GUIDANCE DOCUMENT

Improvement, Verification, and Refinement of Spatially Explicit Exposure Models in Risk Assessment

FishRand-Migration Probabilistic Bioaccumulation Module

ESTCP Project ER-200917

MARCH 2015

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Distribution Statement A

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FISHRAND-MIGRATION (FR-M)
Probabilistic Fish Bioaccumulation Module

USER'S MANUAL
Version 4.0

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LIST OF ACRONYMS

BAF	BioAccumulation Factor (ratio of lipid-normalized tissue concentration to freely dissolved water concentration)
BP	Bioaccumulation Parameters
BSAF	Biota Sediment Accumulation Factor (ratio of lipid-normalized benthic invertebrate tissue concentration to TOC-normalized sediment concentration)
COC	Chemical of Concern
EH	Exposure History
FR-M	FishRand-Migration
K_{ow}	Octanol Water Partition Coefficient
PDF	Probability Density Function
TOC	Total Organic Carbon
USACE	United States Army Corps of Engineers
USEPA	United States Environmental Protection Agency

1 PREFACE

This *FISHRAND-MIGRATION Probabilistic Fish Bioaccumulation Module - User's Manual*, outlines the mathematical framework for the modeling approach, presents the equations and operational mechanics of the model, and provides stepwise user instructions.

Drawing from user-defined input parameters, FISHRAND-MIGRATION (FR-M) is a software tool to estimate body burdens of organic chemicals in fish under current and future exposure scenarios. Based on the Gobas (1993 and 1995) modeling approach, FR-M is a mechanistic, time-varying exposure model that employs mass balance principles, species-specific foraging and life history data, site-specific chemistry and biological characteristics to predict population distributions of aquatic food web concentrations and associated uncertainty. The user enters data on biota-sediment accumulation factors for infaunal organisms, lipid content, chemical concentrations in associated physical media, total organic carbon in sediment, chemical assimilation efficiency, fish residence time and octanol water partition coefficients. FR-M also accounts for the influence of species-specific migratory and foraging behaviors and spatial heterogeneity of contamination and habitat quality to incorporate greater realism into exposure estimates.

2 INTRODUCTION

2.1 Background

The FishRand-Migration (FR-M) model is a spatially-explicit aquatic bioaccumulation model originally developed to support decision making at the Hudson River Superfund Site (assuming single, non-spatially explicit reach-wide exposure concentrations in sediment and water) and used to compare remedial alternatives (and no action) on the basis of predicted fish tissue concentrations. Since its original development, the model has been expanded and augmented to include a spatially-explicit component to better characterize exposures for migratory and wide-ranging fish species.

The sediment and water concentrations of contaminants to which aquatic organisms are exposed in areas of localized contamination are a function of spatial factors together with species biology. Species with overlapping foraging areas may experience significantly different contaminant exposures from the same site due to local variability in species behavior and contaminant distributions as they overlap with preferred foraging and migratory areas. Predicted exposure estimates and subsequent human health and ecological risk projections typically assume static exposures of receptors to contaminant concentrations characterized by descriptive statistics such as a mean or maximum. The level of health protection is unknown, and the results may not be representative of actual exposures experienced by aquatic organisms in a dynamic system. In addition, these static exposures do not account for uncertainty and variability in the underlying input parameters.

The FR model assumes that the fish caught by anglers or ecological receptors are sampled from a population of fish, and so every individual fish can be thought of as coming from a population distribution. Computationally, this assumption leads to a set of nested Monte-Carlo subroutines shown in Figure 2. Conceptually, the FR-M model begins by defining a hypothetical population of fish. These fish are randomly placed on the modeling grid according to the model input parameters. The fish are allowed to forage over the grid (within their defined foraging areas) for the time period specified by the analyst. At the end of that time period (e.g., one week or one month), all the fish are “gathered up” and again randomly dispersed over the modeling grid. For each time interval, the predicted body burden of the individual fish contributes to the population distribution. Strictly speaking, the FR-M model does not track individual fish; individual fish are represented mathematically by the number of simulations specified by the analyst (e.g., the number of Monte Carlo draws).

The modeling grid in FR_M is defined by a map that can be imported from a variety of graphical formats such as JPEG or GIF files. Contaminant concentrations in sediment and water and physical locations are defined on the map as modeling zones using a polygon drawing tool. The user specifies the aquatic food web, which can include benthic and pelagic invertebrates, phytoplankton, forage fish, and piscivorous fish. The mathematical engine for the model is based on the Gobas model developed by Dr. Frank Gobas and colleagues at Simon Frasier

University (Gobas, 1993; Gobas et al., 1995; 1999; Gobas and Wilcoxson, 2003; Arnot and Gobas, 2004).

Fish, like terrestrial receptors, are known to preferentially forage in particular areas based on features of the landscape (e.g., particular substrates, presence of specific kinds of aquatic vegetation, physical disturbances, such as fallen trees, etc.). The FR-M model allows fish to be "attracted" to these physically defined features again using the map-based polygon tool. In this case, the random dispersal of fish over the modeling grid is weighted toward these attractive areas (e.g., the probability that the fish will land near these areas is increased rather than completely random). It is possible to define attraction factors using analogous methods to the habitat suitability index utilized in terrestrial systems, but there are no formal methods or databases incorporated in FR-M (e.g., the analyst must make this determination outside the software).

FR-M predicts fish body burdens in aquatic food webs given site-specific exposure conditions. One key aspect to this is having an understanding of the relationship between sediment and water. Although fish are primarily exposed to bioaccumulative contaminants through sediment sources, there can be significant dynamics that allow sediments to release contaminants, for example, through various flux mechanisms resulting from disequilibrium between sediment and water, which may be important to capture with respect to exposure. FR-M is not a sediment fate and transport model – these issues need to be addressed outside the FR realm.

FR allows users to specify probability distributions for model inputs, and users can specify whether an input predominantly contributes to "uncertainty" or population "variability." Uncertainty and variability should be viewed separately in risk assessment because they have different implications to regulators and decision makers (Thompson and Graham, 1996). For example, there is "true" uncertainty (e.g., lack of knowledge) in the estimated concentrations of sediment and water to which aquatic organisms are exposed. Concurrently, there is variability across inputs -- stochasticity -- contributing to contaminant bioaccumulation. Variability is a population measure, and provides a context for a deterministic point estimate (e.g., average or reasonable maximum exposure). Variability typically cannot be reduced, only better characterized and understood. In contrast, uncertainty represents unknown but often measurable quantities. Typically, uncertainty can be reduced by obtaining additional measurements of the uncertain quantity. Quantitatively separating uncertainty and variability allows an analyst to determine the fractile of the population for which a specified risk occurs and the uncertainty bounds or confidence interval around that predicted risk (von Stackelberg et al., 2002b). If uncertainty is large relative to variability (i.e., it is the primary contributor to the range of risk estimates) and if the differences in cost among management alternatives are high, additional collection and evaluation of information can be recommended before making management decisions for contaminated sediments. On the other hand, including variability in risk estimates allows decision makers to quantitatively evaluate the likelihood of risks both above and below selected reference values or conditions (for example, average risks as compared to 95th percentile risks).

