, the std. error of the mean is 0.00



Statistics:	Forecast values
Trials	100,000
Base Case	0.03
Mean	0.06
Median	0.04
Mode	---
Standard Deviation	0.06
Variance	0.00
Skewness	3.61
Kurtosis	28.36
Coeff. of Variation	1.01
Minimum	0.00
Maximum	1.30
Range Width	1.30
Mean Std. Error	0.00

Forecast: SWQC · PFOS (cont'd)

Percentiles:	Forecast values
0%	0.00
10%	0.01
20%	0.02
30%	0.03
40%	0.03

50%	0.04
60%	0.05
70%	0.06
80%	0.09
90%	0.12
100%	1.30

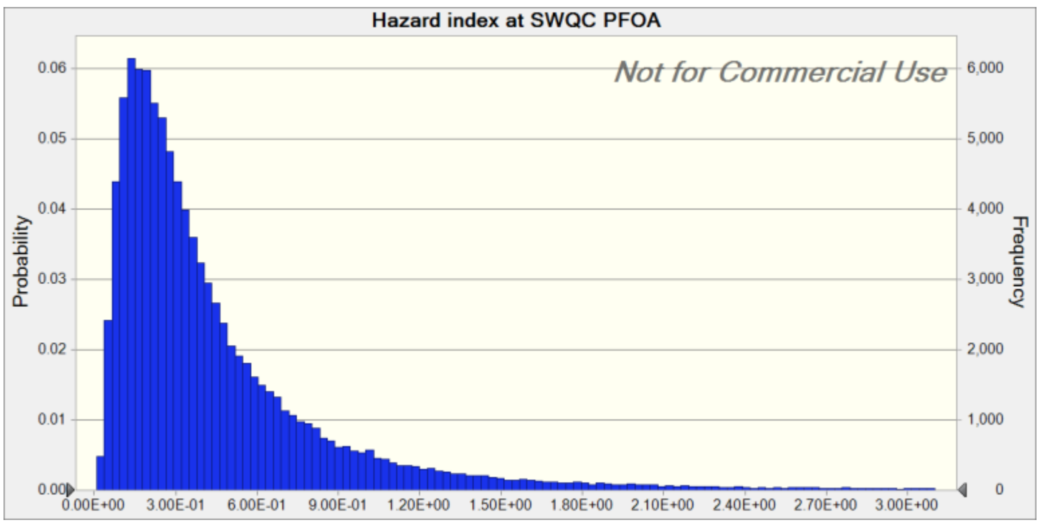
Forecast: Hazard index at SWQC PFOA

Summary:

Entire range is from 8.85E-03 to 1.30E+02

Base case is 4.21E-01

After 100,000 trials, the std. error of the mean is 2.93E-03



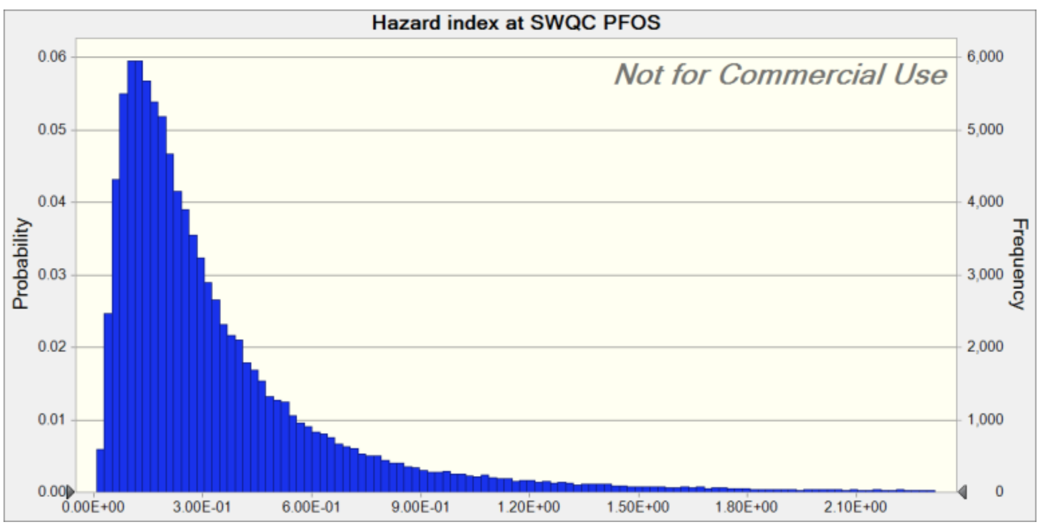
Statistics:	Forecast values
Trials	100,000
Base Case	4.21E-01
Mean	5.04E-01
Median	3.14E-01
Mode	---
Standard Deviation	9.28E-01
Variance	8.60E-01
Skewness	39.79
Kurtosis	4,200.66
Coeff. of Variation	1.84
Minimum	8.85E-03
Maximum	1.30E+02
Range Width	1.30E+02
Mean Std. Error	2.93E-03

Forecast: Hazard index at SWQC PFOA (cont'd)

Percentiles:	Forecast values
0%	8.85E-03
10%	1.08E-01
20%	1.55E-01
30%	2.03E-01
40%	2.54E-01
50%	3.14E-01
60%	3.90E-01
70%	4.94E-01
80%	6.61E-01
90%	9.99E-01
100%	1.30E+02

Forecast: Hazard index at SWQC PFOS

Summary:
Entire range is from 7.67E-03 to 6.68E+01
Base case is 3.28E-01
After 100,000 trials, the std. error of the mean is 2.17E-03



Statistics:	Forecast values
Trials	100,000
Base Case	3.28E-01
Mean	3.93E-01
Median	2.42E-01
Mode	---
Standard Deviation	6.87E-01
Variance	4.72E-01
Skewness	23.39

Kurtosis	1,359.36
Coeff. of Variation	1.75
Minimum	7.67E-03
Maximum	6.68E+01
Range Width	6.68E+01
Mean Std. Error	2.17E-03

Forecast: Hazard index at SWQC PFOS (cont'd)

Percentiles:	Forecast values
0%	7.67E-03
10%	8.16E-02
20%	1.18E-01
30%	1.54E-01
40%	1.94E-01
50%	2.42E-01
60%	3.01E-01
70%	3.83E-01
80%	5.11E-01
90%	7.79E-01
100%	6.68E+01