A CONSISTENT MODEL FOR ECOLOGICAL RISK ASSESSMENT IN TEXAS: THE PROTECTIVE CONCENTRATION LEVEL CALCULATOR APPLICATION

by

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ABSTRACT

Ecological risk assessments (ERA) for contaminated sites can be lengthy, resource-intensive, and prone to subjective interpretation. The Texas Commission on Environmental Quality (TCEQ) periodically publishes the RG-263 document, which is known as the Ecological Risk Assessment Guidance or ERAG, but is entitled "Conducting Ecological Risk Assessments at Remediation Sites in Texas". The ERAG discusses the interactions of the ERA process with the ecological services analysis process and the role the Natural Resource Trustee agencies play in Texas under regulation 30 TAC §7.124. The guidance outlines a three-tiered process:

Tier 1 - Exclusion

Tier II - Screening Level ERA

Tier III - Baseline ERA

The ecological protective concentration level (PCL) calculator and supporting database provide a consistent, scientifically reliable, and technically defensible methodology that streamlines the processes of developing and reviewing ecological risk assessments. The current version is a web-based, user interactive toxicological and species database capable of calculating screening levels (SLs; ERAG Step 6) and protective concentration levels (PCLs; ERAG Step 7) for 105 chemicals of concern (COCs), and for 96 indicator species in seven diverse habitats of Texas. In addition, three

minor habitats provide a representative species selection for risk assessments of areas that cannot be categorized among the seven major habitats, for example, a small man-made stock pond. The web-based tool also supports the risk assessor in developing site-specific Tier III baseline risk assessments. Site-specific input variables can be input by the risk assessor to efficiently re-calculate the PCL. For each species, including the growing list of threatened and endangered (T&E) species, an uptake factors document provides research based support for the default values in the database. For each COC, a fate and transport/toxicological profile was developed based on an exhaustive literature review, which incorporated No Observed Adverse Effect Level (NOAEL), and Lowest Observed Adverse Effect Level (LOAEL)-based toxicity reference values (TRVs) for growth, reproduction, and mortality. The TRVs, in conjunction with species uptake factors and a multimedia bioaccumulation/food web model, are used to calculate the PCL.

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This thesis is dedicated to my family: my wife, Dana for her inexhaustible love, encouragement and support, and to my parents for their encouragement and for teaching me to set the bar high and then go for it.

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CHAPTER I

INTRODUCTION

The Protective Concentration Level (PCL) application (calculator and associated database) resulted from a thirteen year collaborative effort between West Texas A&M University and the Texas Commission on Environmental Quality (TCEQ). The goal was to develop an interactive model capable of producing consistent, scientifically reliable, technically defensible, species-specific PCLs for all habitats in the state of Texas. The project began in 2000 as part of a remedial investigation at the Department of Energy's (DOE) Pantex Nuclear Weapons Plant in Carson County, Texas. The breadth of chemicals of concern (COCs) on site and the amount of time required for developing ecological risk assessments (ERAs) led to the idea of streamlining these assessments using a common framework and database. This application would serve both regulators and potentially responsible parties (PRPs) by streamlining the ERA process, reducing remedial investigation costs, and reducing the time necessary to review ERAs by regulators. Despite the availability of TCEQ ERAG documents (2001, 2006, 2014, 2016), which provide specific procedures for conducting ERAs, assessments typically vary widely in their methods, sources of data, and assumptions. Almost as much time is spent on reviewing an ERA as is spent conducting an ERA. Project managers and regulators, both with limited time and resources, shared the same vision: streamline, simplify, and optimize the ERA process. The initial scope of the PCL project was simply to derive a list of species-specific PCLs that could be applied to sites in the Texas Panhandle. However, meetings between TCEQ, WTAMU, and the DOE led to the idea that a user-friendly, interactive application would allow users to: 1) quickly calculate screening level PCLs, 2) modify PCLs based on site-specific or surrogate species-specific data, 3) see the exact calculations, input data, and references for each PCL, and 4) obtain toxicological profiles, species uptake factors, and habitat food webs used in ERAs. The application would use methods outlined in TCEQ ERAG documents (2001, 2006, 2014, 2016) for calculating species-specific PCLs. Whereas manual PCL development typically takes weeks to months, the PCL application would theoretically be able to determine a PCL in seconds. Since the PCL application would be based on a single equation with established, pre-agreed upon literature sources for exposure and toxicity data, regulators would not have to spend an inordinate amount of time tracking down literature sources, validating exposure factors and verifying PCL calculations.

Meetings between TCEQ, DOE, WTAMU staff, and other members of the TCEQ Ecological Working Group led to a clarification of objectives and needs of the application:

- Calculate ecological species-specific PCLs using methods outlined in the TCEQ ERAG document.
- Clearly outline the methods and data used in calculating ecological PCLs
- Allow users to modify input data in case of disagreement with default values, or if more appropriate site-specific data is available

Further discussions led to the development of a PCL equation and agreement on the format of the user interface and documentation (uptake factors and toxicological profiles), and default literature sources for input data. Due to the breadth of the project, tasks were divided into seven major parts for the ecological risk team:

1. Development of the PCL equation
2. Screening of COCs and development of fate and transport/toxicological profiles
3. Selection of representative habitats and development of habitat-specific food webs and feeding guilds
4. Selection of indicator species based on trophic level and feeding guild
5. Development of species-specific exposure factors
6. Development of a wildlife exposure model
7. Development of a toxicity reference value (TRV) methodology and TRV derivation

The individual component tasks are discussed in the following chapter.

CHAPTER II

METHODS

1. DEVELOPMENT OF THE PCL EQUATION

The first step in developing the quantitative model for the PCL application was to establish an equation for calculating the ecological PCL. Although there are multiple methods of calculating ecological PCLs, the oral dose equation method was chosen by the workgroup due to the simplicity in the calculations, ability to account for exposure through more than one medium, and ability to account for various exposure patterns for different receptors based on spatial and temporal use of the site. The PCL equation is a deterministic model that estimates the COC concentration in soil or sediment that is protective of a toxicological endpoint (e.g., growth, reproduction, or survival) for an ecological receptor (TCEQ 2001, 2016). The PCL is back-calculated from the oral dose equation in which exposure is set equal to a toxicity endpoint (i.e., hazard quotient=1). The model accounts for the toxicity of the COC and the exposure of wildlife to contaminated food, soil/sediment, and water. The PCL equation for soil is a slightly modified form of the equation outlined in the TCEQ (2001, 2016) ERAG document and is calculated as follows:

$$PCL_{soil} = TRV - (IR_{water} \text{ x } EPC_{water}) \ / \ (IR_{food} \text{ x } BAF_{soil}) + IR_{soil}$$

Where:

PCL_{soil} = Protective concentration level in soil (mg / kg)

TRV = COC toxicity reference value (mg COC / kg body weight day)

IR_{water} = Water ingestion rate of the receptor (L / kg day)

EPC_{water} = Exposure point concentration for water (mg / L)

IR_{food} = Food ingestion rate of the receptor (kg food / kg BW day)

BAF_{soil} = Bioaccumulation factor (kg soil / kg biota)

IR_{soil} = Soil ingestion rate of the receptor (kg soil / kg BW day)

Similarly, the PCL equation for subaqueous sediments is calculated as follows:

$$PCL_{sediment} = TRV - (IR_{water} \times EPC_{water}) / (IR_{food} \times BAF_{sediment}) + IR_{sediment}$$

Where:

$IR_{sediment}$ = Sediment ingestion rate of the receptor (kg sediment / kg BW day)

$BAF_{sediment}$ = Bioaccumulation factor (kg sediment / kg biota)

All values are based on default literature data but can be modified by the user if he or she disagrees with default input parameters or possesses site- or species-specific data. Furthermore, the PCL values can be adjusted based on bioavailability of the COC or spatial or temporal exposure modifying factors (EMF) as demonstrated in the following equation:

$$PCL_{adjusted} = PCL_{soil/sediment} \times (1 / AUF) \times (1 / EF) \times (1 / \text{Other EMF})$$

Where:

AUF = Area Use Factor, the fraction of home range made up of contaminated area (unitless)

EF = Exposure Frequency, the fraction of time spent in contaminated area (unitless)

Other EMF = Other Exposure Modifying Factors, the fraction of COC that is bioavailable in site soils/sediments (unitless)

For example, the Red Fox (*Vulpes vulpes*) has a default home range of 2,600 acres. Assuming a contaminated area of 30-acres, the AUF would be: 30 acres/2600 acres = 0.012. Since the default values of EF and Other EMF are set to 1.0 (100%), a PCL_{soil} of 100 mg/kg would be adjusted as follows:

$$PCL_{adjusted} = 100 \text{ mg/kg} \times (1 / 0.012) \times (1 / 1.0_{EF}) \times (1 / 1.0_{Other\ EMF}) = 8333 \text{ mg/kg}$$

Default EF values in the PCL are assumed to be 100% and it is assumed that these receptors are exposed within the duration required for toxicity to occur. Similarly, it is assumed that the form of the COC in site soils is 100% bioavailable (Other EMF). Although these assumptions may be conservative, they are consistent with recommendations of the first step of PCL development (required element 6; TCEQ guidance 2014, 2016). All EMF values can be modified by the user to alter the adjusted PCL if site-specific values better represent the site than the default assumptions. However, if site-specific values are used to prepare screening level ERAs for TCEQ review, users will be required to provide a rationale when alterations to default EMF values have been made.

2. CHEMICALS OF CONCERN

The PCL had an initial list of 140 COCs compiled for inclusion in the PCL database using various solid waste management groupings, Resource Conservation and Recovery Act (RCRA) Facility Investigation reports, site wide risk assessments, and work plans. This list was submitted to TCEQ in 2010 for review and was narrowed to 109 COCs common to Superfund sites within the state of Texas. Criteria for inclusion was based on frequency of occurrence, potential for bioaccumulation, toxicity, and fate and transport. The list of 38 inorganic compounds and 71 organic compounds, includes various organochlorine pesticides, dioxins/furans, polycyclic aromatic hydrocarbons, and explosives. An additional 25 COCs were added to the database, which include high molecular weight polycyclic aromatic hydrocarbons, dioxins/furans (using the 2,3,7,8-Toxic Equivalency Quotient methodology [USEPA, 2008]), organotin compounds, and other COCs. It was anticipated that the list of COCs would change over time and this has in fact been the case. The current list of COCs identified by TCEQ for inclusion in the PCL contains 105 COCs (see Appendix A).

Fate and transport/toxicological profiles were developed for each COC based largely on the reviews found in TOXNET (USNLM 2013), which contain detailed information regarding the atmospheric, aquatic and terrestrial fate is outlined, along with information on bioavailability, bioaccumulation, and toxicology. Other COC-specific information, such as Texas Surface Water Quality Standards or Aquatic Surface Water Risk-Based Exposure Limits (used as the default EPC_{water}), bioaccumulation factors, and toxicity reference values are also provided, which are discussed in detail in the following sections.

3. HABITATS

The PCL model addresses all seven major habitats in the state of Texas. In addition, three minor habitats were defined by the TCEQ to provide representative species for ERAs in areas that do not fit a specific habitat characterization. The major habitats and food webs are consistent with the food webs shown in TCEQ guidance (2001, 2016) and include the following:

- Desert-Arid
- Estuarine systems
- Freshwater systems
- Shortgrass prairie
- Shrub-scrub
- Tallgrass prairie
- Upland forest
- Minor habitat – Aquatic and Terrestrial
- Minor habitat – Aquatic
- Minor habitat – Terrestrial

These ten habitats should allow the PCL model to be used for ecological risk assessments at virtually any site within the state of Texas. For each habitat, the food webs outlined by TCEQ (2001, 2016) were uploaded to the database for use and inspection by the user (see Appendix C). These food webs outline all trophic levels, representative feeding guilds in each trophic level, and specific examples of indicator species likely to occur within each feeding guild.

The minor habitats were implemented to facilitate ecological risk assessment of fragmented or isolated ecological areas that are not easily categorized as one of the seven major habitats. Such areas include small man-made stock ponds and unmaintained grassy areas next to lay down yards. The minor habitats contain species that are representative of a variety of aquatic and terrestrial feeding guilds.

4. SELECTION OF INDICATOR SPECIES

Where COCs exceed ecological screening benchmarks for a particular community or feeding guild within a habitat, TCEQ (2001) requires selecting an indicator species to represent each feeding guild and/or trophic level. The indicator species is used as a surrogate to represent the potential risk to entire feeding guilds. For example, to be protective of invertivorous birds, the American Woodcock (*Scolopax minor*) could be used as an indicator species.

To adequately protect each feeding guild, a minimum of two indicator species from each feeding guild of each habitat were selected for incorporation into the PCL. As per TCEQ guidance (2001, 2016), the criteria for indicator species selection were based on:

- Common Occurrence
- Range
- Ecological Relevance
- Exposure Potential
- Sensitivity
- Social / Economic Relevance
- Threatened & Endangered (T&E) Status
- Availability of Natural History Information

Commonly used species were also included (e.g. the American Robin (*Turdus migratorius*), Least Shrew (*Cryptotis parva*), and Belted Kingfisher (*Megaceryle alcyon*) based on agency recommendations. A total of 96 indicator species have been incorporated into the database, including 46 birds, 26 mammals, 20 reptiles, and 4 amphibians. Included in the count are 11 threatened or endangered species 7 of which are birds, 1 is a mammal and 3 are reptiles. In the future, additional species of fish and benthic invertebrates will likely be added pending methodology for calculating sediment-based PCLs for aquatic receptors.

5. DEVELOPMENT OF SPECIES-SPECIFIC EXPOSURE FACTORS

It is assumed that the major route of exposure for ecological receptors is through oral ingestion of soils/sediments, water, and food. Dermal and inhalation exposures are not considered due to the lack of data on uptake factors and insignificance of exposure to airborne COCs over chronic time periods (Sample and Suter 1994). However, if these pathways are considered significant for a particular COC at a site, alternative methods of PCL development are recommended.

The species-specific exposure factors required for developing a PCL are body weight, ingestion rates (food, water, and soil/sediment), home range, and dietary composition. These factors were largely gathered from peer-reviewed literature or widely used government documents as listed in Table 1.

Water ingestion rates

Water ingestion rates were estimated for mammals and birds using allometric models based on body weight derived by Calder and Braun (1983). These models were normalized to body weight as presented below:

$IR_{water} = 0.099 \times (BW)^{0.90} / BW$ (Mammals)

$IR_{water} = 0.059 \times (BW)^{0.67} / BW$ (Birds)

Where:

IR_{water} = water ingestion rate L / kg day

BW = body weight of the organism (kg fresh weight)

Food ingestion rates

Food ingestion rates were derived from species-specific empirical data available in the literature (USEPA 1993, Sample and Suter 1994). However, when species-specific empirical values were not available, they were estimated from allometric regression models based on metabolic rate (Nagy 2001). Nagy developed 90 equations in the exponential form for mammals, birds and reptiles, which were normalized to body weight as per the following equation:

$IR_{food} = a \times (BW)^{b} / BW$

Where:

IR_{food} = food ingestion rate (kg food / kg body weight day)

BW = body weight (kg)

a, b = taxon-specific scaling factor (unitless)

Selection of the appropriate allometric equation depended on the organism's body weight, diet, and taxon. Preference was given to equations that demonstrated a high correlation with measured values (i.e., high r values). Kilograms dry matter intake (DMI) per day was used due to the variable water content in fresh matter intake (FMI) values and because bioaccumulation factors were based on dry weight.

In 2013 Larry Champagne of the TCEQ communicated to the PCL development team that taxon-specific scaling factors had fallen out of general use in the environmental community and were no longer recommended by TCEQ. In response to this trend, the PCL calculations were modified to no longer take into account taxon-specific scaling factors thus setting the value to 1 for both a and b scaling factors, and the scaling factors were removed from the data table.

Soil/sediment ingestion rates

Wildlife may ingest soil or sediments intentionally or incidentally during feeding, grazing, preening, cleaning, or burrowing. Since soils and sediments may contain high COC concentrations, direct ingestion may be a significant exposure pathway. Therefore, USEPA (1993), Beyer et al. (1994) and Beyer and Fries (2003) were used to estimate the percentage of soil in diet for a variety of wildlife species. Additionally, current literature was reviewed to determine if there was any new and relevant information. If a value for percent soil in diet was not available for a particular organism, a surrogate organism was chosen based on its diet, burrowing, foraging or nest-building habits, and other relevant life history information. For example, the percent soil in diet for an American Robin (*Turdus migratorius*) was estimated at 5.2% due to its diet of 50% earthworms, based on the diet of the American Woodcock (*Scolopax minor*) which eats 100% earthworms and has approximately 10.4% soil in diet (Beyer et al. 1994).

When the available literature provides a receptor's soil and/or sediment ingestion rate as a percentage of dry matter in the gut, the converted fractional value was multiplied by the food ingestion rate to obtain the soil/sediment ingestion rate:

$$IR_{soil/sed} = IR_{food} \times SID$$

Where:

$IR_{soil/sed}$ = soil/sediment ingestion rate (kg food / kg body weight day)

IR_{food} = food ingestion rate (kg food / kg body weight day)

SID = fraction soil/sediment in diet

Home range

Home range is defined as the area encompassed by movement of wildlife on a daily to seasonal basis to find food, water, and shelter (Sample and Suter 1994). Numerous ecological receptors, such as waterfowl and carnivorous birds and mammals, have home ranges that are larger than the size of a typical affected property, which can be assumed to reduce their exposure to COCs compared to receptors with small home ranges. To incorporate exposure modifying factors based on home range, the literature was reviewed to derive applicable home range estimates for each indicator species. Preference was given to values which had been derived using accurate wildlife monitoring techniques, such as radio-tracking, mark-and-recapture, or pit tagging. Home ranges derived during migration or hibernation were not used. When multiple home range values were available, the arithmetic mean was used.

6. DEVELOPMENT OF A WILDLIFE EXPOSURE MODEL

The PCL model accounts for wildlife exposure to COCs in surface water, soil, and diet. As shown in Equation 1, direct oral exposure to ambient surface water and soils/sediments, and indirect oral exposure to COCs bioaccumulated in diet are used to calculate the PCL.

Exposure to surface water

As a conservative measure, oral exposure to surface water was considered in the PCL model. As oral exposure to surface water increases, the overall PCL decreases. This is because as the dose through surface water increases, the exposure to contaminated soils and diet must decrease in order for the dose to equal the TRV. To simplify the exposure model, one surface water-based exposure point concentration (EPC_{water}) was incorporated. As a conservative measure, the default EPC_{water} value is set to the TCEQ (2010) freshwater chronic surface water quality standard for the COC. When surface water quality standards were not available, the EPC_{water} was derived using the freshwater chronic aquatic surface water Risk-Based Exposure Limit (RBEL). This incorporates some conservatism in the model by accounting for potential exposure that does not occur through exposure to soils or sediments. Although higher values of EPC_{water} decrease the final PCL, the overall contribution of exposure through water to the dose at the default EPC_{water} is typically small (~1-2% of total dose). Eventually, the EPC_{water} may be a user-modified value so that the user can account for site-specific surface water concentrations above or below the default EPC_{water} value.

Exposure to COCs in diet

Dietary composition data was obtained from various literature sources (EPA 1993, Sample and Suter 1994). The fraction in diet made up by a particular food item (e.g., plants, soil invertebrates) was ideally determined as the percent mass in the specific organism's gut. Dietary data that represents an organism's diet over the course of the entire year were preferred. Many organisms alter their feeding habits seasonally based on the availability of food at certain times of the year. When data was presented as differing throughout a one-year period, the annual mean percentage of each class of food item was determined and incorporated as the dietary fraction. Preference was given to data based on organisms found in Texas or from similar habitats to those found in the state. If the dietary composition data was reported as a percent frequency, best professional judgment was used to estimate the percent mass of food items in the gut. If the percent mass of certain class of food was less than 5% (e.g., plant material made up 3% of the organism's diet), that mass was considered to be insignificant for modeling purposes.

Dietary composition data must match up with the five chemical-specific BAF pathways (plants, soil invertebrates, small mammals, fish, or benthic invertebrates). For example, a Common Yellowthroat (*Geothlypis trichas*) forages entirely on arboreal and aerial insects. However, due to the lack of BAFs for arboreal and aerial insects, the warbler's diet was simplified to 100% soil invertebrates. Similarly, various carnivores prey on terrestrial reptiles. However, since chemical-specific BAFs are not widely available for reptiles (but are widely available for small mammals), the fraction in diet made up by reptiles was included as small mammals. While there is a degree of uncertainty in assuming that BAFs for small mammals are similar to those of reptiles, there is currently too little data available to develop BAF pathways for reptiles. A separate BAF pathway for aerial insects and arthropods may be incorporated based on the availability of literature data (USACHPPM 2004). Other assumptions similar to those aforementioned are listed in Table 2. Note that, if this data is available for a particular COC/receptor pair, the user can input literature values to further refine the PCL.

COC food web model

In order to relate COC concentrations in the diet of ecological receptors to the PCL, media-to-receptor bioaccumulation factors (BAFs) were incorporated. The dietary BAF (BAF_d) is defined as the ratio of the COC concentration in the receptor's diet to that in the underlying media:

$$BAF_d = C_{diet} / C_{media}$$

Where:

BAF_d = the bioaccumulation factor that relates the concentration of COC in diet to that of the underlying media (soil or sediment)

C_{biota} = the COC concentration in the diet of the receptor (g / kg body weight)

C_{media} = the COC concentration in the underlying media (g / kg soil or sediment)

For receptors that forage on only one type of food (e.g., herbivores), the BAF_d would be equal to the BAF for the corresponding food type. For example, the BAF_d for an herbivore would be equal to the $BAF_{soil\text{-}to\text{-}plant}$. However, the majority of receptors forage on more than one food type, and so the BAF_d is the weighted average of the BAF for each corresponding food item as shown in the following equation:

$$BAF_d = \sum_{i=1}^{m} (BAFi \times F_i)$$

Where:

BAF_i = the bioaccumulation factor for food item (i) (kg soil/sediment / kg biota)

F_i = the fraction in diet of food item (i) for the ecological receptor (unitless)

Initially, three BAF_i (soil-to-plants, soil-to-invertebrates and water-to-fish) were arbitrarily incorporated in the bioaccumulation model. In 2012 at the request of TCEQ, the model was expanded and modified to include four soil-based BAF_i values (plants, earthworms, soil arthropods, and small mammals) and two subaqueous sediment-based BAF_i values (benthic invertebrates and fish). Since the PCL model assumes a constant, no-threshold relationship between concentrations in media and concentrations in biota, linear and log-linear regression models were not incorporated.

Extraction and selection of BAF_i values

There were two steps to the development of BAF_i values for a particular COC: extraction of BAF_i values from literature sources, and selection of the representative BAF_i.

Extraction of BAF_i values from literature sources

Literature containing bioaccumulation data first had to meet several acceptance criteria to be considered for incorporation into the model. First, unless the data was contained in a widely used secondary literature source (e.g. USEPA 2007, 1999; Sample et al. 1998a,b; Bechtel-Jacobs 1998a,b) the literature source had to be the primary source of the bioaccumulation data. The source must report the 1) chemical form and concentration, 2) exposure duration (if the study was controlled), 3) scientific and/or common name of the species used, and 4) method of chemical analysis. The method had to be an EPA SW-846 or otherwise reliable method based on known extraction and analytical techniques.