2.2 Purpose and Scope

The FR-M model provides a more realistic simulation of how population exposures in aquatic food webs occur by developing a probabilistic analytical framework that simulates random fish movements over a grid or polygon map, and allows for fish congregating or preferentially feeding in particular areas within the study area through the use of user-defined modeling zones. The model also allows fish to move in and out of the modeling grid if that reflects their particular life histories. The probabilistic framework provides population estimates of tissue concentrations with associated uncertainty that provide greater flexibility for analysts in estimating subsequent human health and ecological risks.

2.3 Application

FR-M can be a valuable tool for ecological and human health risk assessors. The model can be used to estimate aquatic food web concentrations under different scenarios. The impact of different remedial strategies can be explored by applying sediment clean-up levels. The time-varying features in the model enhance the analytical and risk management power.

2.4 Installation and Requirements

FR-M requires Windows and Microsoft Excel (2003 or higher) for the report viewer. FR-M requires 100 MB of free hard drive space for most calculations. The required hard drive space required is dependent on the complexity of the user-defined model. FR-M generates output files in Microsoft Excel; **when generating output files, the user should not work, open, or save any other Excel files**.

If previous versions of FishRand or FR-M are installed, run the uninstall function to remove these versions before installing the latest version. In addition, after removing the program, confirm that all program files have been deleted from the Program Files folder on your computer (e.g., C:\ drive).

FR-M is distributed in a self-extracting setup file. Within this file, click on setup.exe to install the program. The setup will create a desktop shortcut and move files to the appropriate folders. Project-specific data files may be stored in any folder.

3 MODEL STRUCTURE

3.1 Overview

FR-M uses time-varying water and sediment concentration data to generate fish tissue concentrations[1]. The model is constructed using a set of compartments. The two primary diet compartments are pelagic biota (both invertebrate and phytoplankton) and benthic

[1] NOTE: Fish tissue concentrations are simulated in the same way regardless of position in the food chain

invertebrates. Tissue concentrations are assumed to be in equilibrium with the media concentrations, i.e. pelagic biota tissue concentrations are assumed to be in equilibrium with dissolved water concentrations and benthic invertebrate body burden concentrations are assumed to be in equilibrium with sediment concentrations (USEPA 2000). Depending on the specific diet preferences, forage fish consume biota from the two compartments. There can be multiple types for each compartment, e.g., worms, mollusks, shrimp, phytoplankton, etc. Piscivorous fish consume biota from these two compartments as well as forage fish, depending on species-specific diet preferences. Chemical uptake can occur through the diet or through the water column for both forage fish and piscivorous fish. Conceptually, the various inputs and outputs of FR-M are summarized in Figure 1.

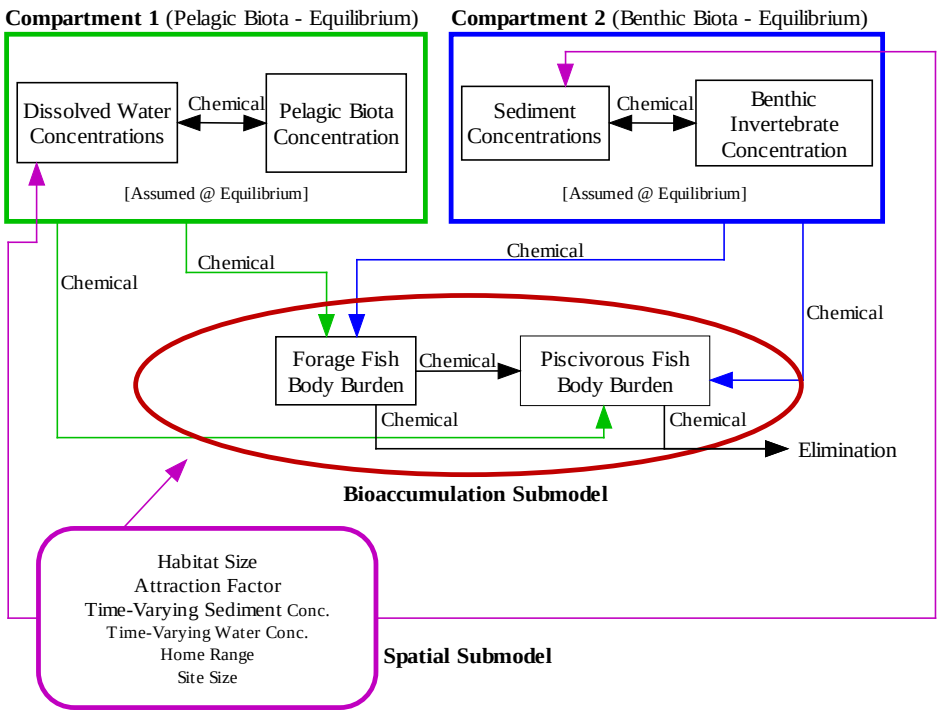


Figure 1. Schematic summary of calculation pathways within FISHRAND

In addition to assessing the bioaccumulation of chemicals, FR-M contains a spatial submodel. The spatial submodel improves the realism of the modeling process by incorporating foraging behaviors that may impact exposure. The spatial submodel includes:

a consideration of seasonal migration (relative abundance);

a consideration of the influence of home range size compared to the size of the site (home range in meters);

a consideration of the influence of habitat quality on exposure expressed as differential attraction to certain areas within the site (species-specific attraction factors); and,

the influence of time-varying concentrations on the species exposure given the seasonal movements and impacts of habitat quality on foraging (tine-varying and spatially-defined sediment and water input concentrations).

In the sections that follow, the model structure is described in more detail. As mentioned previously, the FR-M model is based on the Gobas model (Gobas, 1993; Gobas et al. 1995; 1999). The FR-M model has been applied to specific projects (USEPA 2000) and is also discussed in von Stackelberg et al. (2002a,b) and Linkov et al. (2002).

3.2 Equilibrium Partitioning (Prey Item Calculations)

The base of the food web, including pelagic and benthic invertebrates and plankton (e.g., zooplankton, phytoplankton) assumes that these compartments are in equilibrium with either sediment or water, depending on the dominant exposure route. Pelagic invertebrate and phytoplankton concentrations are estimated using equilibrium partitioning based on a freely dissolved water concentration, while benthic invertebrates are related to dry weight sediment concentrations. FR-M provides three options for generating invertebrate tissue and plankton concentrations. They include:

Entry (or selection) of a Biota Sediment Accumulation Factor (BSAF) for sediment or Bioaccumulation Factor (BAF) for water. Time-varying tissue concentrations are calculated using the BSAF and time-varying sediment concentrations or BAF and time-varying water concentrations;

Estimation through equilibrium partitioning from sediment (BSAF=1) or water (BAF = 1) to tissue, yielding time-varying tissue concentrations that track the sediment OR water concentration; and,

Input of co-located tissue and sediment (or water) concentrations (measured data). Such sets of measured tissue concentrations and medium concentrations are usually time independent (i.e. time varying tissue measurements are not collected on the same time scale as time-varying sediment or water measurements). All pairs of measured medium and tissue concentrations (or BAF/BSAF values estimated from measurements) are assigned equal statistical weights and are used to construct a mixture distribution of BAF/BSAF reflecting central tendency and measurement uncertainty in BAF/BSAF.

The US Army Corps of Engineers provides guidance regarding bioaccumulation testing (USEPA/USACE 1991). The equilibrium partitioning models for phytoplankton and pelagic invertebrate tissue concentration estimation use the octanol water partition coefficient (Log K_{ow}) in combination with the lipid content and freely dissolved water concentration. For sediment dwelling organisms, the percent lipid, total organic carbon, and chemical concentration in sediment are applied.

3.3 Bioaccumulation Submodel

Time-varying biota tissue chemical concentrations are calculated using the following differential equation:

$$\frac{dC_f}{dt} = k_1 * C_{wd} + k_d * C_{diet} - (k_2 + k_e + k_m + k_g) * C_{fish}$$

where:

k_1 = gill uptake rate (L/Kg/d)

C_{wd} = freely dissolved concentration in water (ng/L)

k_d = dietary uptake rate (d^{-1})

C_{diet} = concentration in the diet (μg/kg)

k_2 = gill elimination rate (d^{-1})

k_e = fecal egestion rate (d^{-1})

k_m = metabolic rate (d^{-1})

k_g = growth rate (d^{-1})

C_{fish} = concentration in fish (μg/kg)

3.4 Rate Constants

Four rate constants are required for model operation. Gobas (1993) discusses each in detail. The rate constants include chemical uptake via water and the diet, the fecal egestion rate and a growth rate constant. The equations for each are presented below and are discussed in greater detail in Gobas (1993; 1995) and Arnot and Gobas (2004). Several of the coefficients for these rate constants can be user modified based on site-specific and species-specific data.

3.4.1 Direct Uptake from Water

This rate constant is used to estimate the rate at which chemicals in water cross the gill interface and includes a gill ventilation rate as well as a cross gill diffusion rate. The equation is:

$$K_1 = \frac{1}{V_f / Q_w + V_f / Q_L * K_{ow}}$$

where:

k_1 = gill uptake rate (d^{-1})
K_{ow} = octanol/water partition coefficient
Q_w = transport rate in the aqueous phase (L/day)
Q_L = transport rate in the lipid phase (L/day)
V_f = fish weight in kg (described by a distribution in FR-M)

The two transport rates are described by:

$Q_w = 88.3*V_f^{0.6}$

$Q_L = Q_w/100$

The gill elimination rate is described by:

$$k_2 = \frac{k_1}{L_{fish} * K_{ow}}$$

where:

L_{fish} = fish lipid content

3.4.2 Uptake from Prey Consumption

The rate at which chemicals in prey items are transported into a consumer is dependent on the food ingestion rate, the rate of diffusion across the intestinal wall, and the fecal egestion rate. Gobas (1993) assumes that the efficiency of the uptake from food is related to the transport of the chemical in aqueous and lipid phases within the gut.

$$K_d = \frac{E_d * F_d}{V_f}$$

where:

k_d = dietary uptake rate constant (d^{-1})
E_d = uptake efficiency (unitless)
F_d = food ingestion rate (kg food/day)
V_f = fish weight (kg)

The uptake efficiency, E_d, is defined by:

$$E_d = \frac{1}{5.3x10^{-8} * K_{ow} + 2.3}$$

The food ingestion rate, F_d in [kg food/day] is defined by:

$F_d = 0.022*V_f^{0.85}*e^{0.06T}$

where:

F_d = food ingestion rate (kg food/day)
V_f = fish weight (kg) (described by a distribution in FR-M)
T = monthly mean water temperature (deg C)

3.4.3 Fecal Egestion Rate Constant

The rate at which biota release waste is defined by:

$k_e = 0.2*k_d$

where:

k_e = fecal egestion rate (d^{-1})
k_d = dietary uptake rate constant (d^{-1})

3.4.4 Growth Rate Constant

FR-M uses the growth rate constant presented in the original Gobas Model (1993). It is defined by:

For temperatures greater than 10^oC ($T>10^oC$), the growth rate constant, k_g, is given by:

$K_g = 0.01*V_f^{-0.2}$

Where:
V_f = fish weight (kg) (User input)

For temperatures less than or equal to10^oC ($T\leq10^oC$), the growth rate constant, k_g, is given by:

$K_g = 0.002*V_f^{-0.2}$

3.5 Spatial Submodel

The spatial submodel is described in detail in Linkov et al. (2002) and von Stackelberg et al. (2002b). The method is derived from an approach originally formulated for terrestrial habitats (Freshman and Menzie, 1996). The spatial submodel employs fish foraging behaviors to calculate the probability that a fish will be exposed to a chemical concentration in water and/or sediment. The spatial submodel uses time-varying sediment and water chemical concentrations, size of the site and so-called "hotspots" or modeling zones, attraction factors, migration habits of the fish, and fish home range sizes to evaluate the probability that a fish will be exposed to chemicals in the site.

A polygon tool is used to define hot spots and other spatially-dependent inputs within the study area.

The concentrations of chemicals in sediment (C_s) and in water (C_{wd}), water temperature, and sediment organic carbon content are considered as random variables described by data-based parametric probability distributions. In addition, the variability associated with the migratory habits of the fish population as well as the possible differential attractiveness of particular areas within the site are taken into account. Finally, population heterogeneity in bioaccumulation by individual fish is modeled in the bioaccumulation submodel.

The variability of chemical accumulation in the population of fish has two independent origins: 1) variability associated with the migratory and foraging strategy of each individual fish in the population (resulting in variable exposure histories); and, 2) variability in the parameters associated with chemical uptake for each individual fish. Accordingly, the model is based on the following general decomposition of the probabilities:

$$PDF(C_f \mid t) = \int_{\substack{Exposure \\ Histories}} \int_{\substack{Bioaccumulation \\ parameters}} PDF(C_f \mid t, EH, BP) \cdot dP(EH) \cdot dP(BP) \qquad (1)$$

where:

PDF(C_f | t) = probability density function (PDF) of chemical concentration in fish (C_f) accumulated at each time period *t*

EH = exposure history: the time series of chemical concentrations in local sediments and water, prior to the time period *t* (based on the migratory and localized foraging history of the fish)

BP = the set of individual bioaccumulation parameters

PDF(C_f | t,EH,BP) = conditional PDF of chemical concentration in fish given the exposure history *EH* and a set of values of the bioaccumulation parameters *BP*

d*P(EH)* = the probability of given exposure history *EH*

d*P(BP)* = the probability of given set of values of the bioaccumulation parameters *BP*

The integral in equation (1) employs a Monte Carlo assessment to generate random realizations of exposure histories (EH), i.e. random fish locations within the site or outside of the site, and bioaccumulation features (BP), i.e. random values for the parameters affecting assimilation and elimination of chemicals.