To derive sediment-based BAF values for non-ionic organic COCs, lipid- and organic carbon-normalized biota sediment accumulation factors (BSAFs) were extracted because 1) BSAFs account for site- and species-specific differences in organic carbon and lipid content, respectively, 2) BSAFs exhibit much lower variability than BAFs and 3) BSAFs can be adjusted based on site-specific organic carbon levels. To be incorporated into the PCL model, BSAFs were converted to BAFs based on default lipid contents of 5% for fish and 2% for benthic invertebrates (wet weight) based on data reported in USACE (2013). A default sediment-organic carbon content of 1% (dry weight) was used based on TCEQ (2006) and USEPA (1999) recommendations, however the user can re-calculate the BAF if organic carbon at the site differs from the default value.

Selection of the representative BAF_i

Following compilation of BAFs from literature sources, the representative BAF is chosen. When the sample size was adequate ($n \geq 10$), the median BAF was selected because: 1) the median is not sensitive to outliers (unlike the arithmetic mean), 2) the median represents the point at which 50% of all observations are above and 50% of observations are below, and 3) the median is the measure of central tendency used in the development of other ecological screening or clean-up levels (USEPA 2007, LANL 2012). When the sample size was moderate ($7 \leq n < 10$), the 90^{th} percentile value was used. When the sample size was small ($n < 7$), the maximum value was used.

Note that, in some cases the chosen value was not determined to be a conservative representation of the most appropriate BAF. For example, if the median BAF was representative of values derived at a highly contaminated site (where BAFs tend to be lower), an alternate statistic (e.g., the arithmetic mean) may be chosen. If deviations from the decision tree are made, an appropriate rationale or justification must be provided.

Several COCs did not have empirical bioaccumulation data available, which prompted development of a framework for selecting another BAF. In the absence of empirical data for organic COCs, a valid physicochemical (e.g., Log K_{ow}-based) model could be used as long as models met acceptance criteria ($r^2 \geq 0.2$ and $p \leq 0.05$; USEPA 2007). Otherwise, empirical BAFs for a surrogate chemical could be used as long as the surrogate chemical exhibits similar structure, toxicity, and behavior (e.g., Log K_{ow} or K_{oc}). If a surrogate chemical could not be used, the 90^{th} percentile value of empirical

BAFs for a chemical class could be used as a last resort. This method was more frequently used for inorganics, when a lack of physicochemical models and appropriateness of surrogate chemicals prompted the use of 90^{th} percentile values. The decision tree for selecting a representative BAF is presented in Fig. 1.

7. DEVELOPMENT OF A TOXICITY REFERENCE VALUE (TRV)

Methodology and TRV Derivation

The TCEQ (2001) ERAG states that, for each COC with a complete exposure pathway, "a toxicity reference value (TRV) should be developed from published studies and/or developed for potential receptor species." Based on methodology outlined in Calabrese and Baldwin (1993), Simini et al. (2000) and discussions with the TCEQ Ecological Working Group, a methodology for developing TRVs was agreed upon and incorporated into the database.

The three main types of TRVs considered relevant to the survival of a species' population are growth, reproduction, and mortality, so all three TRV types were incorporated into the model. For a screening level ecological risk assessment, TCEQ (2001) requires TRVs to be developed based on no observable adverse effect levels (TRV_{NOAEL}) and lowest observable adverse effect levels (TRV_{LOAEL}). The Step 6 (Screening Level) PCL is calculated using the TRV_{NOAEL} whereas the Step 7 PCL is calculated using the average of the TRV_{NOAEL} and TRV_{LOAEL}. This value is referred to as the average TRV ($TRV_{AVERAGE}$).

Decision hierarchy for TRV selection and use of uncertainty factors

The calculation of a soil- or sediment-based PCL is most sensitive to the TRV (Allard et al. 2010, Regan et al. 2002). The appropriateness of the TRV also contributes the most uncertainty to the development of the PCL. Whenever possible, TRVs were derived from studies in which both a TRV_{NOAEL} and TRV_{LOAEL} had been identified. However, when a TRV_{NOAEL} was not available, it was estimated by multiplying the TRV_{LOAEL} by 0.1. When a TRV_{LOAEL} was not available, it was estimated by multiplying the TRV_{NOAEL} by 10 (note, however, that this extrapolation is more likely to overestimate the "true" TRV_{LOAEL} and was not used frequently). TRV_{NOAEL} and TRV_{LOAEL} values could also be estimated by multiplying an acute LD_{50} by 0.01 or 0.1 respectively, however this method was used as a last resort as it tends to produce particularly conservative TRV_{NOAEL} and TRV_{LOAEL} values. The decision tree in Fig. 1 shows the hierarchy of decision-making used to derive TRV_{NOAEL}s.

Before selecting appropriate TRVs, selection criteria were developed to ensure TRVs were of high enough quality to develop a defensible PCL. At the very least, TRVs had to:

- Be primary literature published in either a peer-reviewed journal or document from a U.S. government agency (e.g., U.S. Environmental Protection Agency, Department of Defense, Agency for Toxic Substances and Disease Registry) where all relevant exposure and effect information is clearly outlined:
    - "Relevant exposure and effect information" includes chemical form (e.g., salt or oxidation state for metals); test species common/scientific name, age, sex; test endpoint and effect type; method and frequency of dosing; number of doses used; whether nominal doses were confirmed analytically; exposure duration; and whether statistics were used to identify the TRV
- Be based on exposure through food or drinking water:
    - TRVs based on intravenous or intraperitoneal exposure were not considered due to irrelevance of these exposure pathways to the dose

- TRVs based on inhalation were not incorporated based on the assumption that exposure of ecological receptors at a hazardous waste site to COCs is oral in nature, and because there is a great deal of uncertainty in extrapolating from TRVs based on inhalation to TRVs based on oral exposure

- Report either a NOAEL, LOAEL, or LD_{50}

After studies containing TRVs were screened, a TRV was selected based on several evaluation criteria similar to the data evaluation factors and categories outlined in USEPA (2003). TRVs were not scored quantitatively, however best professional judgment was exercised in selecting the most appropriate TRV based on the following selection criteria:

- Both the TRV_{NOAEL} and TRV_{LOAEL} are reported
- TRV is reported as a dose (mg / kg day) rather than a concentration (mg / kg or mg / L)
    - If TRV is reported as a concentration, a dose can be estimated using the body weights and ingestion rates provided in the study or USEPA (2003) recommended values
- TRV is based on exposure via diet rather than drinking water
- TRV is based on a measured rather than an unmeasured dose/concentration
- TRV is based on exposure to organisms during a critical life stage (e.g., juveniles or reproduction)
- An appropriate range and number of doses were tested
- Statistics were used to identify the TRV_{NOAEL} or TRV_{LOAEL}
- Exposure duration, in order of preference is chronic >>subchronic>> acute
- The effect type measured is relevant to the sustainability of the population
    - For example, the reproduction endpoint: percent of surviving progeny vs. weight of eggs

- The TRV is based on a test organism taxonomically similar to receptor species:
    - TRVs based on cattle and other ruminants were not considered due to a) the difference in body weight between these animals and most receptors, such as shrews and mice, and b) the differences in the digestive systems of ruminants versus most receptors in the database.

When multiple studies containing TRVs were available (as in the Eco-SSL appendices), studies containing only a TRV_{NOAEL} or TRV_{LOAEL} were screened out. Of the TRVs that remained, the TRV_{NOAEL} and TRV_{LOAEL} from each study were averaged to calculate the $TRV_{AVERAGE}$ and the median of the $TRV_{AVERAGE}$ values was chosen. If the median value lay between two $TRV_{AVERAGE}$ values (i.e., anytime there was an even number of $TRV_{AVERAGE}$ values), both the USEPA Eco-SSL data evaluation score and expert judgment was used to select the appropriate TRV. When all criteria were equal (which was rare), the more conservative value was chosen. All TRVs incorporated into toxicological profiles underwent internal review at WTAMU prior to being uploaded to the database for external review.

Secondary literature sources containing large amounts of peer-reviewed TRVs were often used to locate primary studies. The main secondary literature sources included USEPA (2007), Sample et al. (1998a,b), and LANL (2013). When TRVs could not be obtained from these sources, various online databases were searched using the chemical's name, synonyms, and Chemical Abstract Services Registry Number (CASRN).

For all TRVs selected for incorporation into the COC's toxicological profile, the following information was reported: CASRN, chemical name/form, surrogate (test species), effect type, effect measure, TRV type (NOAEL/LOAEL/LD_{50}), body weight, food or water ingestion rate (if needed to convert a concentration in food or water to a dose), dosing regime, age of test organism, life stage and sex, exposure duration, uncertainty factors (if used), conversions, end point reference/citation, and basis for selection/comments.

Theoretically, TRVs based on growth and reproduction should be lower than TRVs for mortality since growth and reproduction are typically more sensitive endpoints. However, this was not always the case because TRVs for sublethal endpoints could be based on exposure: a) to a less-toxic form of the COC, b) to adult organisms (whereas TRVs for mortality were based on exposure to neonates or juveniles), c) to a less-sensitive test species, or d) over a short-term (subacute or subchronic) duration. Some COCs simply did not appear to cause adverse effects on growth or reproduction below lethal levels due to differing mechanisms or modes of action. In these cases, (i.e., if TRVs for growth or reproduction exceeded TRVs for mortality), critical TRVs were selected based on what would be critical to the survival or sustainability of the population. If critical TRVs were selected, they are provided in the toxicological profile along with a rationale explaining why those TRVs were selected.

In accordance with USEPA (2007) guidance, TRVs were not adjusted for body weight using allometric scaling. Allometric equations for adjusting TRVs from test species to wildlife species developed by Sample and Arenal (1999) were developed for acute endpoints, and were not considered appropriate for extrapolating chronic TRVs across body sizes.

CHAPTER III

MODEL IMPLEMENTATION

1. PROOF OF CONCEPT

From 2003 through 2008, the initial efforts to collect the data necessary to compute protective concentration level values used Excel spreadsheets to record the data for the PCL. As the quantity of data grew, so did the incidence of error associated with manual entry of the data. In 2008, Dr. Rogers discussed the data issues with Dr. Musa Jafar of the Computer Information Systems department at West Texas A&M University. Dr. Jafar enlisted the help of Dr. Russell Anderson in the design and construction of a relational database to manage the data and a java web application tool to derive and present PCL calculations. Called a "Proof of Concept" model the java web application was designed to demonstrate the efficacy of the PCL model, a purpose for which it was immensely successful.

In April of 2010, Drs. Jafar, Anderson and Rogers published a paper in the *Journal of Information Systems Applied Research* entitled "Superfund Site Analysis Using Web 2.0 Technologies (Anderson, Jafar and Rogers, 2010). The paper describes the design and construction of a web based tool that would provide a central repository for the collection, validation, organization and presentation of the available toxicological research data. Of primary concern to the original team were the issues of data integrity, “model implementation, and tool availability and usability” (Anderson, Jafar and Rogers, 2010). The plan was implemented in three phases, 1) data cleansing , 2) database schema design and construction and 3) PCL Calculator design and implementation.

2. DATA CLEANSING

In the first step, the data collected by graduate students in Excel spreadsheets was classification of the types of data errors that were present and then defining methods to programmatically or manually resolve the errors. Data duplication was identified as the number one data error. Dr. Jafar “estimated that 75% of the data in the original spreadsheets was redundant” (Anderson, Jafar and Rogers, 2010). The initial data collection effort was based upon manual entry of data into spreadsheets which resulted in data entry errors such as extra spaces, alpha or numeric characters where they should not be, misspelled words, and naming inconsistencies. The majority of the issues could be resolved through the use of Excel formulas that remove leading or trailing spaces, formulas that validate the alphanumeric integrity of specific values and spell check for the common misspellings. Naming inconsistencies proved to be particularly difficult to eliminate completely which was the case with the species name, “Mourning Dove” versus the often encountered “Morning Dove”. As confidence in the raw data increased, the team was able to transition to the second phase, database schema design and construction.

3. COMPUTATIONAL DATA

The initial data collected for COCs, species, body weight, reported toxicity value and toxicity type was supplemented with the additional data required to calculate adjusted PCL values including water and fat solubility of the COC (log K_{ow}), trophic level of the species (used to determine bioaccumulation of COC), food, water and soil and sediment ingestion percentages, percentage of bioaccumulation in the diet and percentage of time spent in the contaminated area. Using the methodology described earlier, the varying toxicity values collected from the literature were converted to uniform toxicity reference values (TRVs) for each of the eighty-five common species, ten threatened or endangered species and fifty-three surrogate species.

The PCL calculator page combines the TRV value developed for the selected COC with each of the receptor species in the selected habitat into COC/Receptor pairs. The combination is then used to calculate NOAEL (No Observable Adverse Effect Level), LOAEL (Lowest Observable Effect Level) and PCL (i.e. one-half the value of the combined LOAEL and NOAEL) for each of the three PCL Types; growth, reproduction and mortality. The result of this is the generation of approximately 10,000 PCL values for each habitat/COC pairing, setting the total number of calculated PCLs at over 31,000. These numbers are expected to increase as additional COCs are identified and as future research provides additional COC/Receptor pairs data.

4. DATABASE DESIGN AND CONSTRUCTION

The physical MySQL database is composed of 16 tables, 5 of which are the primary data tables with the remaining tables containing application support data used to manage the users of the system, maintain user usage log data, provide a system for user feedback, store version history data and provide static reference values for animal classification, the PCL type and COC concentration type indexes. The 5 primary data tables can be described as follows:

- Chemical – contains the list of COCs, identified by the CAS registry number, a unique number for each. This data table also contains the adjustment factors specific to each COC.
- Species – contains the list of species, both primary and surrogate along with the adjustment factors specific to each.
- Concentration – contains the TRVs from the literature. Identified by a compound key consisting of the "CAS number, common species name, concentration type (LOAEL, NOAEL, LD50) and PCL type (mortality, reproduction or growth). [1]" This table contains the additional data of "TRV, body weight of test subjects, and bibliographic reference information[1]".
- SurrogateAssignment – associates primary species with surrogate species when TRV data for the primary species is missing. "Identified by CAS number, common species name, concentration type (LOAEL, NOAEL, LD50), and PCL type (mortality, reproduction or growth).[1]"
- Habitat – lists the species included in each habitat. Identified by the unique habitat ID

The referential connections between the data elements in the primary data tables can be seen in the data table diagram in Appendix F. Once the structure of the database was built it was time to upload the collected and cleansed Excel data. The spreadsheets were saved as a series of comma delimited value (csv) files and then manually converted into SQL INSERT statements for each of the primary tables. Transference of the data to the MySQL data tables revealed referential errors as primary and foreign key constraints were violated. As the application moved from prototype to product, the responsibility for data entry and integrity was assumed by the administrative editing functions. Currently, data entry validation is performed at the field level of the web pages and again at the server level prior to insertion into the database ensuring the data is proper if not correct.

5. SUPPORT DOCUMENTATION

In support of the database, extensive research documentation was collected for both the species and the chemicals in the database. For each of the ninety-five primary species, the species, default values for body weight, home range, food ingestion rate, water ingestion rate, soil ingestion rate and dietary composition percentages are given along with the scientific justification for the values. Additional formulae, study details, references and citations are also included in each of the species uptake documents. Literally hundreds of citations are included and tracked in the database (see example in Appendix D).

For each of the 105 chemicals contained in the database a CAS profile document has been created to consolidate the available reference data into one document. The document presents environmental fate and transport data collected from sources such as the Hazardous Substances Data Bank (HSDB), various literature sources, the most recent TCEQ Surface Water Quality Benchmark (SWQB). Bioaccumulation factors (BAF) are modeled using algorithms based upon peer reviewed research available from acknowledged experts and literature sources approved and used by agencies such as the EPA to derive default values and the scientific justifications for each BAF value. In addition to the default values for the various BAFs, default values for the TRVs for each chemical are provided specific to each class of animal along with the basis for the values provided. Each CAS profile ends with a complete list of citations for the document (see example in Appendix E).

The exhaustive documentation of the data values used in the calculator provides both the ecological risk assessor and the reviewing governmental agency a many thousand fold increase in productivity. Risk assessments that once took weeks to create and a month or more to review and validate can be generated in a matter of minutes and validated in a matter of hours because the values used have been either pre-approved by the governmental agencies or in peer reviewed articles and meetings for use in ecological risk assessment.

CHAPTER IV

USER INTERFACE

1. INTRODUCTION

The PCL database user interface has been designed as a user-friendly, interactive, web-based tool that quickly and easily calculates defensible PCLs for use in Texas, in association with the Ecological Risk Assessment Guidelines (ERAG) for the determination of COC screening level (ERAG Step 6) or baseline ecological risk assessments (ERAG Step 7) and to support site-specific ecological risk assessment and determination of PCLs based on site specific data (with justification). A Help page has been developed to guide the user from the initial stages of COC and habitat selection to PCL calculation, adjustment and export (See example, Figure G24). Help pages are available for each of the guest and registered user functions. There are currently three possible user roles available in the PCL, guest, registered and administrator. Each role defines the PCL Calculator functions available to the user;

- Guest users can generate the PCL analysis, view chemical, species and habitat lists and send comments to the PCL Administrators
- Registered users can perform all the functions available to guest users but can also print or export to Excel spreadsheet the generated PCL Analysis.
- Administrator users can perform all the functions available to Registered users but can also Add/Edit/Delete chemicals, species, habitats and user

records, set concentration associations and establish species surrogate assignments.

In 2013, the TCEQ began the process of updating the state's "Ecological Risk Assessment Guidelines" documentation, tying the PCL to the official risk assessment regulations of the state. Work on this effort has continued through 2015 and is nearing completion. When the updated ERAG document is released the PCL Calculator will assume an integral role in the generation of ecological risk assessment document preparation for the state of Texas.

2. FUNCTIONAL DESCRIPTION

The PCL is accessed through the login page (Figure G1). Selecting the "Use as Guest" link allows anonymous access but limited access to the PCL. To gain access as a Registered user requires registration which is accomplished by clicking on the "Register Now" button on the login page which displays the Registration screen (Figure G2). The submission of the registration forms establishes a user record in the database with a "Pending" status. When an Administrator reviews the registration and approves the application, the user status is set to "Active" and the user is sent an email confirming the registration or the registration is denied. Successful login, as guest, registered user or administrator displays the PCL Calculator screen.

To generate a PCL analysis from the PCL Calculator screen, a user begins by selecting 1) the habitat, and 2) the COC (using either the COC name or CASRN). To run an analysis, the user clicks "Next" which opens a pop-up window displaying the PCL calculations for the selected COC and species in the selected habitat. On the "Analysis" page the user sees a list of species with their associated body weights, trophic levels, and ingestion rates. The BAF for each of the five bioaccumulation pathways, along with the species-specific weighted BAF is also displayed. Changing any of the ingestion rates or BAFs will alter the values used in the PCL equation and thereby alter the final PCL. TRVs for growth, reproduction and mortality are shown on the right-hand side of the screen, along with the TRV type (NOAEL/LOAEL) and surrogate used to derive the TRV (e.g. chicken, rat, mouse). The “Computed PCL” can be altered by modifying any of the aforementioned values. The “Adjusted PCL” is also calculated based on exposure modifying factors “Range %”, “Time %”, or “% Bioavailability”. This additional column allows the user to alter default temporal, spatial, or chemical bioavailability assumptions to alter the final PCL.

In addition to the PCL Calculator screen, the guest, registered user or administrator can choose to select from the “Chemical”, “Species”, “Habitat” or “Contact Us” tabs. Selection of the “Chemicals” tab displays the list of chemicals (Figure G9). Clicking on the CAS number for one of the displayed chemicals, opens a pop-up overlay displaying the tox profile for the selected chemical (see example in Appendix E). Selection of the “Species” tab displays the “Species List” screen (Figure G10) where the user can click on a species name to open a pop-up overlay containing the species uptake document for the selected species (see example in Appendix D). Selection of the “Habitats” tab displays the “Habitat List” screen (Figure G11) which lists the habitats included in the database. From the “Habitat List” screen, clicking on the habitat name opens a pop-up overlay containing the food web diagram for the selected habitat (Figures C1-C10). From the “Habitats List” screen, the user can also click on the arrow icon in the Assoc. Species column to open up a list of species associated with the selected habitat (Figure G12). Clicking on any of the associated species listed opens a pop-up overlay containing the

“Species Uptake” document for the selected species (see example in Appendix D). Selection of the “Contact Us” tab displays the “Submit Comments” page (Figure G22) where the user can contact the PCL team to either submit comments or data for incorporation into the database.

Administrative functions in the PCL Calculator web application allow administrator users to add, edit or delete records for chemicals (Figure G13), species (Figure G15), habitats (Figures G17 and G18), PCL concentrations (Figure G14), surrogate assignments (Figure G16) and users (Figure G19). The “User Login Report” (Figure G21) and “View PCL Comments” (Figure G23) screens are also accessible to administrative users. As mentioned previously, the “Pending Users Report” (Figure G20) provides a mechanism for activating user accounts.

3. TECHNICAL DESCRIPTION

Several initial architecture and design approaches for the application were considered including a stand-alone desktop application and a web-based application. The stand-alone application has several advantages to recommend its adoption such as a “richer development environment with ready access to features for designing and creating a more powerful, yet easy to use, user interface. (Anderson, Jafar and Rogers, 2010)” However, when the frequency of data updates was considered, the web-application was determined to have a decided advantage over the stand-alone application from a data update and code maintenance standpoint with a single repository for data and a single application server. The decision was made to develop the PCL with a web-based architecture to be implemented on a Tomcat web server using Java Server Pages (JSP) supported by a few Java servlets to do the heavy lifting.

Initially only the calculator page itself was developed as a proof of concept. Successful development of the prototype system was accomplished by the team of Russell Anderson, Musa Jafar and William Rogers as described in the article “Superfund Site Analysis Using Web 2.0 Technologies” (Anderson, Jafar and Rogers, 2010) and in 2010 was presented to the working group at the Texas Commission on Environmental Quality (TCEQ), the sponsor for the project. Continued sponsorship of the PCL allowed the development team to expand the prototype in 2011 into a robust web application through the inclusion of chemical, species and habitat list pages, identification of user roles and implementation of user id and role maintenance functions. As the TCEQ working group continued to request revisions that would refine the functions of the calculator and the availability of specific functions based upon user role. To date, 3 roles have been established, Administrator, Registered User and Guest.

Under the Guest role a user can view the Chemical, Species and Habitat lists and generate a PCL calculator page based upon the selection of Habitat, COC and PCL Type(s). The Guest can modify values on the calculator page. Registered Users have the rights granted to Guests, but can also print or export the calculator results to an Excel spreadsheet. Users with the Administrator role are either members of the WT development team or TCEQ officials. Options available to Administrator users include all of those available to Registered users and the ability to edit COC, species, habitat, concentration and surrogate assignment data. Administrators can also add, modify or delete user accounts.

CHAPTER V

DISCUSSION

1. TESTING

Testing of the PCL calculator was initially done by installing individual copies of the application on laptops or workstations of the TCEQ working group members. This group is chaired by a member of the TCEQ Ecological Risk Assessment Group and is comprised of ecological risk professionals from federal and state government agencies. Presentations of the PCL were given at the Texas Commission on Environmental Quality Trade Fairs in 2007, 2008, 2012 and 2015, where the audience was solicited "for comments on the usefulness and applicability of the site."(Anderson, Jafar and Rogers, 2010) In total, approximately 1000 conference participants attended the sessions. "The general consensus was that the site provided a valuable and user-friendly risk assessment tool."(Anderson, Jafar and Rogers, 2010) Since 2012 the site has been available to the TCEQ group and selected members of the ecological risk assessment community through a web site established and maintained by West Texas A&M University. In 2015, as TCEQ was finalizing the revisions to the Ecological Risk Assessment Guidelines document, the members of the TCEQ working group were invited to register as users in order to assist TCEQ in validating the accuracy of the ERAG document and the efficacy of the PCL Calculator application. To date, the working group has discovered a few minor discrepancies between the ERAG and the PCL. All known issues have been resolved. The version currently on the web application server is PCL 1.7.