In addition to capturing the impact of migratory behaviors on exposure, the spatial submodel also incorporates the impact of heterogeneous chemical distribution across the site. Areas with a unique chemical distribution compared to the remainder of the site are referred to as modeling zones. Differential attraction to defined modeling zones versus the remainder of the site is captured through the application of an attraction factor. Using attraction factors, the probability of finding a fish within a particular modeling zone compared to finding a fish within the remainder of the site is defined by:

$$\text{Prob(modeling zone)} = \frac{AF_i * MZ_i^{\,2}}{S^2 + \sum_{i=1}^{N} AF_i \times MZ_i^{\,2}}$$

where:

AF_i = attraction factor (unitless; ratio of abundance within hotspot to abundance outside of the i-th modeling zone)
MZ_i^2 = i-th modeling zone area (km^2)
S^2 = site background (site without defined modeling zones) area (km^2)

3.6 Population Distributions and Associated Uncertainty

Parameters within FR-M are categorized as either variable (reflect population heterogeneity or stochasticity) or uncertain (reflect a lack of knowledge attributable to precision and bias) (von Stackelberg et al. 2002a). FR-M employs distributions to define model parameters; but point estimates may also be applied. Inputs may be defined as predominantly uncertain (e.g. Log K_{ow}, organic carbon, chemical concentrations, etc.) or variable (e.g. percent lipid, body weight, water temperature, etc.), but not both. As shown in Figure 2, FR-M then employs a nested Latin Hypercube/Monte Carlo approach to quantitatively evaluate uncertainty and variability. In this approach, uncertainty and variability are assessed separately (Cohen et al. 1996; Burmaster and Wilson 1996; von Stackelberg et al. 2002a). The nested Monte Carlo approach holds uncertain values constant and then runs the model by selecting values from the distributions for variable parameters for a user-selected number of iterations. Then another set of values are selected from the distribution for uncertain parameters, the values are again held constant while the variable parameter loop is completed. This nested Monte Carlo analysis continues until the specified number of iterations for the uncertain parameters are completed. Each set of iterations repeats across time periods.

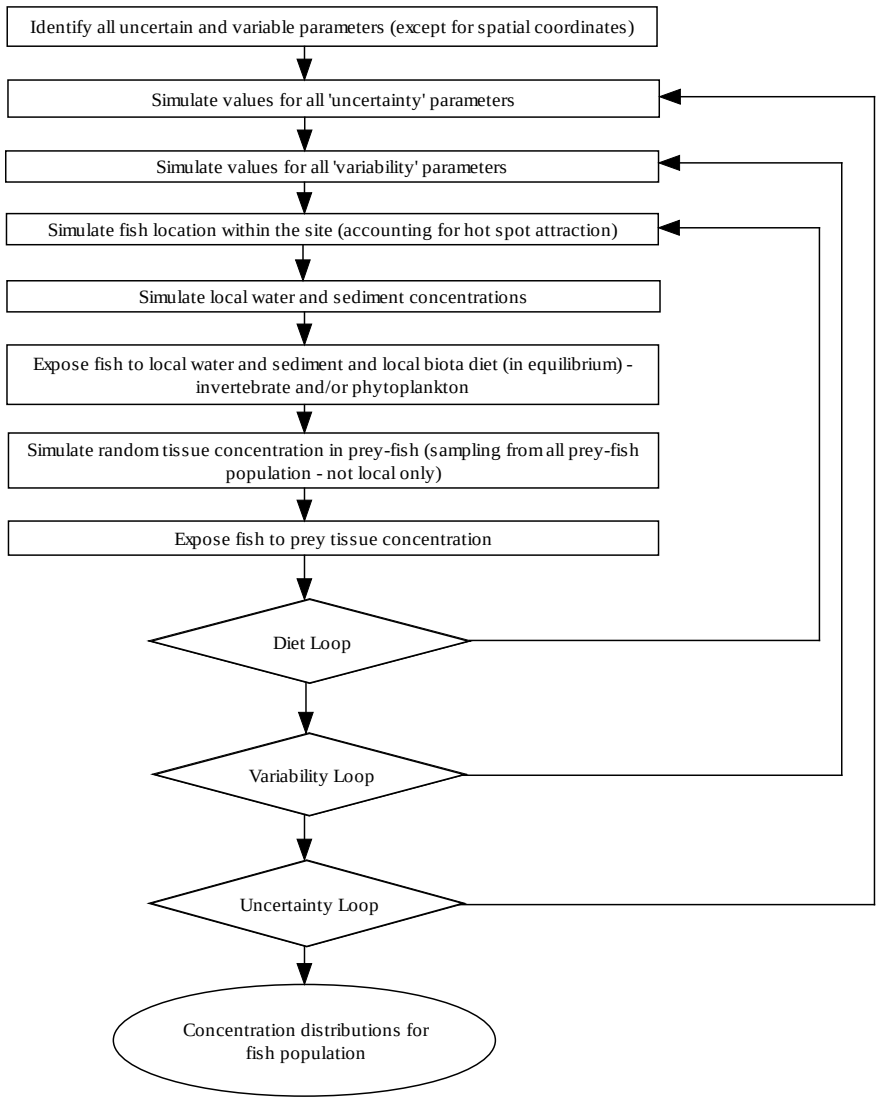


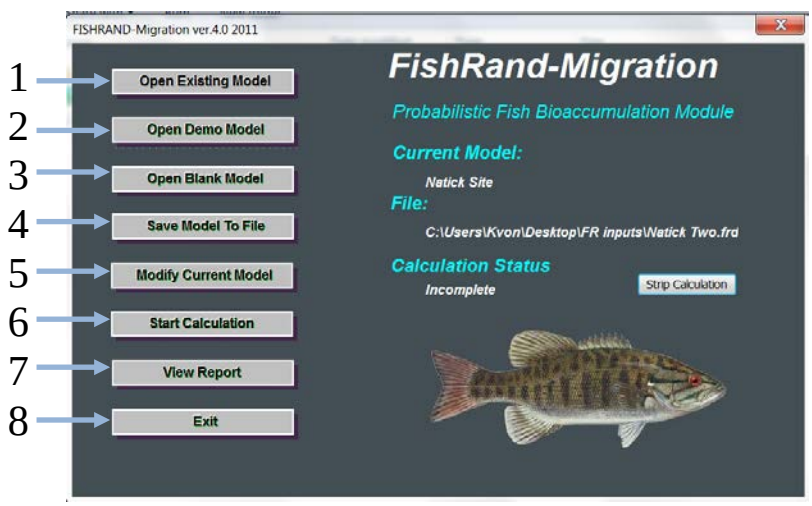
Figure 2. Nested Monte Carlo Approach Schematic

In addition to the variability loop discussed above, there is also an internal simulation loop capturing variability in prey body burdens (forage fish with an exposure history that is not correlated with the exposure of the piscivorous fish) and generating spatial simulations for fish

positions within the site with corresponding body burdens of local biota (invertebrates and plankton).

4 Stepwise Instructions

FR-M is organized around the home screen. From this screen a user may open existing models, save a model to a file, open a demonstration model, create a new model, modify the open model, start/run calculations and view reports. Each function is operated by directly clicking on the button/icon of interest. In addition, this screen reports the name of the current model (data from previous FR-M activity remains loaded until a user selects a new dataset to load or create from a blank input). FR-M is designed with an integrated guided input interface. The interface directs the user to enter specific pieces of information required to operate the model correctly. The guided input, in addition to other functions is accessed via the home screen. The function of each button on this screen is:



Open Existing Model (1): If a model data set has already been started and saved to an external file, this button allows a user to reopen that file and modify inputs, complete inputs, run the calculation and view the report;

Open Demo Model (2): FR-M includes two demonstration data sets. Access these datasets while learning how to use FR-M. Each dataset includes different combinations of inputs and modeling options to illustrate model functionality;

Open Blank Model (3): To load a blank model file and begin a new project, click this button;

Save Model to File (4): This button provides a user with an opportunity to save the input files, as well as the calculation file (after running the model), to an external file;

Modify Current Model (5): When opening an existing data file or returning to an active file, this button is used to access and modify the inputs in the file in the guided input;

Start Calculation (6): After data entry is complete, the model may be run. In order to run the model, *Finish* must have been clicked within the guided input to confirm that

data entry is complete. A set of calculation options are available to the user (discussed in detail in the Sections that follow);

View Report (7): After completing the calculations, the *View Report* button generates a summary report including inputs, tabular results and graphical results. Users are offered a number of statistical and summary options (discussed in detail in the Sections that follow); and,

Exit (8): To close the model, click *Exit*. Note: save all model data and outputs prior to exiting the program.

In addition to the function buttons on the home screen, additional information is provided to the user.

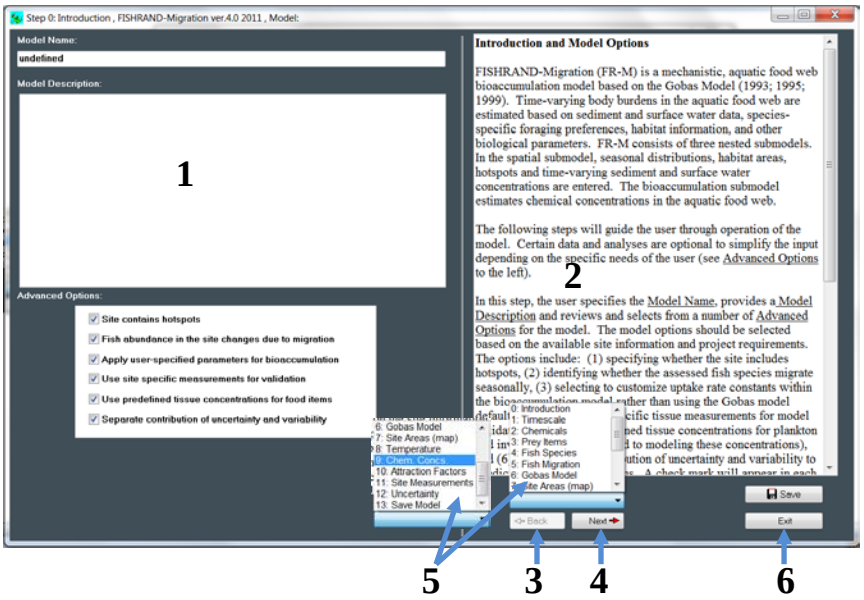
Current Model (9): This is the name of active model. The name is entered in the initial guided input step;

File (10): The file name is also provided to assist users in tracking which data set is active at any given time;

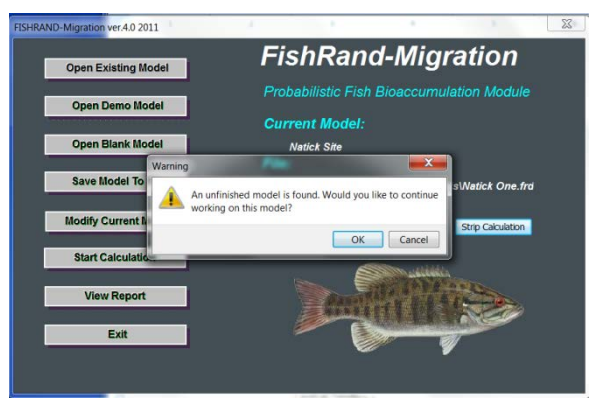
Is Calculation Complete (11): Before a report can be generated, the calculations must be completed. This information box indicates whether the model has been run for the current input file.

Each screen in the guided input requires the user to supply specific inputs needed to run the model. Users are given the opportunity to determine the complexity of each model run, which is dependent on the specific question being framed, the available data and user preferences. As a result, the number of steps in a specific guided input series is customized based on the desired level of complexity and/or flexibility selected by the user. The number of guided input steps will vary depending on the parameters that a user selects (from 8 to 14 steps) (see Section 3.1 for additional detail). Use of parameters such as migratory characteristics of the assessed species or the presence of hotspots is optional. The guided input is used to populate the model. Once completed, the user will exit the guided input and initiate model calculations from the FR-M home screen.

In the following sections, the input screen and a description of the input data for each step are provided. For organizational purposes, we list all possible guided input steps; note that the exact number of steps depends on the number of advanced options chosen by the user. The program will modify the step numbers depending on which parameters apply to a given model run.



The general structure of the guided input screens is displayed to the left. Data entry fields occupy the left-hand side of the screen **(1)**, while step-specific guidance text describing the required data is provided on the right-hand side of the screen **(2)**. On some input screens, clicking on a data entry screen on the left-hand side of the screen will activate an additional data entry pop-up on the right-hand side. A user can toggle between the guidance text and the pop-up data entry window. The *Back* **(3)** and *Next* **(4)** buttons are used to navigate between guided input steps. All guided input steps are available from every screen (**5**). *Save* and *Exit* (**6**) are also available from every screen. They differ in how they save the data. *Save* will always lead to a dialog box asking the user to name the file, while *Exit* will bring the user back to the main menu and will save all data entry up to that point in the "current model" – if that is a model that has been opened from a file, or previously saved, clicking on *Exit* from any screen will automatically overwrite the file contents and save data entry up to that point to the current file without notifying the user that a file could be overwritten. FR-M stores all data input while working on an active data set – if that dataset has not been named, FR-M will recover data entry from an unfinished temporary file and users will be given the option of continuing to work on this data file if it is not actively saved. This is shown in the figure below. To summarize:



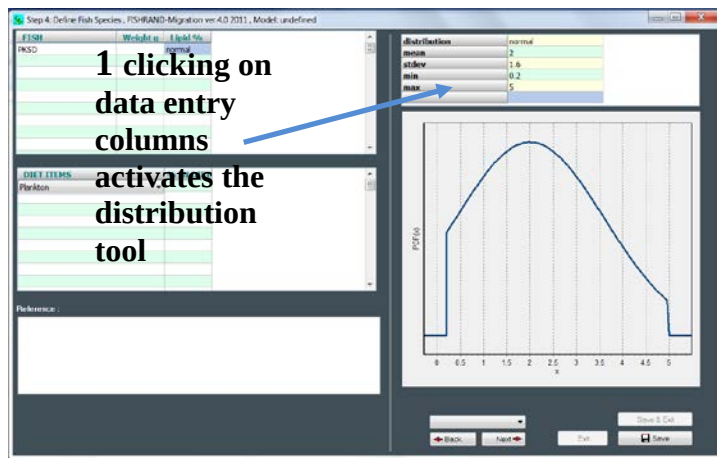
Save: this option is available on each input screen and allows a user to save the data entered through the guided input step *preceding* the active step to an external file. Data entry must be completed in order to run the model, but this feature allows a user to backup work, create duplicate input files, etc.