2. FUTURE DEVELOPMENT

The development of additional functionality in the PCL Calculator application has been considered. One such development would be a function that would allow submission of additional COCs, receptor species, PCL concentration and surrogate assignment data based upon new research or field observations from the community of ecological risk assessors. When complete, this function will allow submission of data and provide a mechanism for the administrators of the system to review and approve the submitted data for addition to the PCL database. This process has been inspired by the functionality of the GenBank web site for the collection of DNA sequences (NCBI 2013). Other possibilities include the design and implementation of an interface to a GIS mapping application which could allow ecological risk assessors to prepare contamination site maps tied directly to the risk assessment, data driven dynamic generation of the species uptake, and tox profile documentation as a replacement for the current pdf files and dynamic generation of complete, validated risk assessment documentation.

3. CONCLUSION

Automation of the ecological risk assessment process in conjunction with the compilation of peer reviewed current research documents has been a goal of the ecological risk assessment profession and the governmental agencies responsible for evaluation and approval of ecological risk assessments for decades. Attempts to provide data useful to ecological risk assessors by numerous academic and governmental agencies have been met with varying degrees of success, however in each case, the attempt fell short due to the difficulty in providing a model that is precise enough to satisfy regulators and yet flexible enough to allow for site variations and consistently accurate enough to provide useful results.

The Protective Concentration Level calculator application represents an innovative, comprehensive, accurate and accepted methodology for achieving remarkable increases in the productivity of professionals and government agencies that constitute the Community of Ecological Risk Assessors. With the continued support of the TCEQ, the Environmental Sciences Department at West Texas A&M University will continue to refine the process, data and supporting research documentation that is available from the PCL application.

Although the PCL database is specific to the habitats found in the state of Texas, the design is flexible enough to be applicable to any state, federal or even international entity with a minimum amount of fine tuning. In fact, several states, the United States Environmental Protection Agency and other federal agencies have expressed interest in the PCL Calculator providing a potential avenue of expansion for the application.

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APPENDIX A

CHEMICALS OF CONCERN

CAS	Chemical Name
79-34-5	1,1,2,2-TETRACHLOROETHANE
75-34-3	1,1-DICHLOROETHANE
120-82-1	1,2,4-TRICHLOROBENZENE
95-50-1	1,2-DICHLOROBENZENE
107-06-2	1,2-DICHLOROETHANE
540-59-0	1,2-DICHLOROETHENE
99-35-4	1,3,5-TRINITROBENZENE (TNB)
106-46-7	1,4-DICHLOROBENZENE
118-96-7	2,4,6-TRINITROTOLUENE (TNT)
121-14-2	2,4-DINITROTOLUENE
35572-78-2	2-AMINO-4,6-DINITROTOLUENE
19406-51-0	4-AMINO-2,6-DINITROTOLUENE (4-AM-DNT)
67-64-1	ACETONE
309-00-2	ALDRIN
84-65-1	ANTHRAQUINONE
7440-36-0	ANTIMONY
12672-29-6	AROCLOR 1248
11097-69-1	AROCLOR 1254
11096-82-5	AROCLOR 1260
7440-38-2	ARSENIC
22541-54-4	ARSENIC (AS ARSENIC III)
7440-39-3	BARIUM
71-43-2	BENZENE
7440-41-7	BERYLLIUM
92-52-4	BIPHENYL, 1-1
117-81-7	BIS(2-ETHYLHEXYL) PHTHALATE (DEHP)
85-68-7	BUTYL BENZYL PHTHALATE
7440-43-9	CADMIUM
75-15-0	CARBON DISULFIDE

CAS	Chemical Name
57-74-9	CHLORDANE
7647-14-5	CHLORIDE (AS SODIUM CHLORIDE)
67-66-3	CHLOROFORM
18540-29-9	CHROMIUM, HEXAVALENT
7440-47-3	CHROMIUM, TOTAL
16065-83-1	CHROMIUM, TRIVALENT
7440-48-4	COBALT
7440-50-8	COPPER
172306-86-4	COREXIT 9500
CAS	Chemical Name
60617-06-3	COREXIT 9527
57-12-5	CYANIDE
108-94-1	CYCLOHEXANONE
50-29-3	DDT AND METABOLITES
319-86-8	DELTA-HCH (DELTA-HEXACHLOROCYCLOHEXANE)
84-74-2	DI-N-BUTYL PHTHALATE
117-84-0	DI-N-OCTYL PHTHALATE
132-64-9	DIBENZOFURAN
60-57-1	DIELDRIN
84-66-2	DIETHYL PHTHALATE
131-11-3	DIMETHYL PHTHALATE
1746-01-6	DIOXINS AND FURANS (AS 2,3,7,8-TCDD TEQs)
115-29-7	ENDOSULFAN
72-20-8	ENDRIN
7421-93-4	ENDRIN ALDEHYDE
53494-70-5	ENDRIN KETONE
100-41-4	ETHYL BENZENE
7782-41-4	FLOURIDE
58-89-9	GAMMA-HCH (LINDANE)
76-44-8	HEPTACHLOR
118-74-1	HEXACHLOROBENZENE
2691-41-0	HMX (OCTAHYDRO-1,3,5,7-TETRANITRO-1,3,5,7-TETRAZOCINE)
67-63-0	ISOPROPANOL (ISOPROPYL ALCOHOL OR 2-PROPANOL)
7439-92-1(T)	LEAD (TOTAL)
7439-96-5	MANGANESE
7439-97-6	MERCURY (TOTAL INORGANIC)
78-93-3	METHYL ETHYL KETONE

CAS	Chemical Name
108-87-2	METHYLCYCLOHEXANE
75-09-2	METHYLENE CHLORIDE(DICHLOROMETHANE)
22967-92-6	METHYLMERCURY
110-54-3	N-HEXANE
91-20-3	NAPHTHALENE
7440-02-0	NICKEL
98-95-3	NITROBENZENE
29082-74-4	OCTACHLOROSTYRENE
106-44-5	P-CRESOL
87-86-5	PENTACHLOROPHENOL
014797-73-0	PERCHLORATE
108-95-2	PHENOL
7723-14-0	PHOSPHORUS, TOTAL (AS P)
1336-36-3(D)	POLYCHLORINATED BIPHENYLS (PCBs), DIOXIN-LIKE (AS 2,3,7,8-TCDD TEQs)
1336-36-3	POLYCHLORINATED BIPHENYLS (PCBs), TOTAL
130498-29-2	POLYCYCLIC AROMATIC HYDROCARBONS, TOTAL
130498-29-2(HMW)	POLYCYCLIC AROMATIC HYDROCARBONS-HIGH MOLECULAR WEIGHT
130498-29-2(LMW)	POLYCYCLIC AROMATIC HYDROCARBONS-LOW MOLECULAR WEIGHT
7757-79-1	POTASSIUM NITRATE
121-82-4	RDX (HEXAHYDRO-1,3,5-TRINITRO-1,3,5-TRIAZINE OR CYCLONITE)
7782-49-2	SELENIUM
7440-22-4	SILVER
7440-24-6	STRONTIUM
100-42-5	STYRENE
7757-82-6	SULFATE AS SO4 (AS SODIUM SULFATE)
608-73-1	TECHNICAL HEXACHLOROCYCLOHEXANE (t-HCH)
127-18-4	TETRACHLOROETHYLENE
479-45-8	TETRYL
7440-28-0	THALLIUM
108-88-3	TOLUENE
8001-35-2	TOXAPHENE
688-73-3	TRIBUTYLTIN
79-01-6	TRICHLOROETHYLENE
75-69-4	TRICHLOROFLUOROMETHANE

CAS	Chemical Name
88-06-2	TRICHLOROPHENOL, 2,4,6-
7440-61-1	URANIUM, TOTAL
7440-62-2	VANADIUM
75-01-4	VINYL CHLORIDE
1330-20-7	XYLENES, TOTAL
7440-66-6	ZINC

APPENDIX B

RECEPTOR SPECIES

Species Name (scientific name)	Class Name	Species Type	Soil Type
AMERICAN CLAWED FROG (Xenopus laevis)	AMPHIBIAN	CM	TR
BARRED TIGER SALAMANDER (Ambystoma mavortium)	AMPHIBIAN	CM	TR
CENTRAL NEWT (Notophthalmus viridescens louisianensis)	AMPHIBIAN	CM	TR
LEOPARD FROG (*Lithobates* *sp.)*	AMPHIBIAN	CM	AQ
WOODHOUSE TOAD (Anaxyrus woodhousii)	AMPHIBIAN	CM	TR
AMERICAN KESTREL (Falco sparverius)	BIRD	CM	AQ
AMERICAN ROBIN (Turdus migratorius)	BIRD	CM	TR
AMERICAN WIGEON (Anas americana)	BIRD	CM	TR
AMERICAN WOODCOCK (Scolopax minor)	BIRD	CM	TR
BALD EAGLE (Haliaeetus leucocephalus)	BIRD	TE	AQ
BARN OWL (Tyto alba)	BIRD	CM	TR
BARN SWALLOW (Hirundo rustica)	BIRD	CM	TR
BELTED KINGFISHER (Megaceryle alcyon)	BIRD	CM	AQ
BEWICK S WREN (Thryomanes bewickii)	BIRD	CM	TR
BLACK CAPPED VIREO (Vireo atricapilla)	BIRD	TE	TR
BLACK CROWNED NIGHT HERON (Nycticorax nycticorax)	BIRD	CM	AQ
BLACK DUCK (Anas rubripes)	BIRD	CM	TR
BOBWHITE QUAIL (Colinus virginianus)	BIRD	CM	TR
BURROWING OWL (Athene cunicularia)	BIRD	CM	TR
CANADA GOOSE (Branta Canadensis)	BIRD	CM	AQ
COMMON YELLOW THROAT(Geothlypis trichas)	BIRD	CM	TR
COOPERS HAWK (Accipiter cooperii)	BIRD	CM	TR
CORMORANT (Phalacrocoracidae)	BIRD	CM	AQ
EASTERN LEAST TERN (Sternula antillarum)	BIRD	CM	AQ
GOLDEN CHEEKED WARBLER (Setophaga chrysoparia)	BIRD	TE	TR
GRAY PARTRIDGE (Perdix perdix)	BIRD	CM	TR

Species Name (scientific name)	Class Name	Species Type	Soil Type
GREEN HERON (Butorides virescens)	BIRD	CM	AQ
HORNED LARK (Eremophila alpestris)	BIRD	CM	TR
HOUSE FINCH (Haemorhous mexicanus)	BIRD	CM	TR
HOUSE SPARROW (Passer domesticus)	BIRD	CM	TR
INTERIOR LEAST TERN (Sterna antillarum athalassos)	BIRD	TE	AQ
KILLDEER (Charadrius vociferous)	BIRD	CM	TR
LARK SPARROW (Chondestes grammacus)	BIRD	CM	TR
MALLARD (Anas platyrhynchos)	BIRD	CM	AQ
MARSH WREN (Cistothorus palustris)	BIRD	CM	AQ
MEADOWLARK (Sturnella sp.)	BIRD	CM	TR
MOURNING DOVE (Zenaida macroura)	BIRD	CM	TR
NORTHERN HARRIER (Circus cyaneus)	BIRD	CM	TR
OSPREY (Pandion haliaetus)	BIRD	CM	AQ
RED WINGED BLACKBIRD (Agelaius phoeniceus)	BIRD	CM	AQ
RED-TAILED HAWK (Buteo jamaicensis)	BIRD	CM	TR
REDDISH EGRET (Egretta rufescens)	BIRD	TE	AQ
RING BILLED GULL (Larus delawarensis)	BIRD	CM	AQ
RING-NECKED PHEASANT (Phasianus colchicus)	BIRD	CM	TR
SANDHILL CRANE (Grus Canadensis)	BIRD	CM	TR
SCALED QUAIL (Callipepla squamata)	BIRD	CM	TR
SNOW GOOSE (Chen caerulescens)	BIRD	CM	AQ
SNOWY EGRET (Egretta thula)	BIRD	CM	AQ
SPOTTED SANDPIPER (Actitis macularius)	BIRD	CM	AQ
WESTERN KINGBIRD (Tyrannus verticalis)	BIRD	CM	TR
WHITE FACED IBIS (Plegadis chihi)	BIRD	TE	AQ
WHOOPING CRANE (Grus Americana)	BIRD	TE	AQ
YELLOW CROWNED NIGHT HERON (Nyctanassa violacea)	BIRD	CM	AQ
AMERICAN MINK (Neovison vison)	MAMMAL	CM	AQ
BLACK TAILED JACK RABBIT (Lepus californicus)	MAMMAL	CM	TR
BLACK TAILED PRAIRIE DOG (Cynomys ludovicianus)	MAMMAL	CM	TR
BOBCAT (Lynx rufus)	MAMMAL	CM	TR
COTTON MOUSE (Peromyscus gossypinus)	MAMMAL	CM	TR
COYOTE (Canis latrans)	MAMMAL	CM	TR
DEER MOUSE (Peromyscus sp.)	MAMMAL	CM	TR
DESERT SHREW (Notiosorex crawfordi)	MAMMAL	CM	TR

Species Name (scientific name)	Class Name	Species Type	Soil Type
EASTERN COTTONTAIL (Sylvilagus floridanus)	MAMMAL	CM	TR
HISPID COTTON RAT (Sigmodon hispidus)	MAMMAL	CM	TR
LEAST SHREW (Cryptotis parva)	MAMMAL	CM	TR
LITTLE BROWN BAT (Myotis lucifugus)	MAMMAL	CM	TR
LONG TAILED WEASEL (Mustela frenata)	MAMMAL	CM	TR
MARSH RICE RAT (Oryzomys palustris)	MAMMAL	CM	AQ
MEADOW VOLE (Microtus pennsylvanicus)	MAMMAL	CM	TR
MEXICAN FREE-TAILED BAT (Tadarida brasiliensis)	MAMMAL	CM	TR
MULE DEER (Odocoileus hemionus)	MAMMAL	CM	TR
MUSKRAT (Ondatra zibethicus)	MAMMAL	CM	AQ
NINE-BANDED ARMADILLO (Dasypus novemcinctus)	MAMMAL	CM	TR
RACCOON-SEMI-AQUATIC (Procyon lotor)	MAMMAL	CM	AQ
RACCOON-TERRESTRIAL (Procyon lotor)	MAMMAL	CM	TR
RAFINESQUES BIG EARED BAT (Corynorhinus rafinesquii)	MAMMAL	TE	TR
RED FOX (Vulpes vulpes)	MAMMAL	CM	TR
SOUTHERN SHORT-TAILED SHREW (Blarina carolinensis)	MAMMAL	CM	TR
STRIPED SKUNK (Mephitis mephitis)	MAMMAL	CM	TR
SWAMP RABBIT (Sylvilagus aquaticus)	MAMMAL	CM	AQ
THIRTEEN-LINED GROUND SQUIRREL (Ictidomys tridecemlineatus)	MAMMAL	CM	TR
WHITE FOOTED MOUSE (Peromyscus leucopus)	MAMMAL	CM	TR
AMERICAN ALLIGATOR (Alligator mississippiensis)	REPTILE	CM	AQ
BULL SNAKE (Pituophis catenifer sayi)	REPTILE	CM	TR
COTTONMOUTH WATER MOCASSIN (Agkistrodon piscivorus)	REPTILE	CM	AQ
DESERT SIDE BLOTCHED LIZARD (Uta stansburiana)	REPTILE	CM	TR
DIAMONDBACK TERRAPIN (Malaclemys terrapin)	REPTILE	CM	AQ
EASTERN BOX TURTLE (Terrapene carolina carolina)	REPTILE	CM	TR
GREEN ANOLE (Anolis carolinensis)	REPTILE	CM	TR
LOGGERHEAD SEA TURTLE (Caretta caretta)	REPTILE	TE	AQ
ORNATE BOX TURTLE (Terrapene ornata ornate)	REPTILE	CM	TR
PLAIN BELLIED WATER SNAKE	REPTILE	CM	AQ

Species Name (scientific name)	Class Name	Species Type	Soil Type
(Nerodia erythrogaster)			
PRAIRIE RATTLE SNAKE (Crotalus viridis)	REPTILE	CM	TR
SIX-LINED RACERUNNER (Aspidoscelis sexlineata)	REPTILE	CM	TR
SNAPPING TURTLE (Chelydra serpentine)	REPTILE	CM	AQ
SOUTHERN COPPERHEAD (Agkistrodon contortrix)	REPTILE	CM	TR
SPINY SOFT SHELL TURTLE (Apalone spinifera)	REPTILE	CM	AQ
TEXAS HORNED LIZARD (Phrynosoma cornutum)	REPTILE	TE	TR
TEXAS RAT SNAKE (Elaphe obsoleta lindheimeri)	REPTILE	CM	TR
TIMBER RATTLESNAKE (Crotalus horridus)	REPTILE	TE	TR
WESTERN COACHWHIP (Masticophis flagellum testaceus)	REPTILE	CM	TR
WESTERN DIAMONDBACK RATTLESNAKE (Crotalus atrox)	REPTILE	CM	TR
WESTERN FENCE LIZARD (Sceloporus occidentalis)	REPTILE	CM	TR
YELLOW MUD TURTLE (Kinosternon flavescens)	REPTILE	CM	AQ

CM = Common Species
TR = Terrestrial
TE = Threatened or Endangered
AQ = Aquatic

APPENDIX C

FOOD WEB DIAGRAMS

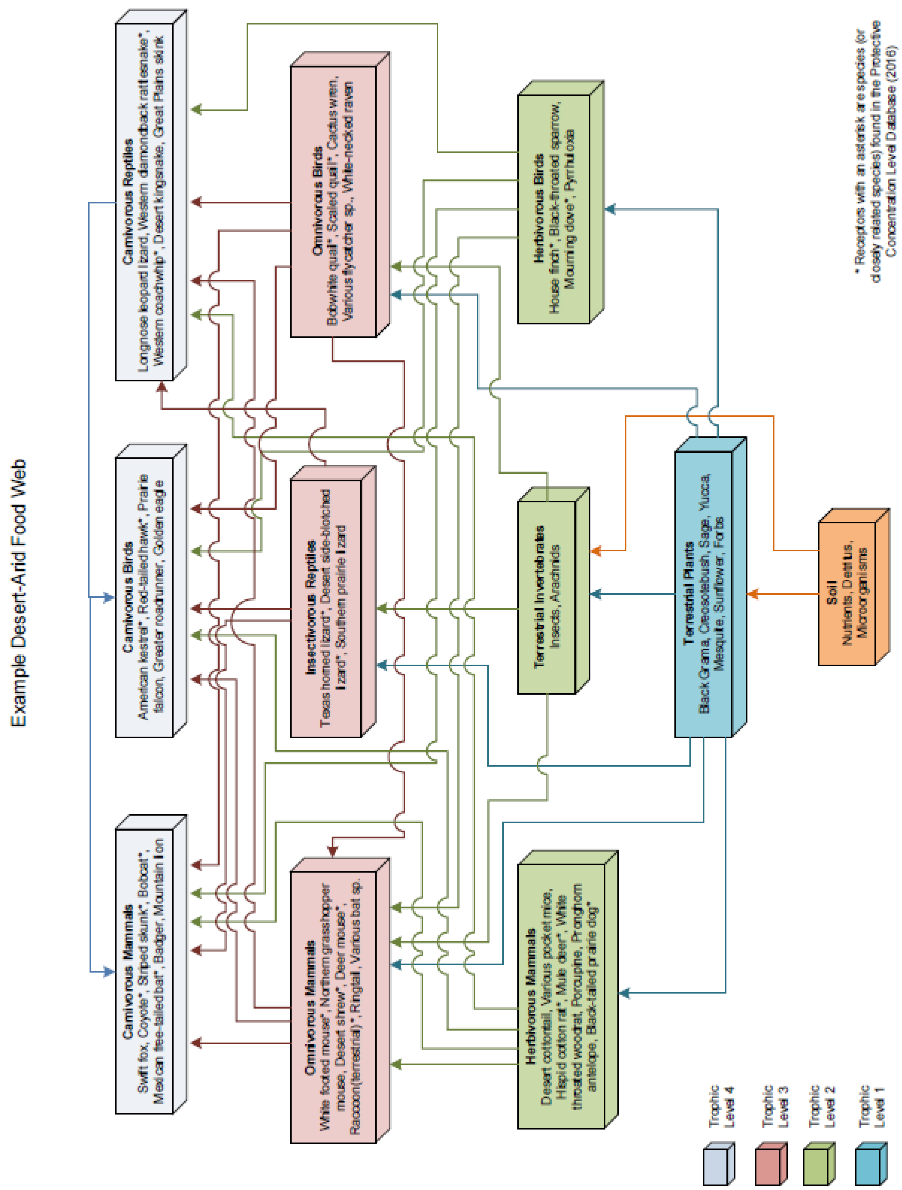

Figure C1 – Desert/Arid Food Web diagram

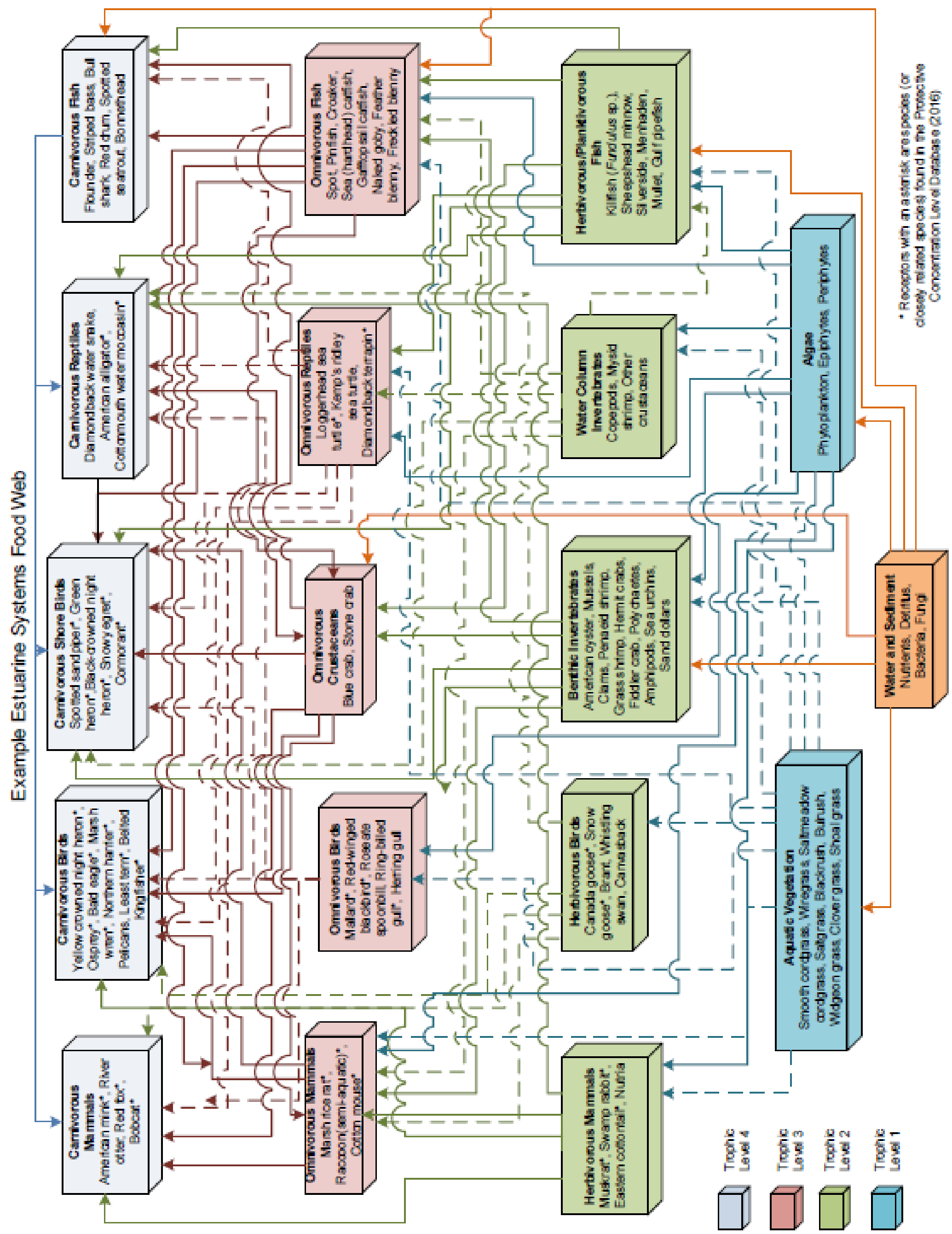

Figure C2 – Estuarine/Wetland Systems Food Web diagram

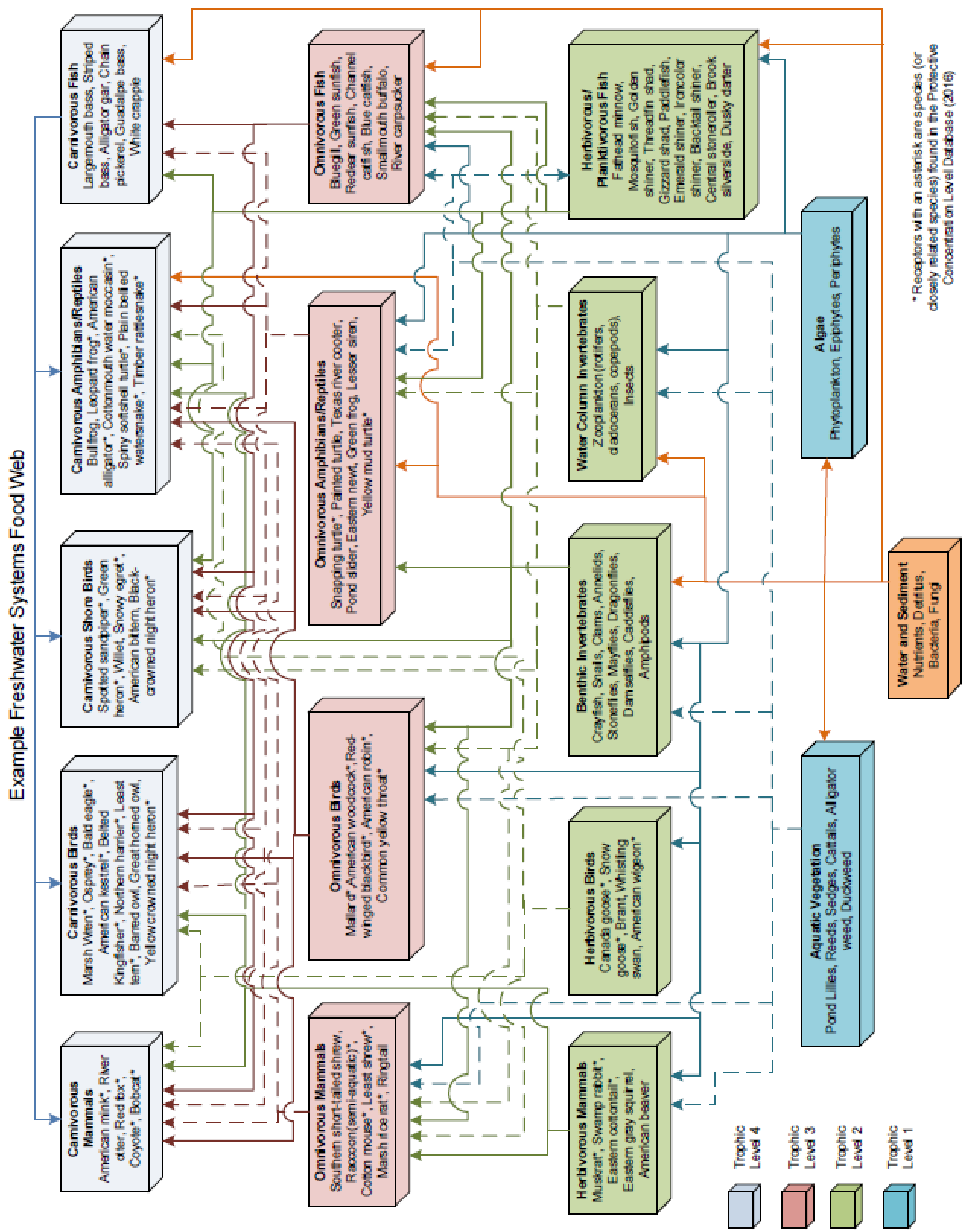

Figure C3 – Freshwater/Wetlands Systems Food Web diagram

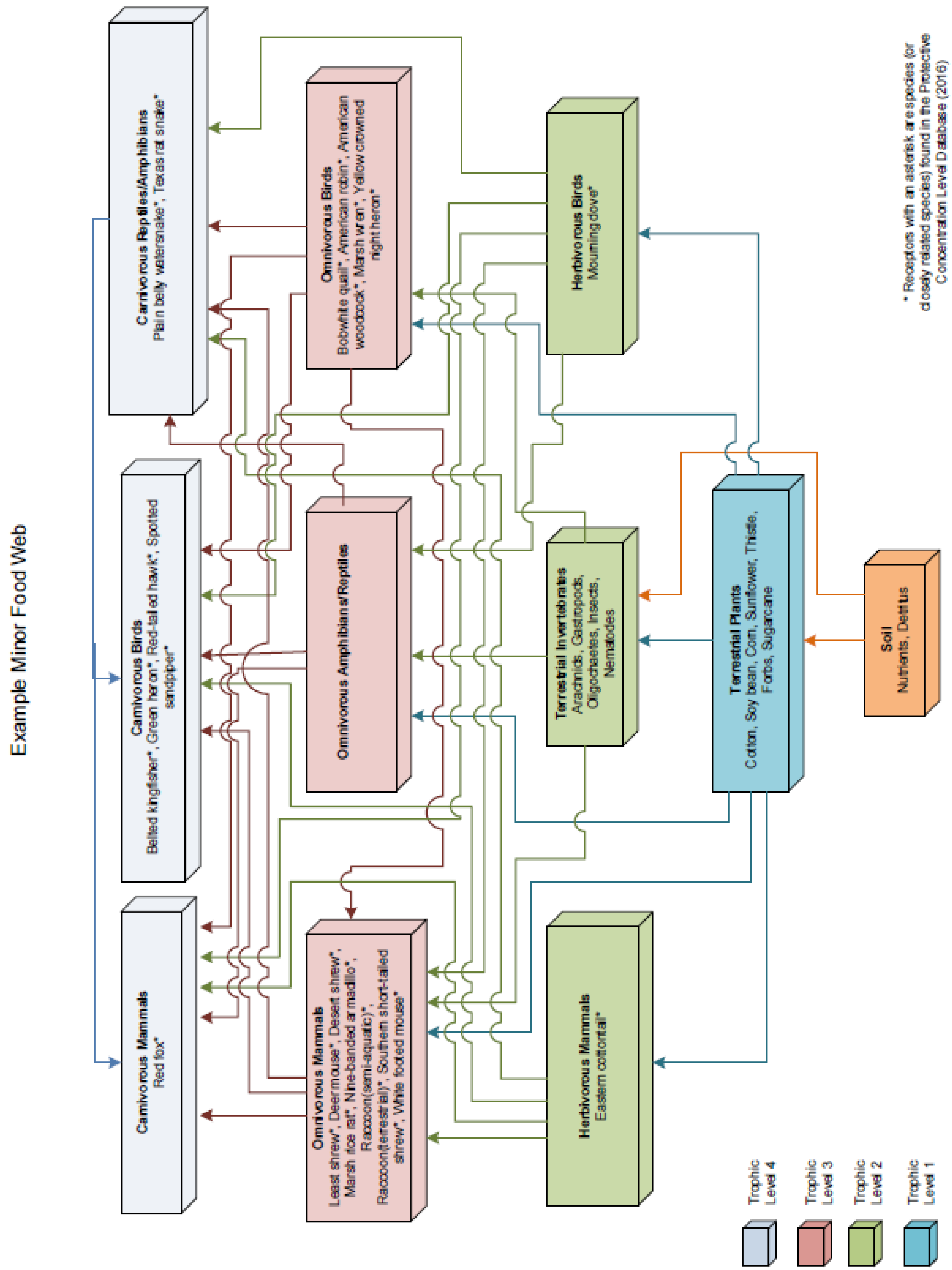

Figure C4 – Minor Food Web diagram

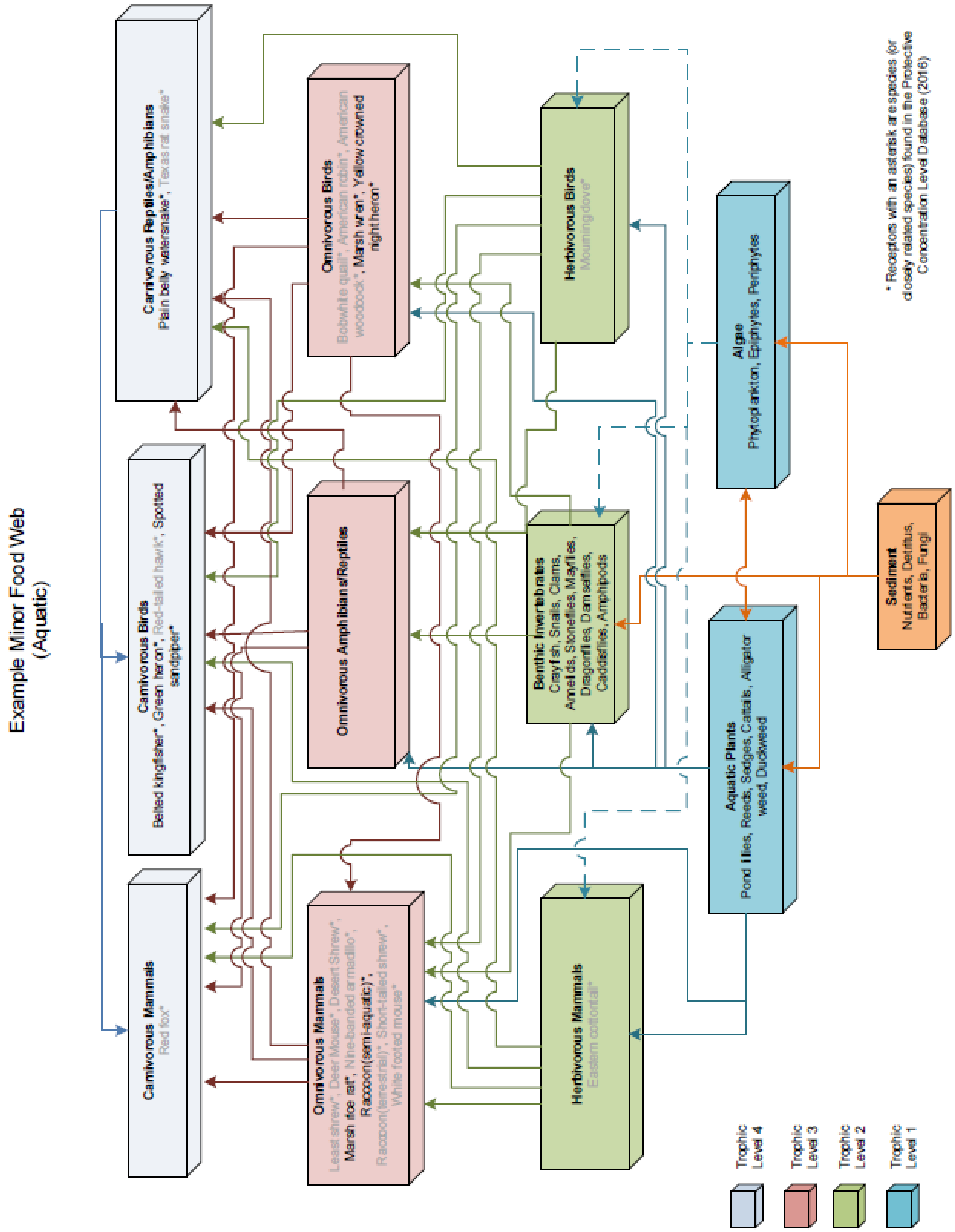

Figure C5 – Minor Food Web (Aquatic) diagram

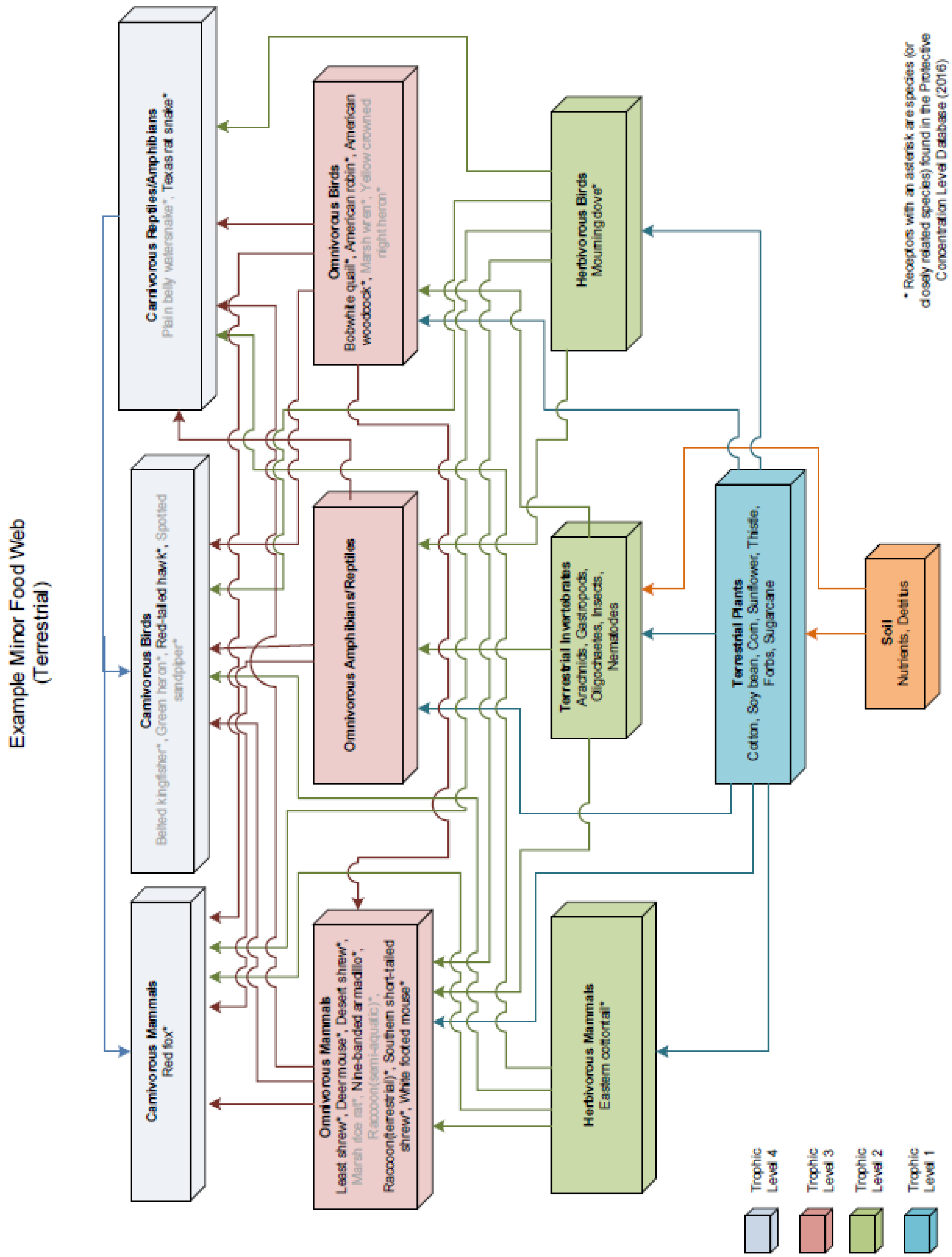

Figure C6 – Minor Food Web (Terrestrial) diagram

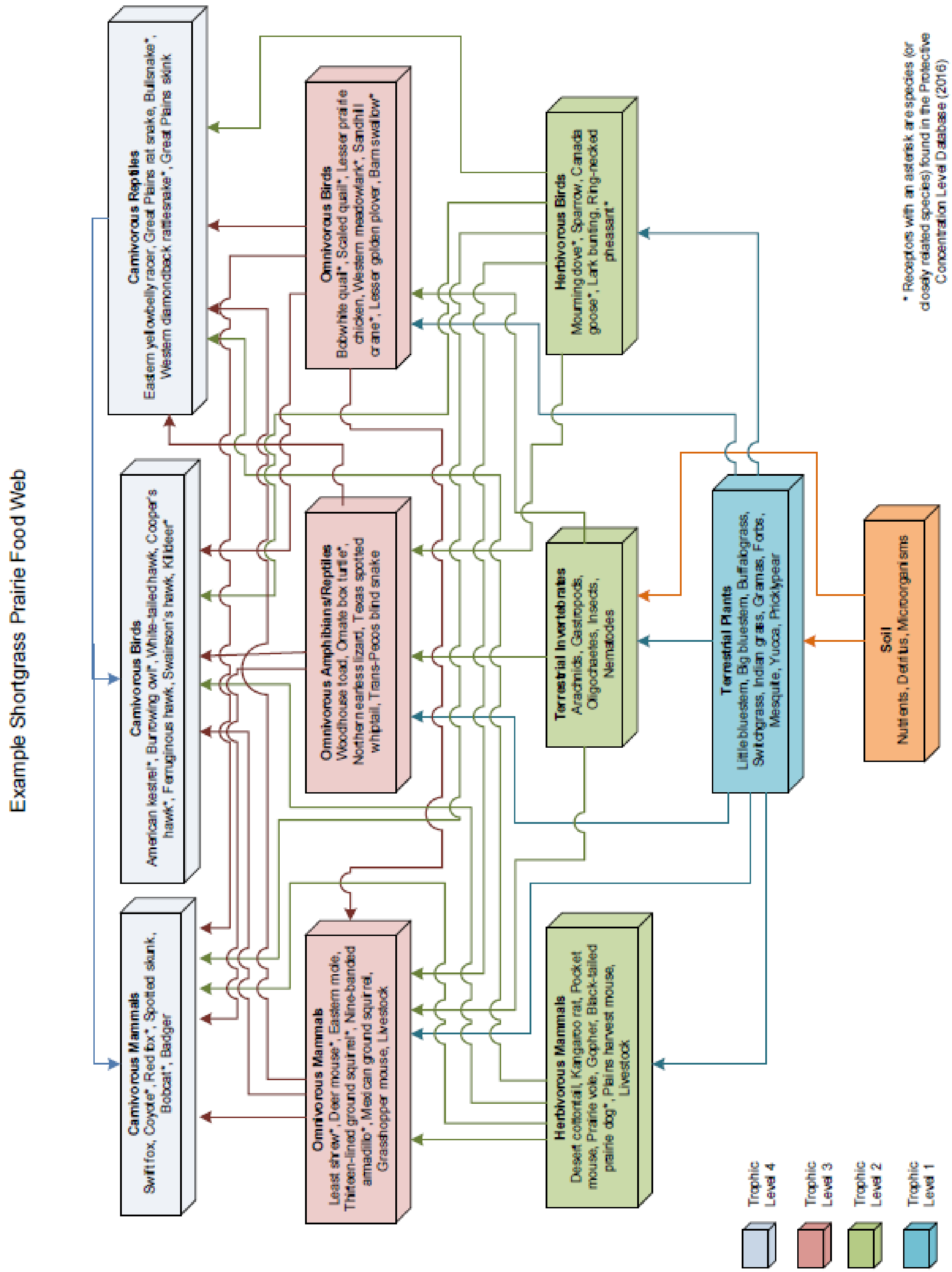

Figure C7 – Shortgrass Prairie Food Web diagram

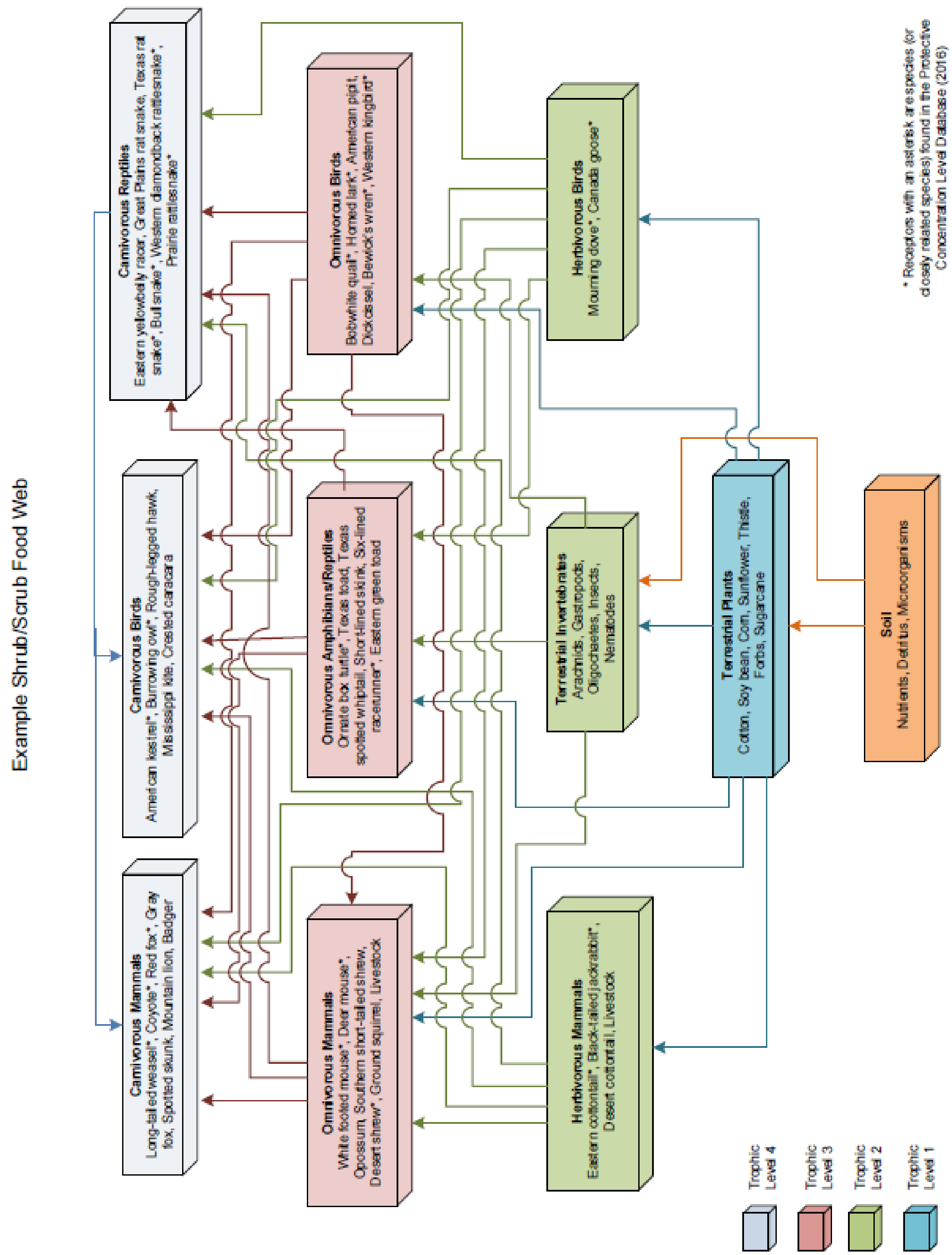

Figure C8 – Shrub/Scrub Food Web diagram

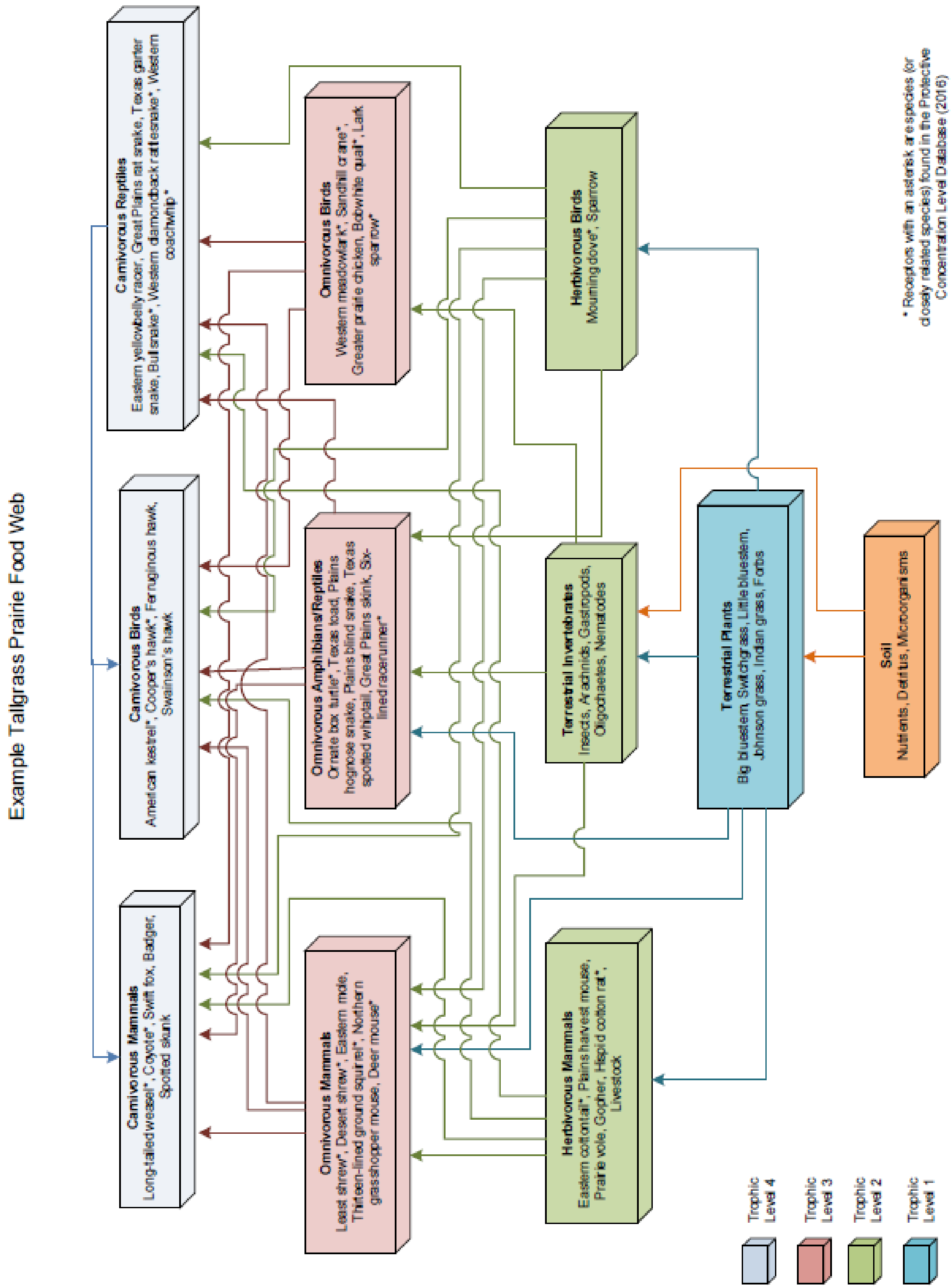

Figure C9 – Tallgrass Prairie Food Web diagram

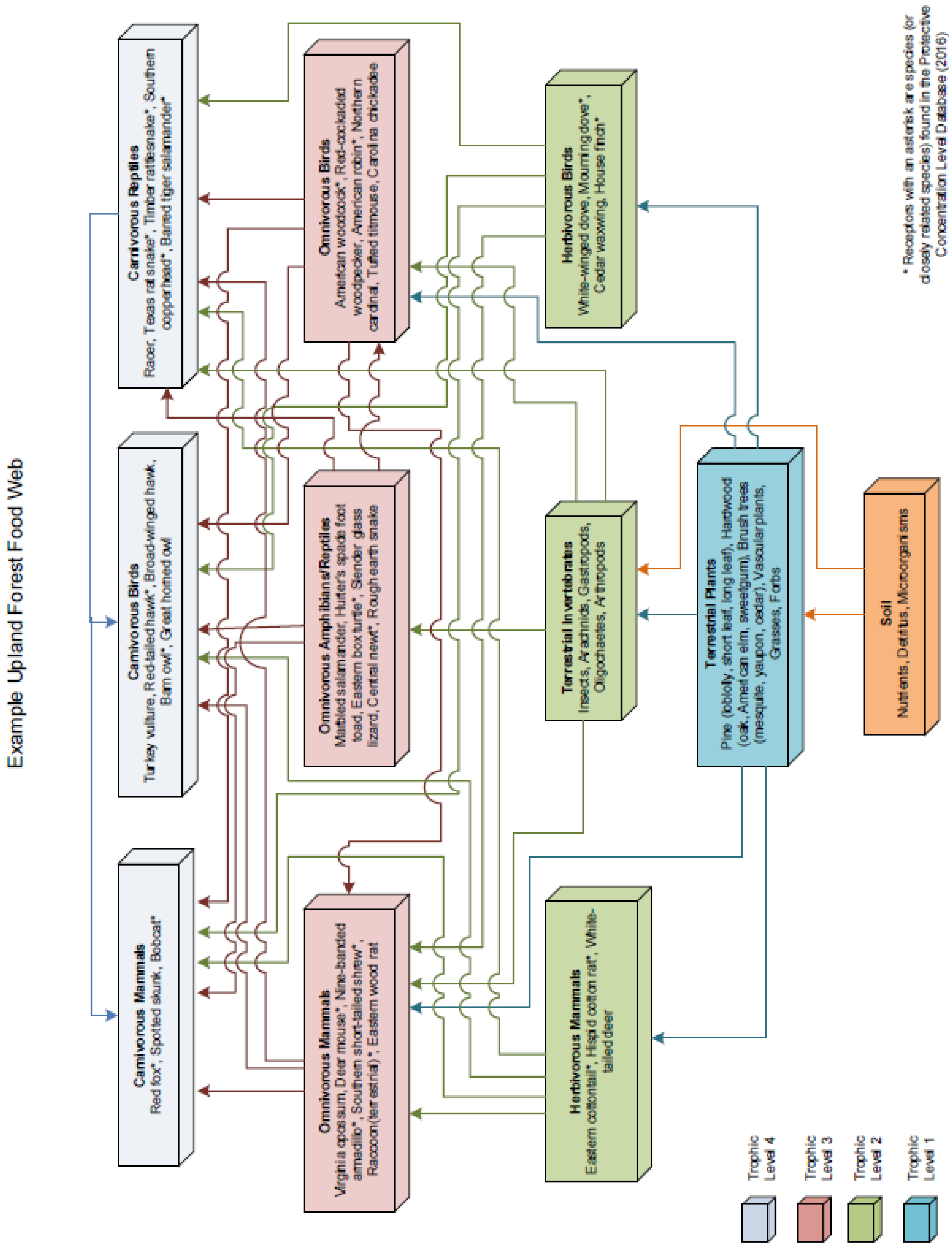

Figure C10 – Upland Forest Food Web diagram

APPENDIX D

EXAMPLE OF SPECIES UPTAKE PROFILE DOCUMENT

Coyote
Canis latrans

Factors	Age/Sex/ Cond./ Season	Mean	Range	Location	Reference
Body Weight (kg)	AM AF AM AF AM	13 11 13 11 13.9	 12-15.3	Iowa Kansas Oklahoma	Sample et al. (1997) from Bekoff (1982) Halloran and Glass (1959)
Home Range (acres)*	AM AF Coyotes in pairs Coyotes in packs	Up to 16,800 Up to 8,900 7,440 3,530			Sample et al. (1997) from Bekoff (1982) Sample et al. (1997) from Bekoff (1982)
Food Ingestion Rate (kg/kg-d)	A A	 0.018 0.0318	0.009-0.011[1] 0.032-0.038[2]	 Desert Calculated	Sample et al. (1997) from Litvaitis and Mautz (1980) Golightly and Omart (1983) Huegel and Rongstad (1985) Nagy (2001) using equation for carnivorous mammals
Water Ingestion Rate (L/kg-d)		0.0766		Calculated using allometric equation	Calder and Braun (1983)
Soil Ingestion Rate (kg/kg-day)		0.000889			Beyer et al. (1994) using surrogate of red fox (2.8% soil in diet)

*Highly variable.

[1]Converted from wet weight to dry weight assuming 68% moisture content of prey (small mammals; Sample et al. 1997).

[2]Authors estimated that coyotes consume 10-12% of their body mass in prey daily (0.1 – 0.12 kg/kg-d fresh wt.); values were converted to dry weight assuming 68% moisture content (Sample et al. 1997).

Dietary composition	Spring	Summer	Fall	Winter	Location/Habitat (measure)	Reference
Mammals	77.1	65	72.2	82.7	Missouri (% volume)	Sample et al. (1997) from Korschgen (1957)
-lagomorphs	48.6	35.2	47.7	58.1		
-livestock	16.5	17.5	7.2	7.6		
-mice and rats	5.4	5.6	9	9.5		
-others	6.6	6.7	8.3	7.5		
Birds	17.7	28	13.2	9		
-poultry	17	27.4	12.8	8.5		
Insects	Trace	1.9	3.5	Trace		
Plants	0.2	0.8	6.5	0.9		
Carrion	5	4.3	4.3	6.6		
Misc.	0	0	0.3	0.8		

Coyote Default Values

Body Weight: 13,000 g (13 kg)
Justification: Mean of literature values.
Home Range: 5,485 acres
Justification: Average of values for coyotes traveling in packs or in pairs (Bekoff 1982).
Food Ingestion Rate: 0.0318 kg/kg-d
Justification: Calculated using Nagy (2001) equation for carnivorous mammals. Value is close to the lower-bound value estimated by Huegel and Rongstad (1985).
Water Ingestion Rate: 0.0766 L/kg-d
Justification: Calculated using Calder and Braun (1983).
Soil Ingestion Rate: 0.000889 kg/kg-d
Justification: No empirical data was available for the coyote, so the red fox was used as a surrogate (2.8% soil in diet; Beyer et al. 1994).
Dietary Composition: 100% carnivorous (some plant matter ingested but considered insignificant for modeling purposes [i.e., <5%]).

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Sample BE, MS Aplin, RA Efroymson, GW Suter II, CJE Welsh (1997) Methods and Tools for Estimation of the Exposure of Terrestrial Wildlife to COCs. ORNL/TM_13391. Office of Environmental Policy and Assistance, U. S. Department of Energy. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

APPENDIX E

EXAMPLE OF CAS PROFILE DOCUMENT

FATE AND TRANSPORT/TOXICOLOGICAL PROFILE FOR COBALT

CASRN: 7440-48-4

Texas median soil background concentration is 7 mg/kg (TCEQ 2009). If PCL for soil is below 7 mg/kg, default to this value.

Environmental Fate and Transport (all data from HSDB (2012) unless otherwise noted)

Sources

Cobalt is used in galvanic plating, in the manufacture of tungsten-carbide alloys, in animal feed supplements, and in the production of china and glass (McNeely et al., 1979). Cobalt, in its salt form, is used in nuclear technologies. Radioactive cobalt-60 is used in gamma ray therapy, which has a wide variety of medical applications, for sterilization and preservation, and for water treatment (Hall and Rumack, 1998). Cobalt and cobalt compounds have expanded from use as colorants in glasses and ground coat frits for pottery to drying agents in paints and lacquers, animal and human nutrients, electroplating materials, high temperature alloys, hardfacing alloys, high speed tools, magnetic alloys, alloys used for prosthetics, and uses in radiology. Cobalt is also used as a catalyst for hydrocarbon refining from crude oil for the synthesis of heating fuels. [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V6: 761 (1993)]

Transport and Fate

TERRESTRIAL FATE: Soils with higher pH and contents of clay, natural organics, and hydrous manganese and iron oxides, bind cobalt to a greater degree; as these factors decrease, the mobility of cobalt increases(1). Chelating agents, which are compounds that bind metal ion (i.e., ethylenediamine tetraacetic acid, EDTA), increase the solubility of cobalt and enhance mobility of cobalt in soil(1). Sorption of cobalt onto soils was influenced by the presences of clays and hydrous oxides of iron and manganese(2). Studies suggest that Co^{2+} is being incorporated into the hydrous iron oxide by recrystallization(3). Kd values for cobalt range from 0.2 to 3,800 ml/g(4). Mean Freundlich and n values were 37 liters/kg and 0.754, respectively, in eleven US soils;

Freundlich values ranged from 2.6 to 363 liters/kg and correlated with soil pH and cation exchange capacity(5). In 13 soils from the southeastern US with soil pH's ranging from 3.9 to 6.5, cobalt sorption ranged from 15 to 93%; soil pH explained 84 to 95% of the variation in sorbed cobalt(6). Cobalt compounds would not volatilize from moist or dry soil surfaces, due to their ionic character(SRC).

[(1) Smith IC, Carson BL; pp. 531-62 in the Environment 6 - Cobalt. Ann Arbor, MI: Ann Arbor Sci Pub (1981) (2) Anderson PR, Christensen TH; J Soil Sci 39: 15-22 (1988) (3) Ainsworth CC et al; Soil Sci Soc Am J 58: 1615-23 (1994) (4) Baes CF, Sharp RD; J Environ Qual 12: 17-28 (1983) (5) Buchter B et al; Soil Sci 148: 370-9 (1989) (6) King LD; J Environ Qual 17: 239-46 (1988)]

AQUATIC FATE: The transport and speciation of cobalt in natural waters and sediments is complicated by many factors(1). Anthropogenic pollution appears to enhance the solubility of cobalt in freshwater by forming complexes with the sewage-derived organics(1). The predominate cobalt species in unpolluted freshwater are: Co^{2+}, the carbonate, hydroxide, sulfate, adsorbed forms, oxide coatings, and crystalline sediments(1). In seawater the cobalt species are: $CoCl^{+}$, Co^{2+}, the carbonate and sulfate(1). In aqueous solution, in the absence of complexing agents, the oxidation of the hexaaquacobalt(II) ion to Co(III) is very unfavorable(2). In the presence of complexing agents, such as ammonia which forms very stable complexes with Co(III), the stability of Co(III) is improved(2). Co(III) is inert to ligand exchange relative to Co(II)(2). Cobalt exists in the +2 or +3 oxidation state for the majority of its compounds and complexes(3).