Exit: this option will exit guided input and return to the main screen *without saving* the current input to a file; current input are still available and before opening another file or exiting, the user will be prompted to "continue working on this model?" as shown in the figure above.

Upon exiting the guided input, the *Save As* dialog pops up only if the model is created from scratch. If an external file is already assigned to the model data (due to previous saving or opening of external files), on *Exit* this external file is updated without any additional warnings or dialogs. The external model file will have the extension: *.FRD.

Because FR-M will not run correctly if inputs are not entered correctly, the program contains input alerts. If a user misses an input in any step, an alert will appear when *Next* is clicked. Users will not be permitted to advance to the next step until all inputs have been supplied.

4.1 Deterministic vs. Probabilistic Inputs



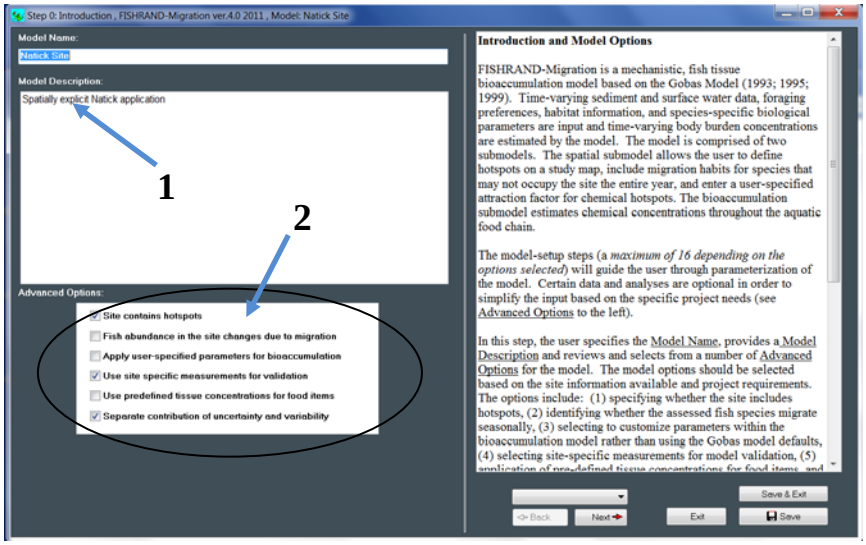
For almost all input variables, users may enter data as point estimates or as distributions, if data allow. Distribution types include uniform, triangular, normal and lognormal. This tool allows a user to select a distribution and displays the required inputs for each specific distribution. A figure of the data distribution is also generated. The tool is accessed by clicking on the value cell on the left side of the screen (**1**). If the input data have a spatial reference, a user may click on the input name to display a map of the data locations. Distributions are parameterized as follows:

- Uniform (min, max); minimum and maximum in native units (e.g., not transformed in any way)
- Normal (μ,σ); mean and standard deviation in native units (e.g., not transformed in any way)
- Triangular (min, mode, max); minimum, likeliest value, and maximum value in native units (e.g., not transformed in any way)
- Lognormal (μ,σ); mean and standard deviation of the natural log transformed data (e.g., LN[x])

4.2 Introduction and Model Option Selection

The first step in the process is to customize the specific model run. Users may select from a number of advanced model options depending on the data available, the project needs, site complexity and the global model run assumptions. FR-M is designed to accommodate a range of different site conditions and parameters. In this step the user creates a model name **(1)** and

provides a model description. The model name entered in this step appears on the home screen.



Below the name and description, a user may review and select among six advanced options.

The options **(2)** include:

- *Site contains hotspots*: This option allows users to define modeling zones within the study area using a map-based input together with a drawing tool. This option assumes spatial heterogeneity across key inputs, analogous to "hotspots";
- *Fish abundance in the site changes due to migration*: This option allows users to specify seasonal migration habits within the fish abundance parameter;
- *Apply user-specific parameters for bioaccumulation*: This option allows users to modify the rate constants in the bioaccumulation model;
- *Use site specific measurements for validation*: This option allows users to automate comparisons between predicted and observed tissue concentrations to visually evaluate model performance;
- *Use predefined tissue concentrations for food items*: This option allows users to enter data for invertebrate and plankton concentrations rather than using equilibrium partitioning to calculate those; and/or,
- *Separate contribution of uncertainty and variability*: This option allows users to specify individual inputs as contributing primarily to uncertainty (lack of knowledge) or variability (population heterogeneity or stochasticity).

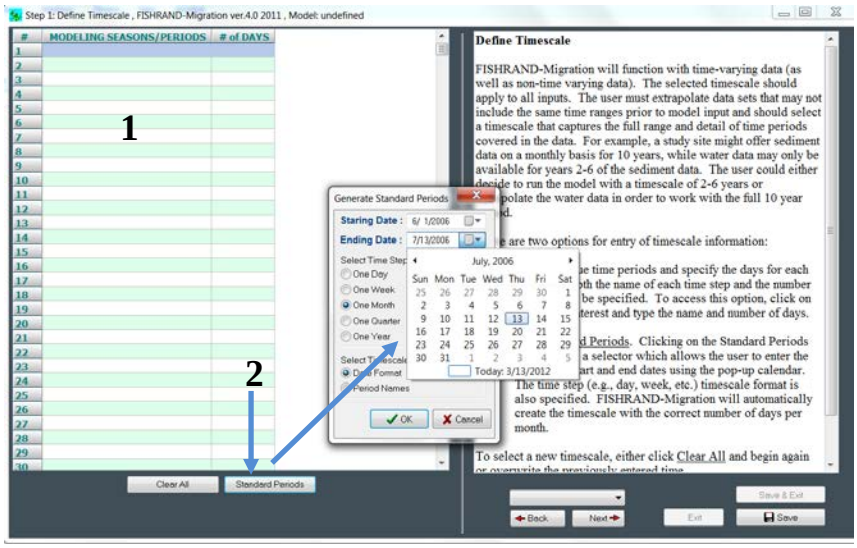
The user may select a subset or all of these options by placing a "✓" in the appropriate selection box. By default, none of these options are selected. The format and number of steps that follow will be determined based on the selection of these options. The step numbers that follow in this User Guide assume that all options have been selected.

When finished specifying the model run name and options, click *Next* to move to the next Step.