[(1) Smith IC, Carson BL; pp. 1-62, 531-62 in the Environment 6 - Cobalt. Ann Arbor, MI: Ann Arbor Sci Pub (1981) (2) Cotton FA et al; pp. 814-835 Advanced Inorganic Chemistry 6th ed. NY, NY: John Wiley and Sons (1999) (3) Richardson HW; Kirk-Othmer Encycl Chem Tech. 4th ed. NY, NY: John Wiley and Sons 6: 778-93 (1993) (4) Gonsior SJ et al; J Environ Qual 26: 957-66 (1997)]

Speciations and Bioavailability

In lower aquatic organisms (i.e., algae and invertebrates) cobalt attains high concentration factors, but the concentrations factors are generally decrease as the higher trophic levels are reached(1). Concentration factors for marine and freshwater fish range from 100 to 4,000 and 40 to 1,000, respectively(1). According to a classification scheme(2), bioconcentration factors <30 are low and from 100-1,000 are high.

[(1) Smith IC, Carson BL; pp. 1-62, 531-62 in the Environment 6 - Cobalt. Ann Arbor, MI: Ann Arbor Sci Pub (1981)]

Toxicological Profile

Summary

Bioaccumulation in the food chain is important in assessing the human exposure to cobalt from the consumption of food. Data are available that indicate that cobalt is not taken up appreciably by plants and does not biomagnify up the food chain. [(Baudin and Fritsch 1987; Baudin et al. 1990; Boikat et al. 1985; Francis et al. 1985; Kloke et al.

1984; Lux et al. 1995; Mascanzoni 1989; Mejstrik and Svacha 1988; Mermut et al. 1996; Palko and Yli-Hala 1988; Smith and Carson 1981; Tolle et al. 1983; Watabe et al. 1984). (ATSDR 2004)]

Plants

The average cobalt concentration for major plant families on the ultrabasic rocks of South Chukotka, an arctic ecosystem in Russia, ranged from <1 to 9.2 ppm(1). Average cobalt concentrations (ug/g) in vegetation collected in Jun and Nov 1988 from Vulcano and Stromboli, two active volcanoes of the Aeolian Islands, Italy, ranged from 0.031-0.057 (*Pinus* sp. needles), 0.025-0.077 (*Spartium junceum*), and 0.055-0.074 (*Genista ephedroides*)(2). Cobalt concentrations in plants ashed at 450 deg C from the Famatina Range (La Rioja, Argentina) ranged from 0.09 to 11.19 ug/g(3). Mean concentrations of cobalt in two seaweeds, *Enteromorpha linza* and *Ulva rigida*, collected in 1982 from Thermaikos Gulf, Greece, a gulf into which industrial waste and sewage is poured, were 0.28 (0.14-0.62) and 0.28 (0.15-0.71) ug/g dry weight, respectively(4). Cobalt concentration in algae collected in 1993/94 from Carouse Lake, Tarn Flat Lake, and Inexpressible Island Lake in Antarctica were 12.5, 13.2, and 19.0 mg/kg dry weight, respectively(5). The mean cobalt concentrations in mushrooms collected in primary forests of Latin America was 10.57 (0.21-148.00) ppm dry weight(6). Cobalt concentrations ranged from 0.050-3.470 mg/kg in 50 medicinally important leafy materials(7).
[(1) Alexeeva-Popova NV et al; Sci Total Environ 160/161: 643-52 (1995) (2) Bargagli R, Barghigiani C et al; Sci Total Environ 102: 209-22 (1991) (3) Fernandez-Turiel JL et al; Environ Int 21: 807-20 (1995) (4) Haritonidis S, Malea P; Environ Pollut 89: 317-27 (1995) (5) Mentasti E et al; Int J Environ Anal Chem 71: 245-55 (1998) (6) Michelot D et al; Arch Environ Contam Toxicol 36: 256-63 (1999) (7) Reddy PRK, Reddy SJ; Chemosphere 34: 2193-212 (1997)]

Vertebrates

Acute Exposure/ Signs of acute poisoning in animals fed cobalt salts consist of diarrhea, loss of appetite, paralysis of hind legs and lowering of body temp prior to death. With high doses, anuria occurred, and with smaller doses, albuminuria /observed in animals fed cobalt salts/. One of immediate signs is cutaneous vasodilation, especially of nose and ear, within 3 min after administration and persisting for about 1 hr. Blood pressure may fall. Microscopically, all organs are congested, with small focal hemorrhages on serosal surfaces and large hemorrhages in liver and adrenals; bones show hyperplastic marrow. Lungs show alveolar thickening; kidneys, tubular degenerative changes. Fibers of myocardium are pale and shrunken and pancreas show degenerative changes. /Cobalt salts/ [Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology]

REF: HSDB (2012) Hazardous Substance Data Bank< http://www.toxnet.nlm.nih.gov>

ATSDR (2012)Agency for Toxic Substance and Disease Registryhttp://www.atsdr.cdc.gov/toxpro2.html

TCEQ Surface Water Quality Benchmarks (SWQB)

All values listed or calculated in micrograms per liter.

Parameter	CASRN	Freshwater Acute	Freshwater Chronic	Saltwater Acute	Saltwater Chronic
Cobalt [7,9]	7440-48-4	45,000	**1,500**	---	---

[7] Chronic value is a surface water benchmark from the TCEQ Ecological Risk Assessment Guidance (RG-263 and updates).

[9] Acute value derived by the TCEQ Water Quality Division, 2003. In-house water quality chronic and acute values derived for wastewater permits and requests from the Office of Waste based on LC_{50} values in accordance with methodology defined in the TSWQS.

Default SWQB is equal to the freshwater chronic value (1.5 mg/L).

Bioaccumulation Factors (BAFs) for Cobalt

Pathway	Median BAF (range)	Species	Location/Soil or Sediment	Extraction/ Analytical Method	Exposure Duration	Reference
Soil-to-plant	**0.00745** (0.00192-0.0446)	Various, mostly crops and grasses (n=28)	Field/Various soils	Various	Varies – most BAFs from field collected samples	Bechtel Jacobs (1998), App. D, Table D-1
Soil-to-earthworm	**0.122** (0.031-0.321)	Various (n=17)	Various	Various	Various	Sample et al. (1998a), App. C, Table C.1
Soil-to-arthropod	**0.00657** (0.00268 – 0.0375)	Various (n=30)	Oklahoma/NR	NR	N/A – field	USACHPPM (2004) Appendix B
Soil-to-mammal	**0.0205** (0.0101-0.18) 0.021 (0.0134-0.18) 0.0158 (0.0101-0.025)	General (15) Herbivore (10) Omnivore (5)	Field/Various soils	Various	Various	Sample et al. (1998b) Table 7
Sediment-to-benthic invertebrates	**0.300**	N/A	N/A	N/A	N/A	Geometric mean value for inorganics
Sediment-to-fish	**0.171**	N/A	N/A	N/A	N/A	Geometric mean value for inorganics

Cobalt Default Values

Soil-to-plant: 0.00745
Justification: Median value from Bechtel-Jacobs (1998a) post-validation dataset (includes 28 observations).
Soil-to-earthworm: 0.122
Justification: Median of BAFs (n=17) for earthworms from Sample et al. (1998a) Appendix C Table C.1.
Soil-to-arthropod: 0.00657
Justification: Median of 30 BAFs from the Bartlesville, Oklahoma dataset (USACHPPM 2004).
Soil-to-mammal: 0.0205
Justification: Median of the general soil-to-mammal BAFs (n=15) from Sample et al. (1998b). The weighted average could not be calculated due to a lack of data for insectivorous mammals.
Sediment-to-benthic invertebrates: 0.300
Justification: Due to the lack of literature bioaccumulation data, the geometric mean of BAFs for inorganic COCs in the database was used.
Sediment-to-fish: 0.171
Justification: Due to the lack of literature bioaccumulation data, the geometric mean of BAFs for inorganic COCs in the database was used.

Toxicity Reference Values
<u>Birds</u>

CASRN: 7440-48-4
Chemical Form: COBALT
Surrogate: CHICKEN
Effect Type: GROWTH
Effect Measure: BODY WEIGHT CHANGES
NOAEL: 4.10 mg/kg-day
LOAEL: 8.20 mg/kg-day
Body Weight: 0.3738 kg (from study; Ling et al. 1979)
Food Ingestion Rate: 0.030 kg/day (estimated, EPA 2005)
Dosing Regime: *Ad libitum* in diet; 4 doses (0, 50, 100, 200 mg/kg in diet); based on unmeasured concentrations
Age of Test Animal: 1 day
Life Stage and Sex: Juvenile / Males and females
Exposure Duration: 3 weeks
Uncertainty Factors: N/A
Conversions:

NOAEL: (50 mg Co/kg food * 0.030 kg food/d) / 0.3738 kg BW= 4.01 mg/kg-day

LOAEL: (100 mg Co/kg food * 0.030 kg food/d) / 0.3738 kg BW= 8.03 mg/kg-day

Note: calculated NOAEL and LOAEL differ slightly from reported values, likely because body weight and food ingestion rates shown in Appendix 5.1 (EPA 2005) are based on averages whereas EPA actually used values specific to each dose group to calculate the TRVs.

End Point Reference: Ling et al. (1979), EPA (2005)
Basis for Selection/Comments: Four avian growth TRVs are presented in the Cobalt Eco-SSL that report both a NOAEL and LOAEL. Of the two median studies, one reports a questionable food ingestion rate (0.00031 kg/day which is an order of magnitude lower than that of chickens of equal age from other studies). This study was eliminated and thus the other was chosen. The TRVs chosen are also based on a longer exposure period.

CASRN: 7791-13-1
Chemical Form: COBALT CHLORIDE HEXAHYDRATE
Surrogate: CHICKEN
Effect Type: MORTALITY
Effect Measure: MORTALITY
NOAEL: 5.74 mg/kg-day
LOAEL: 11.5 mg/kg-day
Body Weight: 1.042 kg (estimated, EPA 2005)
Food Ingestion Rate: 0.060 kg/d (estimated, EPA 2005)
Dosing Regime: *Ad libitum* in diet; 6 doses (0, 50, 100, 200, 300, 400 mg/kg in diet); based on unmeasured concentrations
Age of Test Animal: 1 day
Life Stage and Sex: Juvenile / Males and females
Exposure Duration: 5 weeks
Uncertainty Factors: N/A
Conversions:

NOAEL: (100 mg Co/kg food * 0.060 kg food/d) / 1.042 kg BW= 5.76 mg/kg-day*

LOAEL: (200 mg Co/kg food * 0.060 kg food/d) / 1.042 kg BW= 11.5 mg/kg-day

Note: calculated value differs slightly from reported value, likely because body weight and food ingestion rates shown (EPA 2005 Appendix 5.1) are based on averages whereas EPA used values specific to each dose group to calculate the TRVs.

End Point Reference: Hill (1974), EPA (2005)
Basis for Selection/Comments: Two avian mortality NOAEL-LOAEL pairs are presented in the Cobalt Eco-SSL. The TRVs from Hill (1974) were chosen because they were the more conservative values, were based on a longer exposure period, and incorporated a larger number of doses.

Mammals

CASRN: 7791-13-1
Chemical Form: COBALT CHLORIDE HEXAHYDRATE
Surrogate: MOUSE
Effect Type: GROWTH
Effect Measure: BODY WEIGHT CHANGES
NOAEL: 19.0 mg/kg-day
LOAEL: 33.0 mg/kg-day
Body Weight: 0.0375 kg (from study; Pedigo et al. 1988)
Water Ingestion Rate: 0.0078 L/d (from study; Pedigo et al. 1988)
Dosing Regime: *Ad libitum* in drinking water; 4 doses (0, 23, 42, 72 mg/kg-day); based on unmeasured concentrations
Age of Test Animal: 12 weeks
Life Stage and Sex: Sexually mature / Males
Exposure Duration: 5 weeks
Uncertainty Factors: N/A
Conversions:

NOAEL: 42.0 mg/kg-day * 45.39% Co/$CoCl_2.6(H_2O)$ = 19.0 mg/kg-day
LOAEL: 72.0 mg/kg-day * 45.39% Co/$CoCl_2.6(H_2O)$ = 33.0 mg/kg-day

End Point Reference: Pedigo et al. (1988), EPA (2005)
Basis for Selection/Comments: The NOAEL and LOAEL reported by Pedigo et al. (1988) was the only NOAEL-LOAEL pair for mammalian growth reported in the EPA (2005) Eco-SSL. TRVs are based on a body weight normalized dose (no concentration-to-dose conversions were necessary).

CASRN: 10124-43-3
Chemical Form: COBALT SULFATE
Surrogate: GUINEA PIG
Effect Type: MORTALITY
Effect Measure: SURVIVAL
LOAEL: 20 mg/kg-day
Body Weight: 0.478 kg (from study; Mohiuddin et al. 1970)
Food Ingestion Rate: 0.037 kg/day (assumed; EPA 2005)
Dosing Regime: Oral in diet; 2 doses (0 and 20 mg/kg-d); based on unmeasured concentrations
Age of Test Animal: NR
Life Stage and Sex: Mature / Males
Exposure Duration: 5 weeks
Uncertainty Factors: N/A
End Point Reference: Mohiuddin et al. (1970), EPA (2005)
Basis for Selection/Comments: The LOAEL from Mohiuddin et al. (1970) was chosen because no NOAEL-LOAEL pairs were available for mammalian mortality in the EPA

(2005) Eco-SSL. Two NOAELs were reported: 19.3 and 81.7 mg/kg-d (the latter of which was based on a subacute [5-day] exposure).

CASRN: 7646-79-9
Chemical Form: COBALT CHLORIDE
Surrogate: RAT
Effect Type: REPRODUCTION
Effect Measure: TESTICULAR DEGENERATION
LOAEL: 20 mg/kg-day
Body Weight: 0.523 kg (estimated; EPA 2005)
Food Ingestion Rate: 0.04 kg/d (estimated; EPA 2005)
Dosing Regime: NR in diet; two doses (0 and 20 mg/kg-day); based on unmeasured concentrations
Age of Test Animal: 100 days
Life Stage and Sex: Sexually Mature / Males
Exposure Duration: 70 days
End Point Reference: Corrier et al. (1985), EPA (2005)
Basis for Selection/Comments: Two NOAEL-LOAEL pairs for mammalian reproduction were provided in EPA (2005), however one NOAEL-LOAEL pair is based on a rat with a questionable body weight (0.021 g at 80 days old; Ref#126) which could not be verified. The other NOAEL-LOAEL pair (based on the "progeny weight" endpoint) could not be verified because the original journal article could not be obtained. However, the TRV shown above is based on the median of the reported LOAELs, a significant endpoint (testicular degeneration), and is within the range of LOAELs reported for other mammalian reproduction endpoints.

Critical TRVs: Since the $TRV_{average}$ for mortality was lower than the $TRV_{average}$ for growth, critical TRV was selected. Although the TRVs for mortality and reproduction are the same (LOAEL = 20 mg/kg-d), following body weight adjustment the mortality TRV will likely come out lower than the reproduction TRV. Since the mortality TRV shown is protective of growth and reproduction, and is based on a potentially more sensitive species (guinea pig), the mortality TRV (LOAEL of 20 mg/kg-d from Mohiuddin et al. 1970) was chosen as the critical TRV.

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Sample BE, Beauchamp JJ, Efroymson RA, Suter GW II (1998b) Development and validation of bioaccumulation models for small mammals. Oak Ridge National Laboratory, Oak Ridge TN. 89 pp

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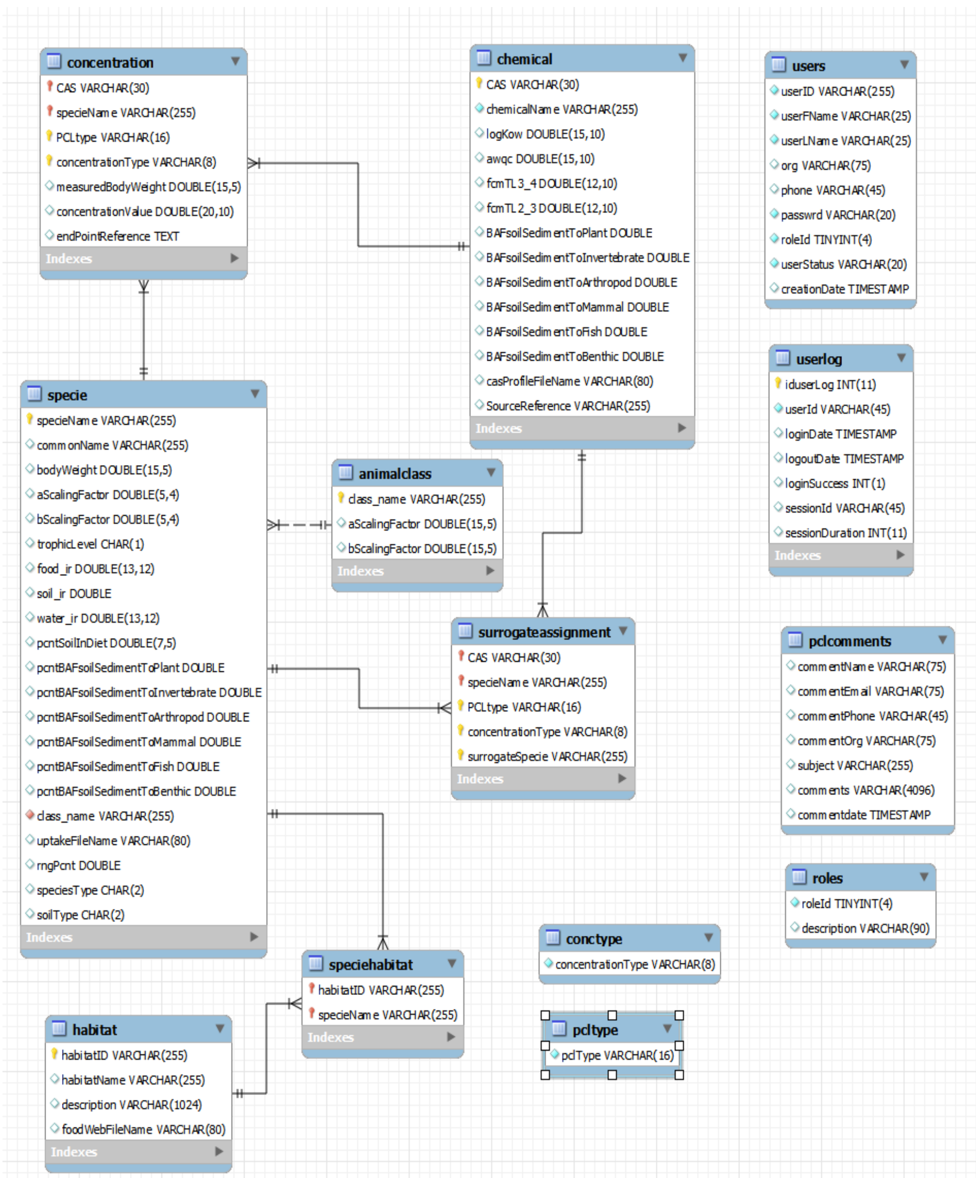
APPENDIX F

DATABASE DIAGRAM



APPENDIX G

USER INTERFACE SCREENS

Login/Registration screens:

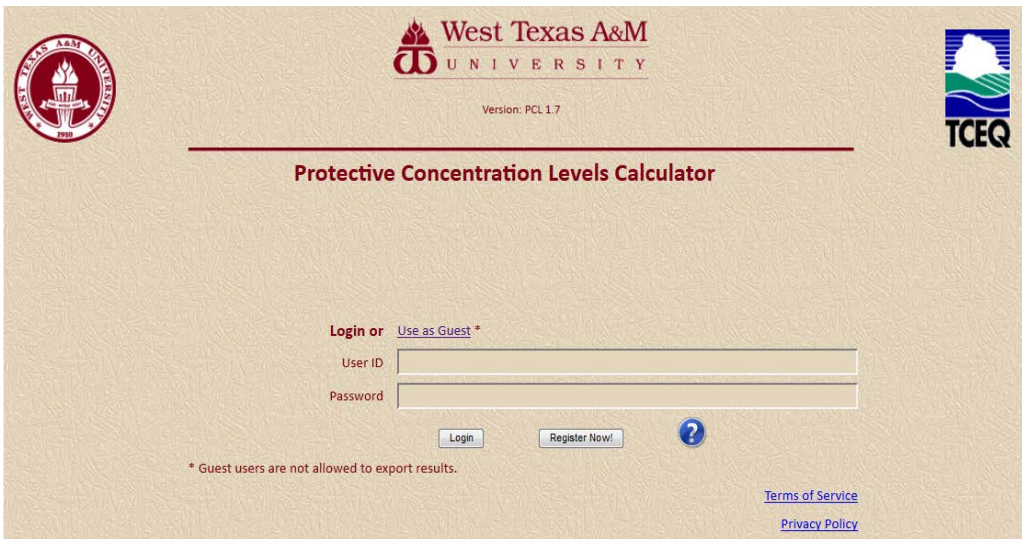


Figure G1 – Login screen

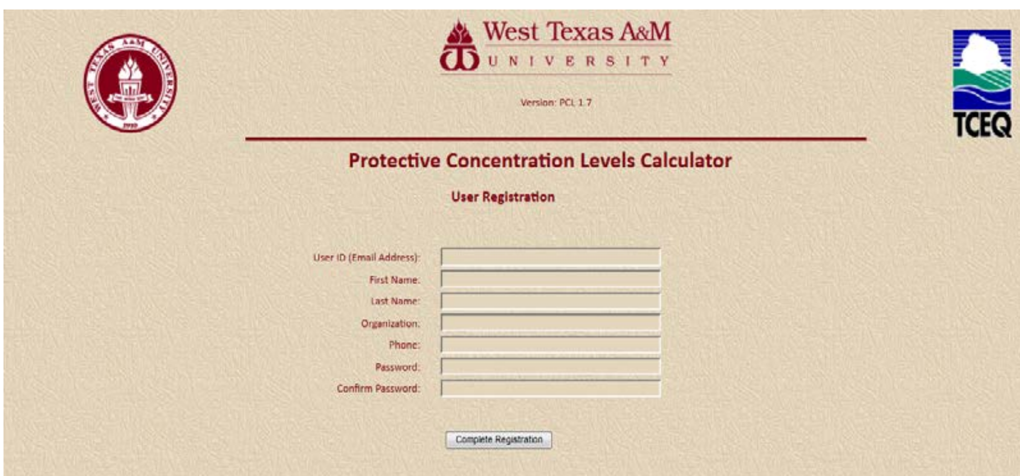


Figure G2 – Registration screen

Calculator screens:

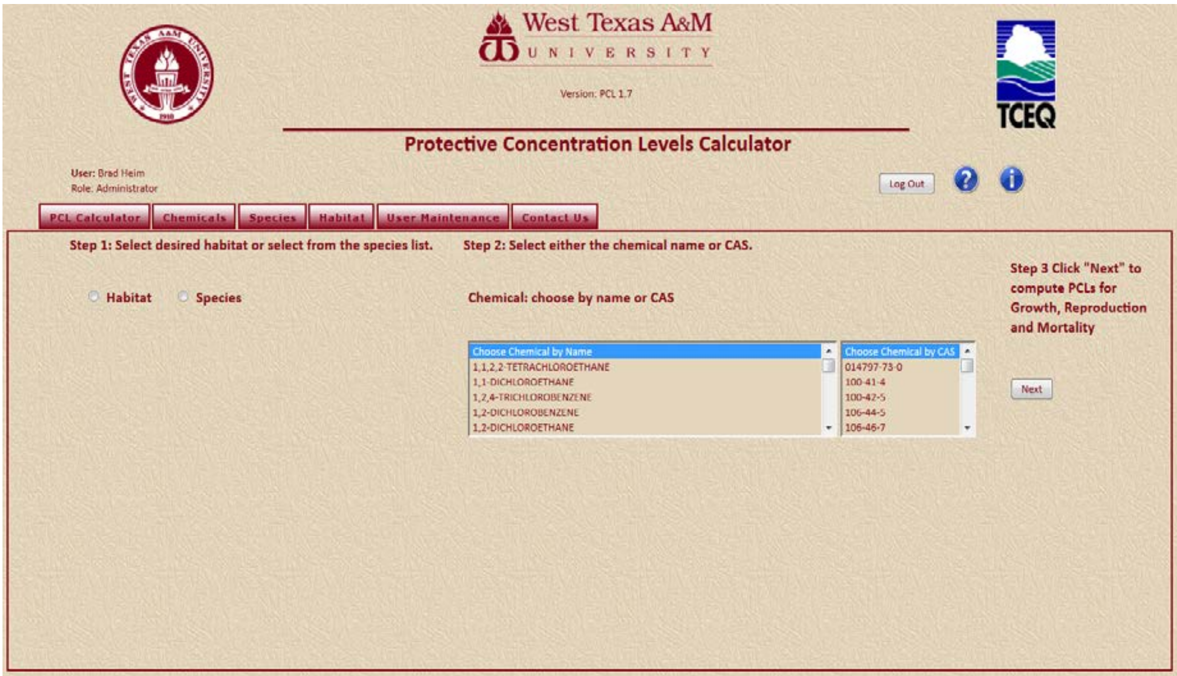


Figure G3 – Calculator selection/initiation screen

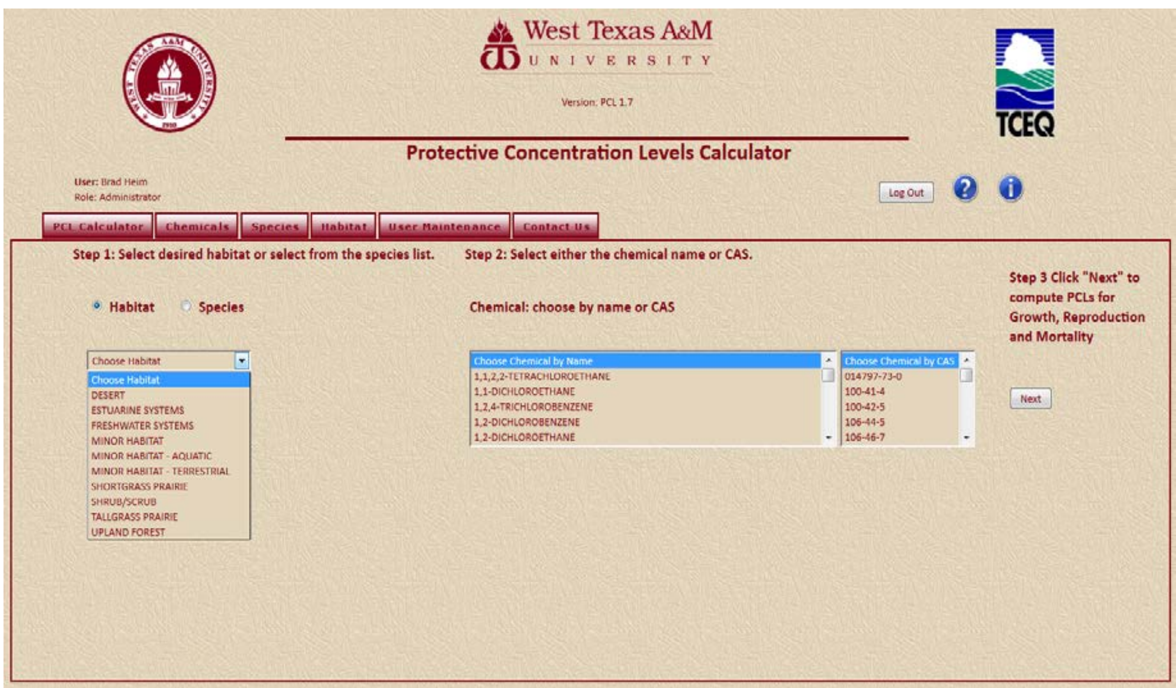


Figure G4 – Habitat selection dropdown

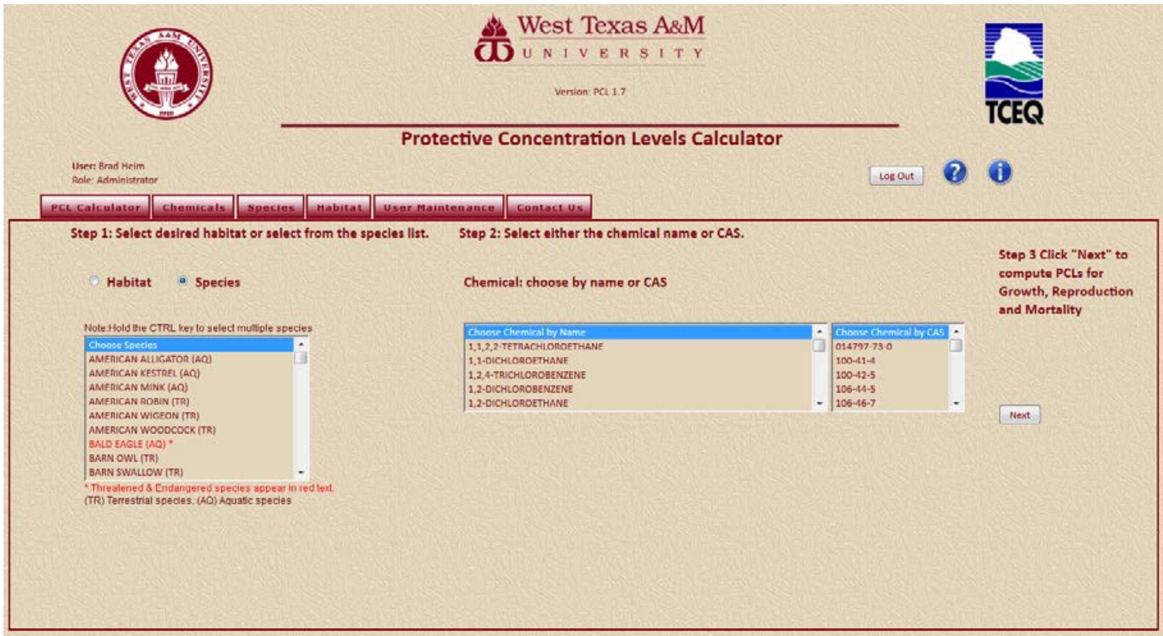


Figure G5 – Species selection dropdown

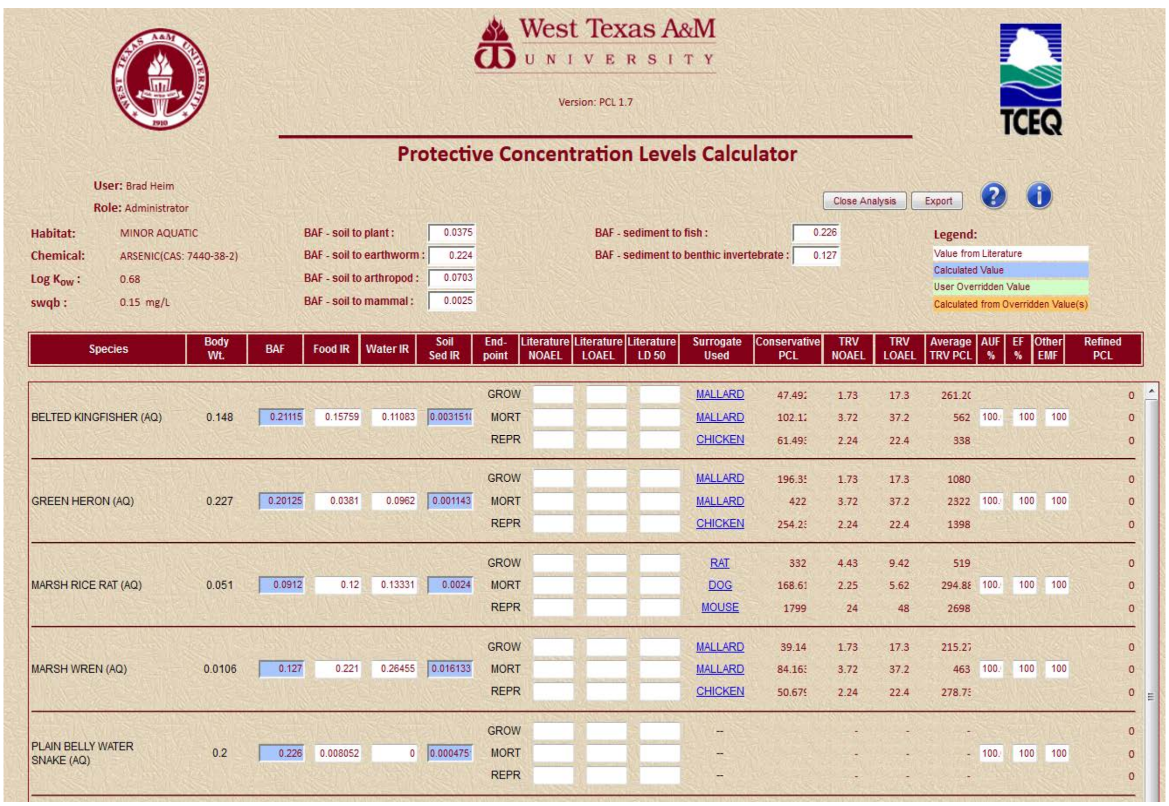


Figure G6 – PCL Calculation Analysis screen

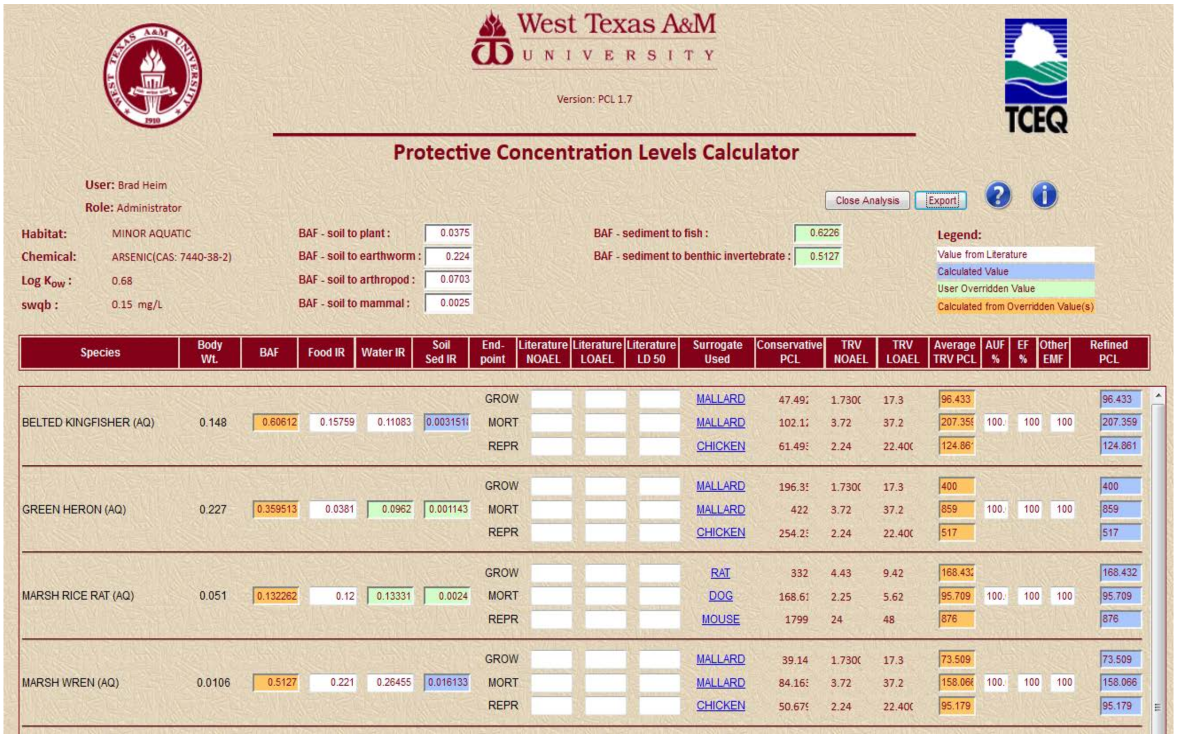
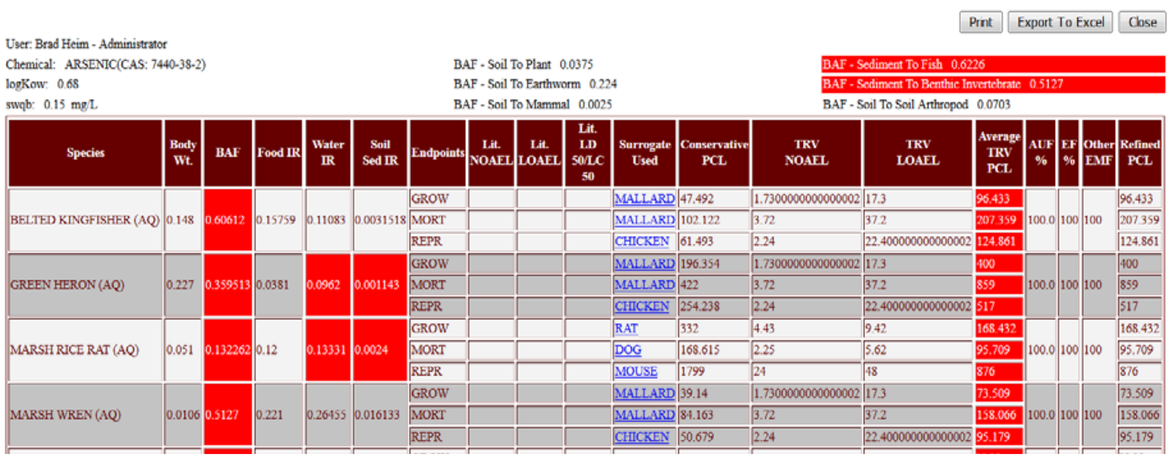


Figure G7 – PCL Analysis Changes Color Coding



Print | Export To Excel | Close

User: Brad Heim - Administrator
Chemical: ARSENIC(CAS: 7440-38-2)
logKow: 0.68
swqb: 0.15 mg/L

BAF - Soil To Plant 0.0375
BAF - Soil To Earthworm 0.224
BAF - Soil To Mammal 0.0025

BAF - Sediment To Fish 0.6226
BAF - Sediment To Benthic Invertebrate 0.5127
BAF - Soil To Soil Arthropod 0.0703

Species	Body Wt.	BAF	Food IR	Water IR	Soil Sed IR	Endpoints	Lit. NOAEL	Lit. LOAEL	Lit. LD 50/LC 50	Surrogate Used	Conservative PCL	TRV NOAEL	TRV LOAEL	Average TRV PCL	AUF %	EF %	Other EMF	Refined PCL
						GROW				MALLARD	47.492	1.7300000000000002	17.3	96.433				96.433
BELTED KINGFISHER (AQ)	0.148	0.60612	0.15759	0.11083	0.0031518	MORT				MALLARD	102.122	3.72	37.2	207.359	100.0	100	100	207.359
						REPR				CHICKEN	61.493	2.24	22.400000000000002	124.861				124.861
						GROW				MALLARD	196.354	1.7300000000000002	17.3	400				400
GREEN HERON (AQ)	0.227	0.359513	0.0381	0.0962	0.001143	MORT				MALLARD	422	3.72	37.2	859	100.0	100	100	859
						REPR				CHICKEN	254.238	2.24	22.400000000000002	517				517
						GROW				RAT	332	4.43	9.42	168.432				168.432
MARSH RICE RAT (AQ)	0.051	0.132262	0.12	0.13331	0.0024	MORT				DOG	168.615	2.25	5.62	95.709	100.0	100	100	95.709
						REPR				MOUSE	1799	24	48	876				876
						GROW				MALLARD	39.14	1.7300000000000002	17.3	73.509				73.509
MARSH WREN (AQ)	0.0106	0.5127	0.221	0.26455	0.016133	MORT				MALLARD	84.163	3.72	37.2	158.066	100.0	100	100	158.066
						REPR				CHICKEN	50.679	2.24	22.400000000000002	95.179				95.179

Figure G8 – PCL Analysis Export page with changes highlighted in red

Reference List Screens:

PCL Calculator | Chemicals | Species | Habitat | User Maintenance | Contact Us

Chemicals List | Add/Edit Chemical | Add/Edit Concentrations

CAS	Chemical Name	logKow	swsh	Bio-Accumulation Factors S2P	S2E	S2A	S2M	S2F	S2BI	Source Reference
79-34-5	1,1,2,2-TETRACHLOROETHANE	2.19	0.465	1.36	6.47	3.25	0.1	0.1	0.1	TRRP, 2014
75-34-3	1,1-DICHLOROETHANE	1.76	2.57	1.36	6.72	3.36	0.1	0.1	0.1	TRRP, 2014
120-82-1	1,2,4-TRICHLOROBENZENE	3.93	0.0515	1.54	10.1	5.05	0.1	0.773	107	TRRP, 2014
95-50-1	1,2-DICHLOROBENZENE	3.28	0.11	2.82	6.45	3.23	0.1	0.62	5.03	TRRP, 2014
107-06-2	1,2-DICHLOROETHANE	1.83	6.3	10.93	14.06	7.03	0.1	0.1	0.1	TRRP, 2014
540-59-0	1,2-DICHLOROETHENE	1.86	14	10.63	9	4.5	0.1	0.1	0.1	TRRP, 2014
99-35-4	1,3,5-TRINITROBENZENE (TNB)	1.45	0	15.6	8.08	4.04	0	0	2.85	TRRP, 2014
106-46-7	1,4-DICHLOROBENZENE	3.28	0.11	2.82	6.91	3.46	0.1	0.341	4.6	TRRP, 2014
118-96-7	2,4,6-TRINITROTOLUENE (TNT)	1.99	0.05	3.53	0.0175	0.00875	0	0	2.85	TRRP, 2014
121-14-2	2,4-DINITROTOLUENE	2.18	1.22	0.577	4.33	2.17	0	2.24	2.85	TRRP, 2014
35572-78-2	2-AMINO-4,6-DINITROTOLUENE	1.84	0.74	1.46	4.33	2.17	0	2.24	2.85	SYRACUSE RESEARCH CORPORATION
19406-51-0	4-AMINO-2,6-DINITROTOLUENE (4-AM-DNT)	1.84	0.74	0.296	3.78	1.89	0	3.89	5.78	ERAP

Figure G9 – Chemicals List screen

PCL Calculator | Chemicals | Species | Habitat | User Maintenance | Contact Us

Species List | Add/Edit Species | Surrogate Assignment

Species Name	Class Name	Habitats	Body Weight	Trophic Level	Ingestion Rates Food	Soil/Sed.	Water	% Soil/Sed. in Diet	% Diet S2P: Plants	S2E: Earthworms	S2A: arthropods	S2M: Small mammals	S2F: Fish	S2BI: Benthic inverts
BARRED TIGER SALAMANDER (TR)	AMPHIBIAN		0.054	4	0.007463	0.000336	0.0	4.5	0.0	0.0	0.0	0.0	0.0	1.0
CENTRAL NEWT (TR)	AMPHIBIAN		0.0026	3	0.01004	0.000592	0.0	5.9	0.0	0.0	0.0	0.0	0.0	1.0
LEOPARD FROG (AQ)	AMPHIBIAN		0.1	4	0.00726	0.000363	0.0	5.0	0.0	0.1	0.9	0.0	0.0	0.0
WOODHOUSE TOAD (TR)	AMPHIBIAN		0.056	3	0.00888	0.00044	0.0	5.0	0.0	0.0	1.0	0.0	0.0	0.0
AMERICAN KESTREL (AQ)	BIRD		0.116	4	0.106	0.002968	0.12011	2.8	0.0	0.0	0.0	1.0	0.0	0.0
AMERICAN ROBIN (TR)	BIRD		0.0773	3	0.242	0.012584	0.157326	5.2	0.5	0.5	0.0	0.0	0.0	0.0
AMERICAN WIGEON (TR)	BIRD		0.755	2	0.07911656	0.002611	0.064734	3.3	1.0	0.0	0.0	0.0	0.0	0.0
AMERICAN WOODCOCK (TR)	BIRD		0.169	3	0.1325	0.01378	0.106084	10.4	0.0	0.9	0.1	0.0	0.0	0.0
BALD EAGLE (AQ)	BIRD		3.75	3	0.053	0.00313	0.0381	5.9	0.0	0.0	0.0	0.0	1.0	0.0
BARN OWL (TR)	BIRD		0.466	4	0.10706848	0.002998	0.075807	2.8	0.0	0.0	0.0	1.0	0.0	0.0
BARN SWALLOW (TR)	BIRD		0.016	3	0.23833	0.023833	0.230936	2.0	0.0	0.0	1.0	0.0	0.0	0.0
BELTED KINGFISHER (AQ)	BIRD		0.148	4	0.1575903	0.003151806	0.11083212	2.0	0.0	0.0	0.0	0.0	0.85	0.15
BEWICK'S WREN (TR)	BIRD		0.01	3	0.273775	0.005475	0.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0
BLACK CAPPED VIREO (TR)	BIRD		0.009	3	0.282	0.00282	0.279	1.0	0.0	0.0	1.0	0.0	0.0	0.0

Figure G10 – Species List screen

Figure G11 – Habitat List screen

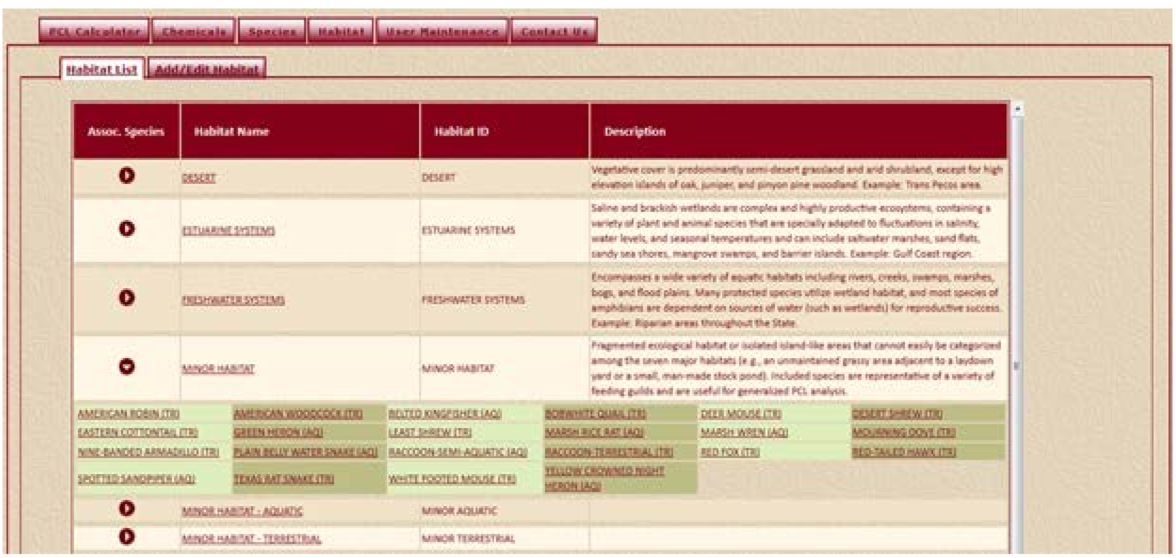


Figure G12 – Habitat List screen with associated species dropdown

Admin Screens:

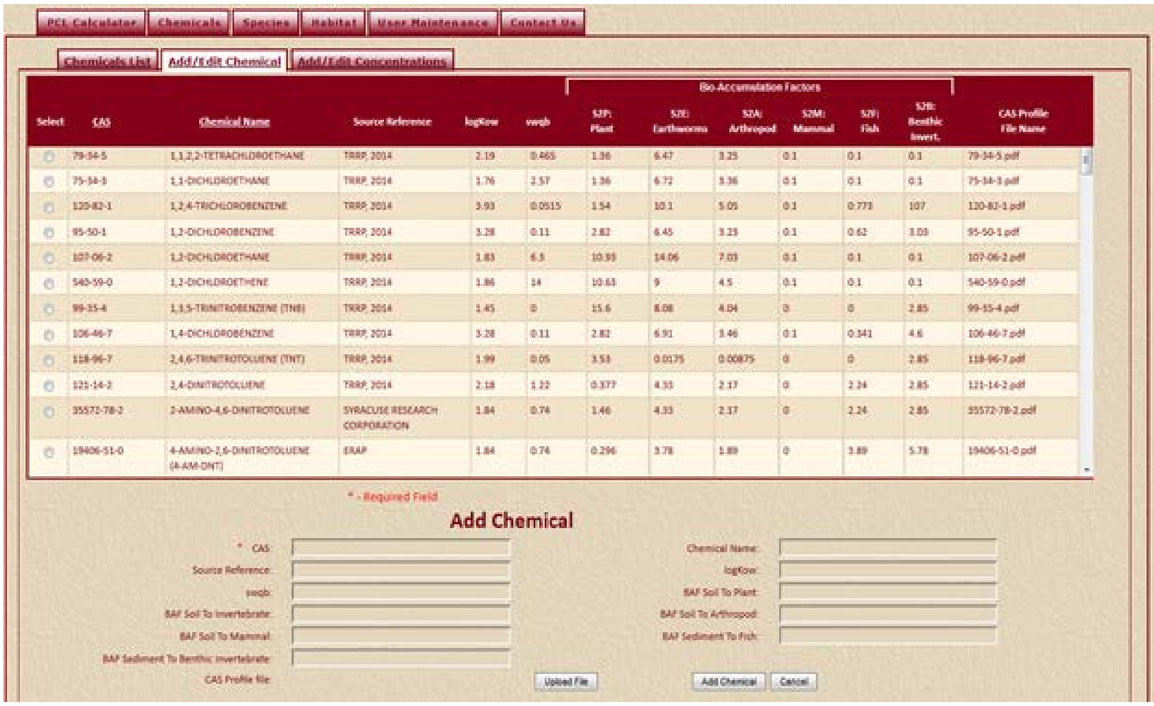


Figure G13 - Add/Edit/Delete Chemical screen

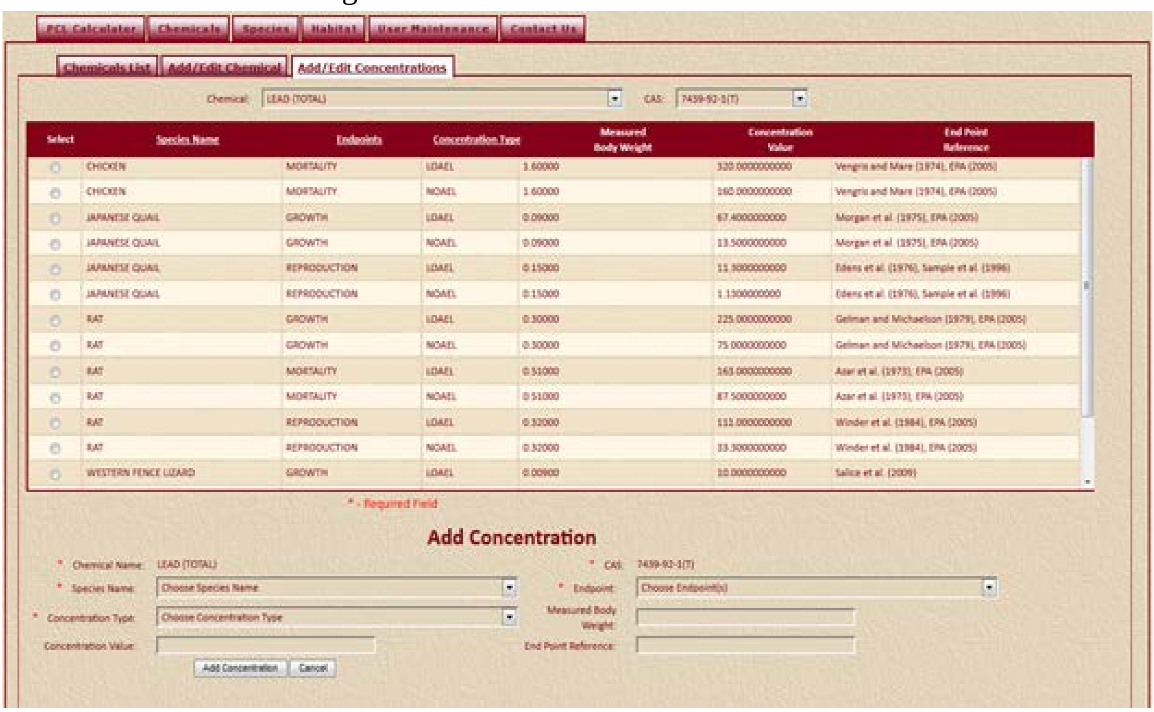


Figure G14 – Add/Edit/Delete Concentration screen

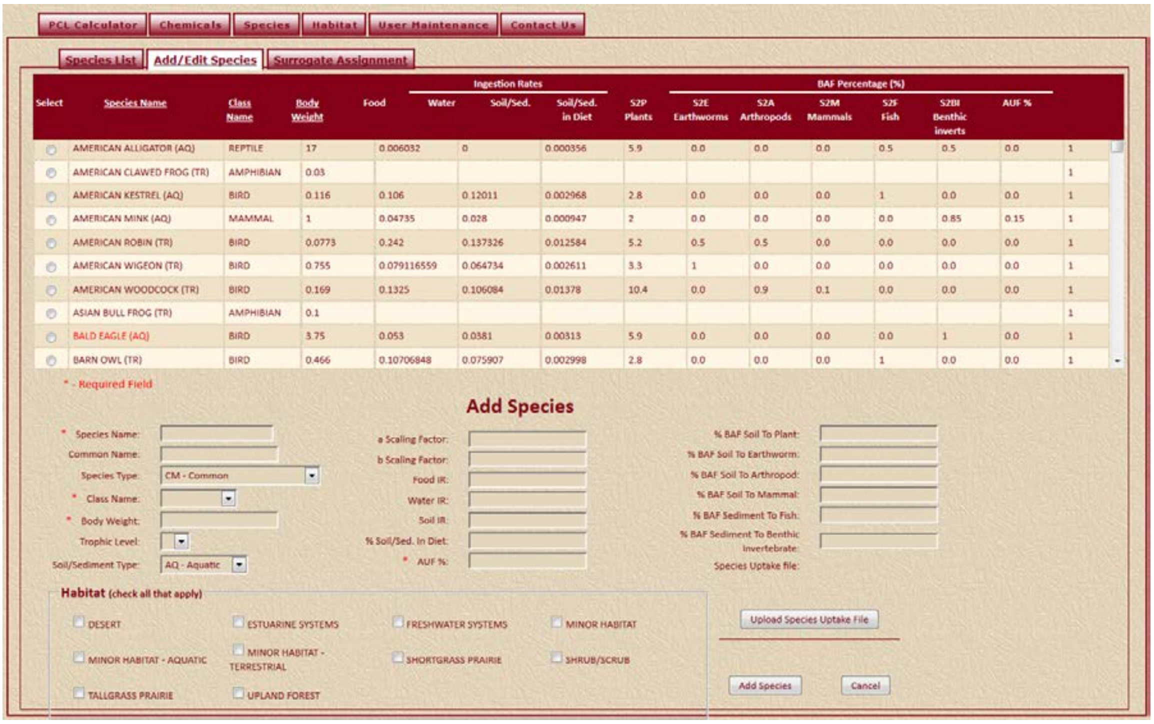


Figure G15 – Add/Edit/Delete Species screen

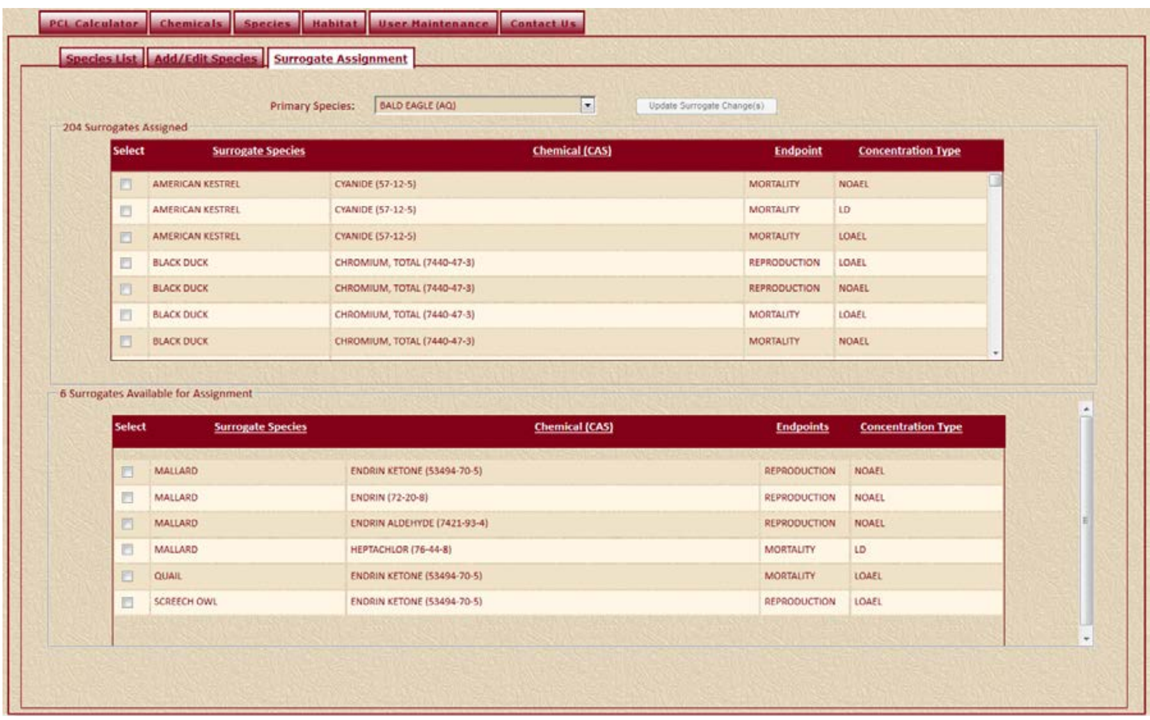


Figure G16 – Assign Surrogates to Primary Species screen

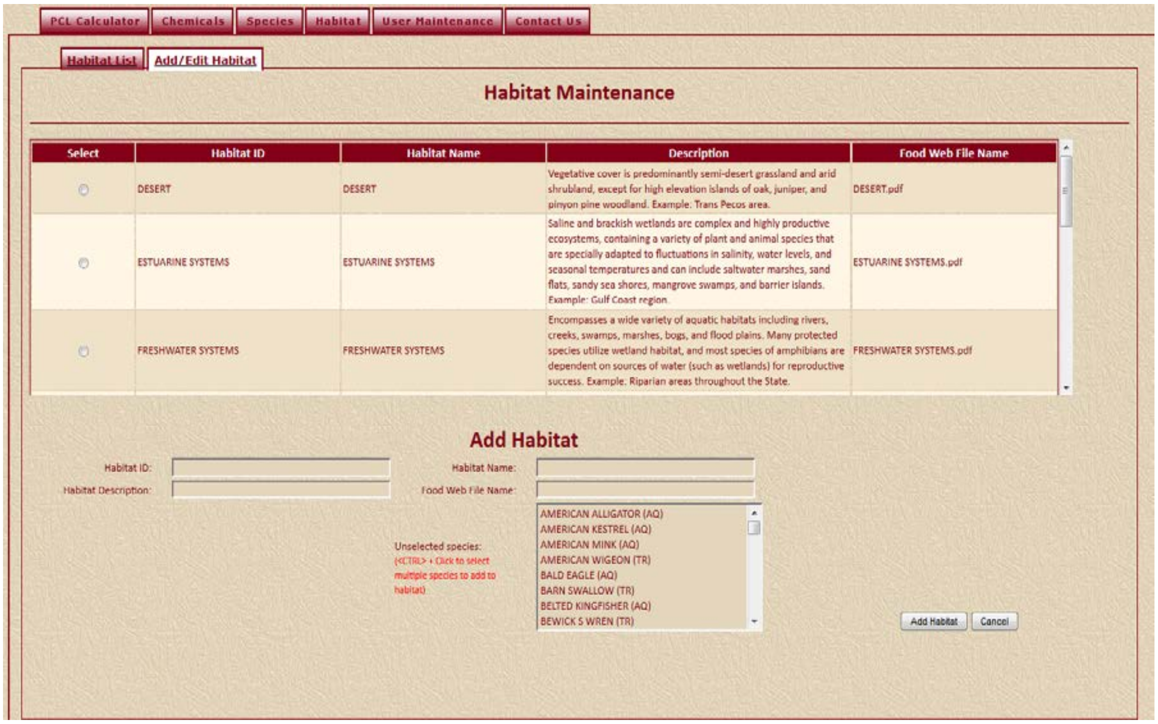


Figure G17 – Add Habitat screen

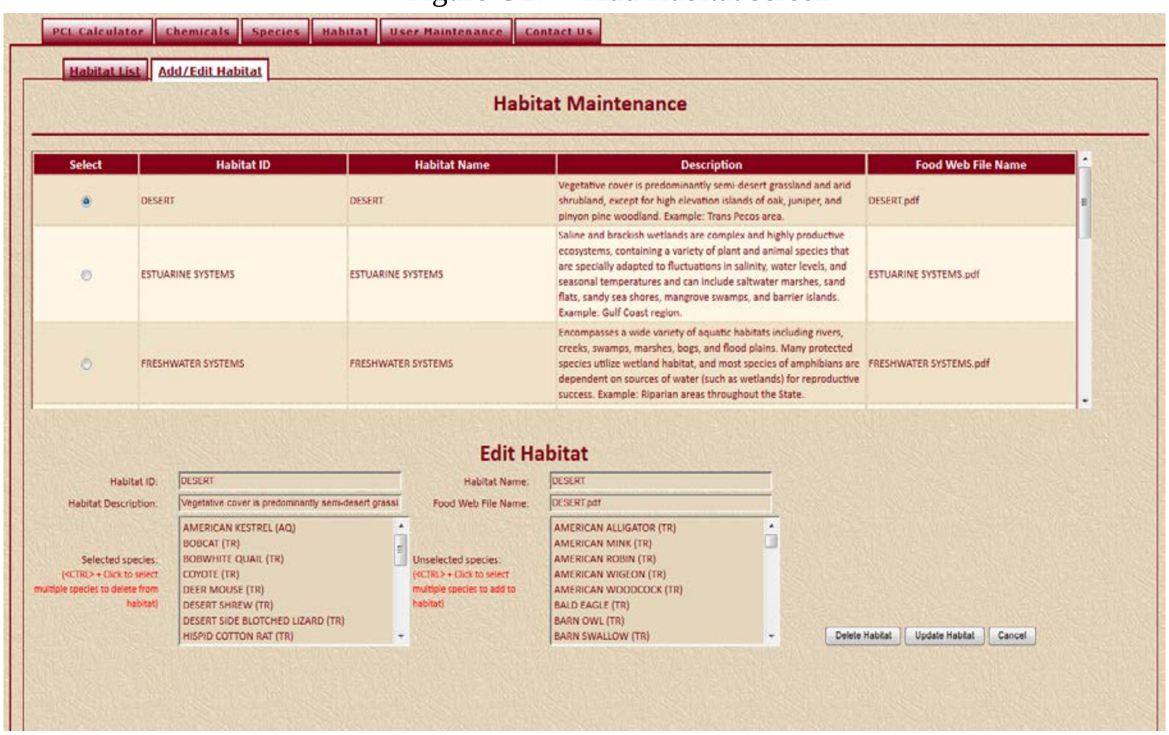


Figure G18 – Edit/Delete Habitat screen

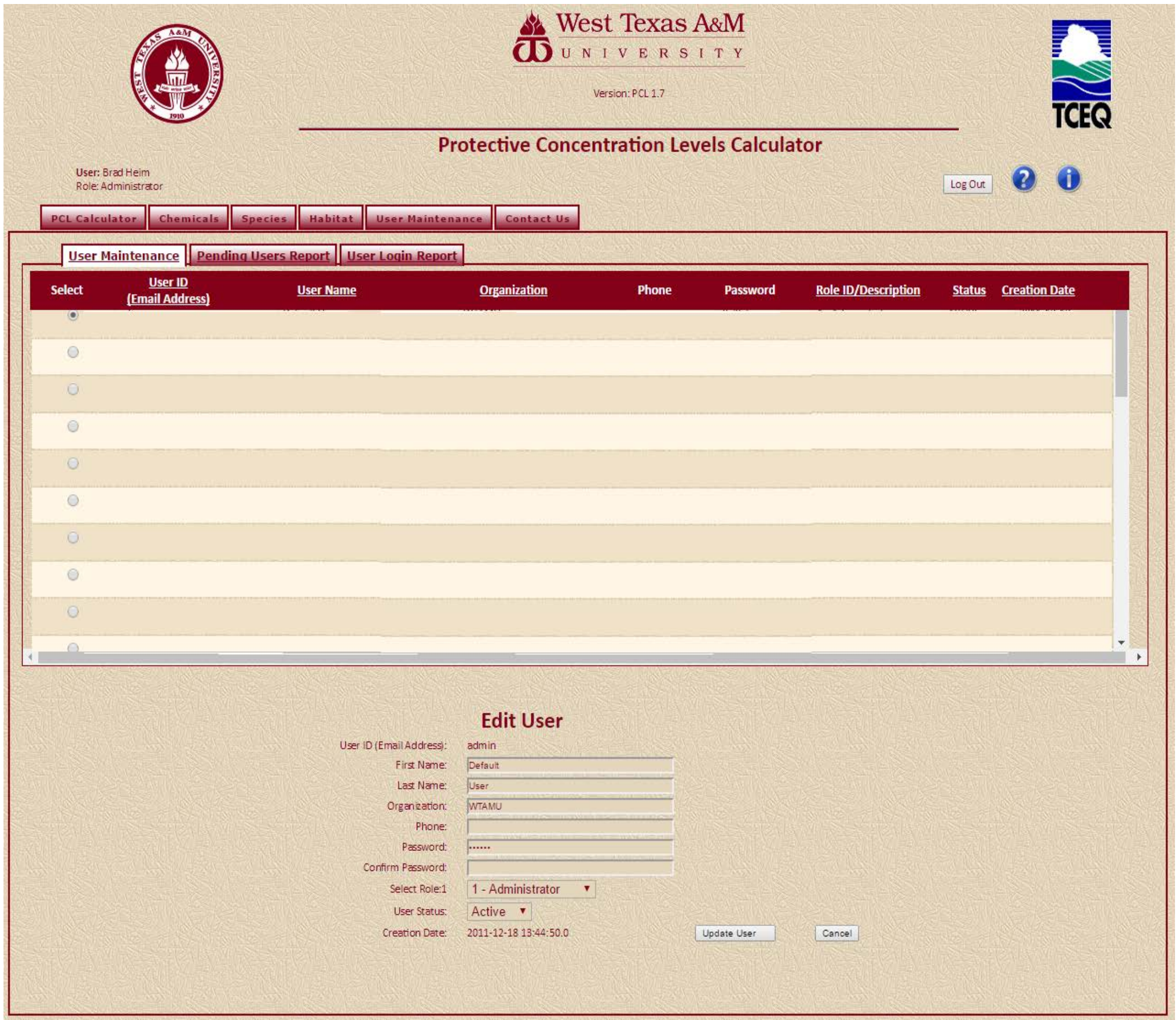


Figure G19 – Add/Edit/Delete User screen

Figure G20 – Pending Users Report screen

Figure G21 – User Login Activity Report screen

Figure G22 – Submit Comments screen

Figure G23 – View Submitted Comments screen

Help Screens:

PCL Help – Calculator

Introduction: The PCL calculator page allows guests, registered users and administrators to create a TCEQ approved, defensible PCL analysis by selecting the appropriate habitat (or individual species) and the Chemical of Concern (COC).

Step 1: Select desired habitat or select from the species list

Click on the Habitat or Species radio button to open the appropriate select list. The Habitat list is a single selection list while the Species list allows multiple selections by depressing the <CTRL> key and clicking on the desired species from the list.

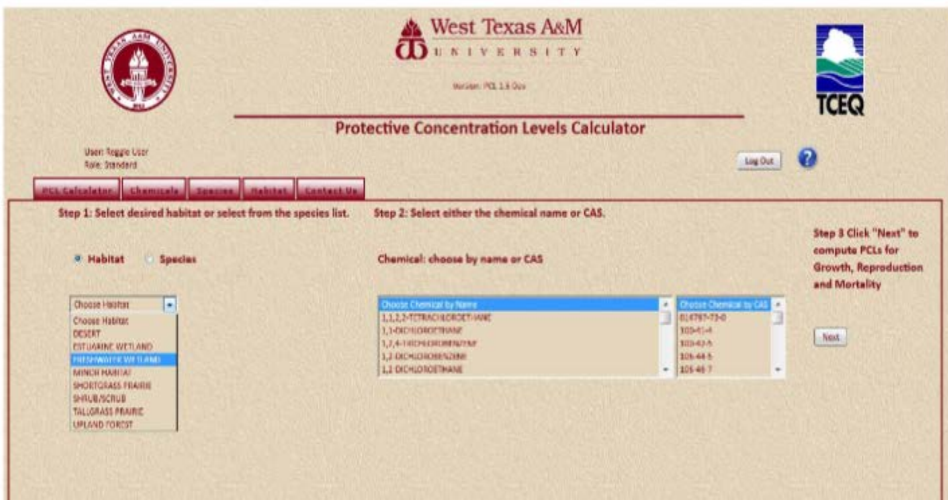
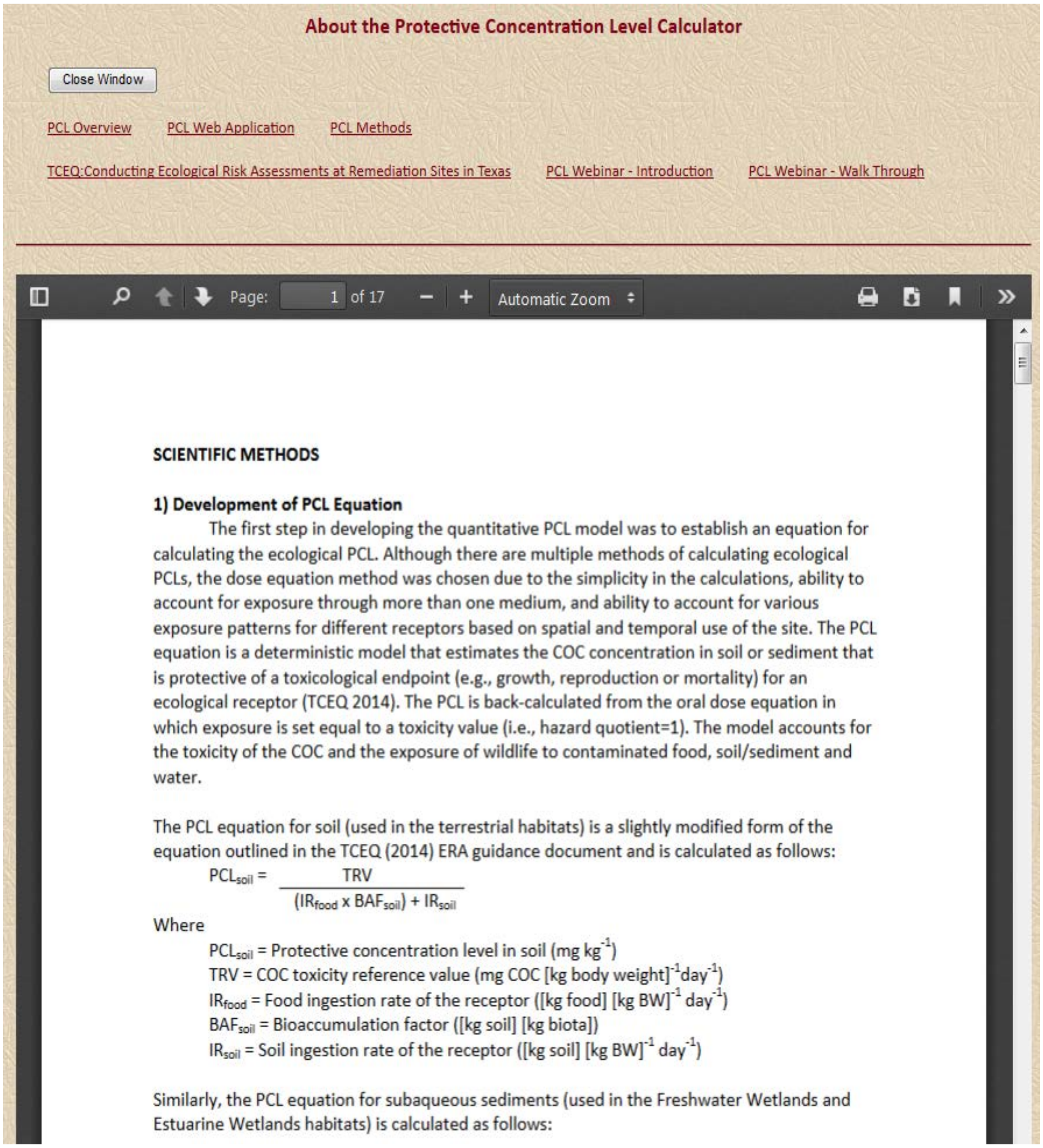


Figure G24 – Example of PCL Help page

Information Screens:



SCIENTIFIC METHODS

1) Development of PCL Equation

The first step in developing the quantitative PCL model was to establish an equation for calculating the ecological PCL. Although there are multiple methods of calculating ecological PCLs, the dose equation method was chosen due to the simplicity in the calculations, ability to account for exposure through more than one medium, and ability to account for various exposure patterns for different receptors based on spatial and temporal use of the site. The PCL equation is a deterministic model that estimates the COC concentration in soil or sediment that is protective of a toxicological endpoint (e.g., growth, reproduction or mortality) for an ecological receptor (TCEQ 2014). The PCL is back-calculated from the oral dose equation in which exposure is set equal to a toxicity value (i.e., hazard quotient=1). The model accounts for the toxicity of the COC and the exposure of wildlife to contaminated food, soil/sediment and water.

The PCL equation for soil (used in the terrestrial habitats) is a slightly modified form of the equation outlined in the TCEQ (2014) ERA guidance document and is calculated as follows:

$$PCL_{soil} = \frac{TRV}{(IR_{food} \times BAF_{soil}) + IR_{soil}}$$

Where

PCL_{soil} = Protective concentration level in soil (mg kg^{-1})
TRV = COC toxicity reference value (mg COC [kg body weight]$^{-1}$day^{-1})
IR_{food} = Food ingestion rate of the receptor ([kg food] [kg BW]$^{-1}$ day^{-1})
BAF_{soil} = Bioaccumulation factor ([kg soil] [kg biota])
IR_{soil} = Soil ingestion rate of the receptor ([kg soil] [kg BW]$^{-1}$ day^{-1})

Similarly, the PCL equation for subaqueous sediments (used in the Freshwater Wetlands and Estuarine Wetlands habitats) is calculated as follows:

Figure G25 – Example of PCL Information page

Webinar Screen:

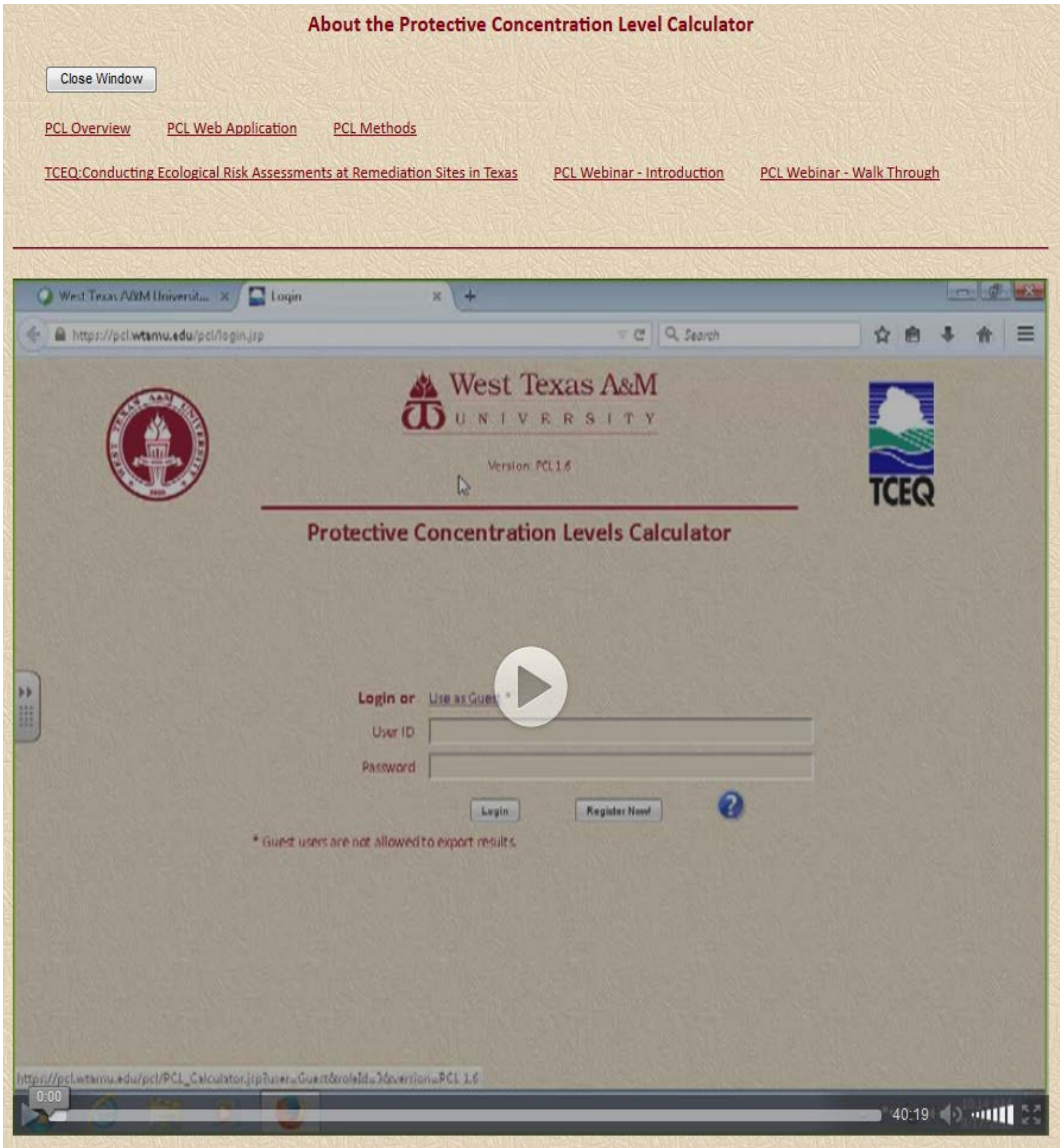


Figure G26 – Example of PCL Webinar Viewing page

APPENDIX H

PCL CITATIONS

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