4.3 Define Timescale

FR-M accepts time-varying input data, and if time-steps are entered, FR-M requires all inputs to follow the same timescale. For example, if annual sediment data are for a five year period, and water concentrations are available monthly over several, but not all, of those years, the user

would specify a monthly timescale and enter the same sediment concentration across the 12 months in the year. The user would also need to fill in the missing water data (the program will not fill in missing data automatically. A user may enter specific time periods and the number of days in each period **(1)**.

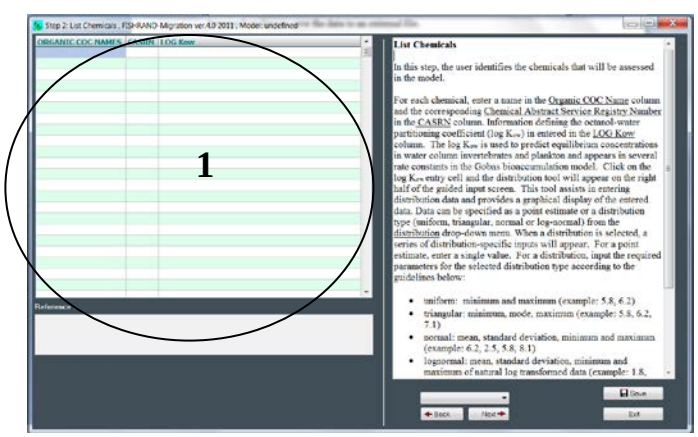


A user may also generate standard periods. By clicking on *Standard Periods* **(2)**, a pop-up selector tool is activated. Using this tool a user enters the starting and ending date, the time step increment (e.g. day, week, month), and the format for the timescale, either date or period names. FR-M will round the time period to the nearest time step increment, e.g. if the time step is one month and a user enters 1/10/04 to 1/25/05, the ending month will be 12/10/04 representing the last complete month.

When the user is collecting data for application in FR-M, he or she should consider standardizing time periods for all data sets. If the time periods differ across data sets, the user is required to reconcile the differences before using FR-M because FR-M will only accept input data with consistent time periods and time steps.

When finished entering inputs for this Step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

4.4 List Chemicals



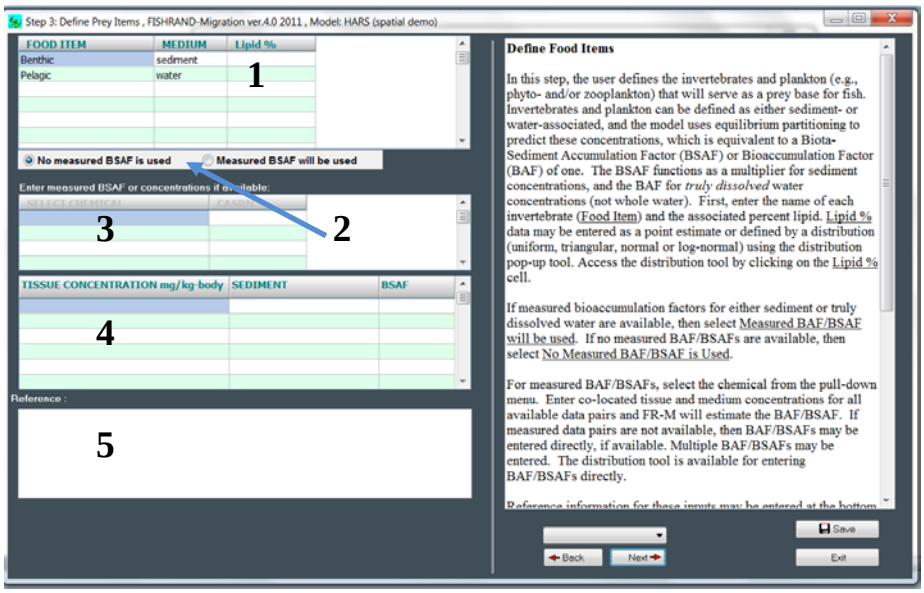
In this step a user names the chemicals that will be assessed in FR-M. The chemical name, chemical abstract service number (CASRN) and the Log octanol water partition coefficient ($LogK_{ow}$) are entered (**1**). The Log K_{ow} data may be entered as a point estimate, or as a distribution (uniform, triangular, normal, lognormal). When a user clicks on the Log K_{ow} entry cell, the distribution input tool

opens. This tool allows a user to select a distribution and displays the required inputs for each specific distribution. A figure of the data distribution is also generated. A single run in FR-M will include all chemicals listed in this step.

When finished entering inputs for this Step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

4.5 Define Prey Items

In this step, prey items such as pelagic or benthic invertebrates, or different kinds of plankton (e.g., phytoplankton) are defined. First **(1)** enter the name of each food item, the medium in which it is found (primary habitat either water or sediment, but not both) and the percent lipid. Percent lipid may be entered as a point estimate or as a distribution. To activate the distribution tool, click on the lipid input cell **(1)**.



Next, specify whether measured BAF data will be used **(2)**. Click either 'No measured BAF is used' OR 'Measured BAF will be used'. If no measured BAF data are used, then the model will estimate food item tissue concentrations using equilibrium partitioning.

If measured BAF values or matching tissue and medium concentrations are available, then highlight the chemical **(3)**. Next, either enter a tissue and medium concentration combination or the BAF **(4)**. A user may enter multiple tissue-medium concentration combinations. Depending on the form of the entered data, FR-M will develop a distribution of BAF/BSAFs from the values and simulate random BAF/BSAFs from the group of entered data **(4)**.

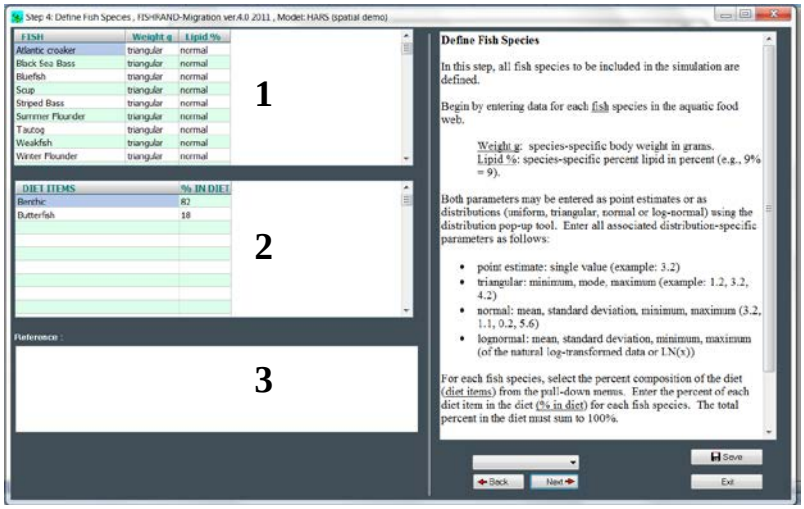
Finally, in this Step a user may record reference information **(5)**. Any text entered here will be tracked and printed on the model report for this data set. Each user determines the format and style of text entered in this section.

When finished entering inputs for this Step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

4.6 Define Fish Species

In this step a user defines the fish species for the FR-M model runs. Tissue concentrations will be estimated for each species entered in this section. In addition to the species name, FR-M requires each species weight, percent lipid and diet composition.

First, enter the fish name (**1**). Users may enter scientific names or common names. Second, enter the body weight in grams. Similar to other data parameters, users may elect to enter a body weight distribution. By clicking on the data entry cell for weight, users access the distribution tool. Third, enter the percent lipid for the fish (**1**).



After entering the weight and lipid data, a user characterizes the diet for each fish species. With the species of interest highlighted at the top of the entry screen, select the species comprising the diet and enter the percent of each species in the diet **(2)**. The only diet items available in the pull-down menu are those entered in the previous step. If a diet item is missing, return to the previous step using the *Back* key, enter the new item, then return to this step and select it. The total percent in diet for each fish species must equal 100% before a user may move to the next step.

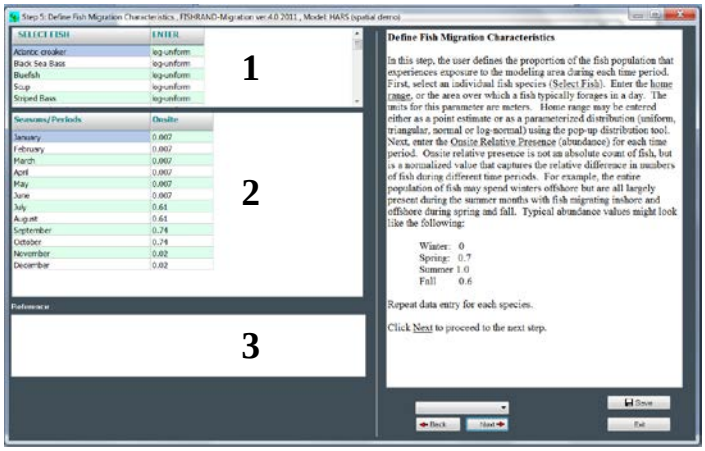
Finally, reference text may be entered in a user-defined format for output in the report **(3)**.

When finished entering inputs for this step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

4.7 Define Fish Migration Characteristics (OPTIONAL)

In this step, fish migration characteristics are entered based on relative abundance as a proportion of the total population. First, select a fish species from the set entered in the previous Step **(1)**. Enter the home range (in meters) for that species. Next, enter the relative abundance for the previously defined seasons or time periods (from Step 1) **(2)**. Abundance, in this case, is defined as relative because it is simply providing an estimate of the likelihood that a species will be found in the site during any given time period/season compared to likelihood of being found during the other time periods. One of the selected time periods should have the maximum relative abundance. Users may choose to enter data as relative to 1, 100 or any

other maximum value, with the remaining time periods being a fraction of the maximum – e.g. 0.5 or 50 in the example.



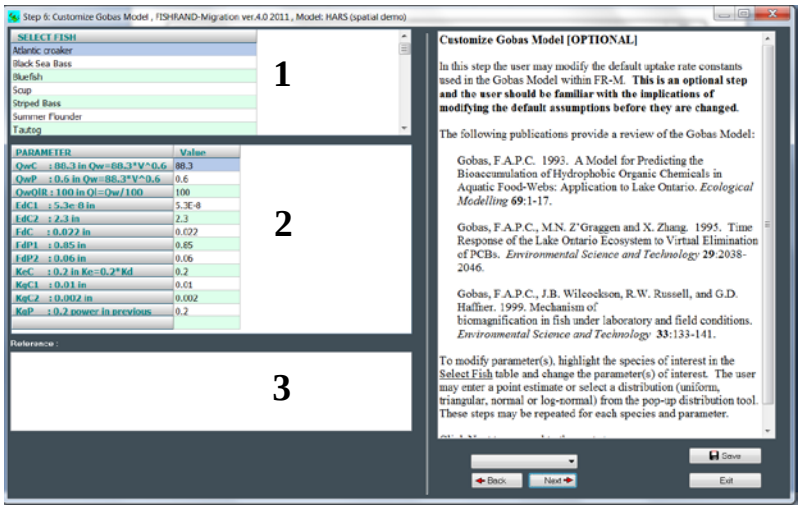
Finally, reference text may be entered in a user-defined format for output in the report **(3)**.

When finished entering inputs for this step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

4.8 Customize Gobas Model (OPTIONAL)

For advanced users who are familiar with the underlying Gobas model structure, the default rate constants may be modified in this step. For detailed bioaccumulation model background information please review Gobas (1993; 1995; 1999).

The parameters may be modified on a species-by-species basis. Select the species **(1)** and then modify the parameters **(2).** Each parameter may be entered either as a point estimate or as a parameterized distribution. References may also be added at the bottom of the screen (**3**).



Caution should be used when modifying the default model parameters.

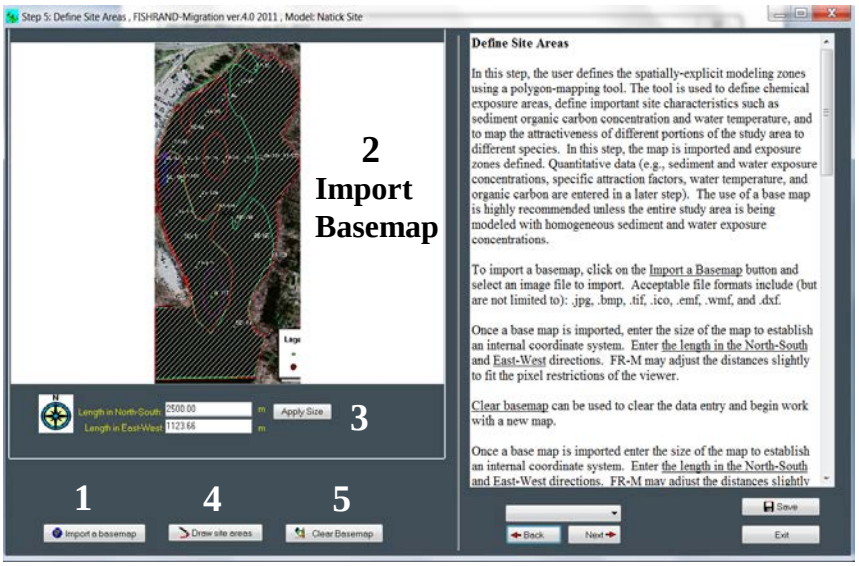
When finished entering inputs for this step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

4.9 Define Site Area and Modeling Zones (OPTIONAL)

A polygon-mapping tool is applied to define the modeling zones within the study area. The tool is used to characterize the chemistry and habitats of a site on a user-supplied base map. Users can define chemical exposure areas and map the attractiveness of different portions of the site

using this polygon drawing tool. FR-M does not link directly to GIS files but allows users to import a base map across a variety of graphical formats, and then essentially draw modeling zones that define chemical concentrations, attraction factors, total organic carbon, miscellaneous site features, and/or water temperature. In this step, a base map is imported **(1)** and modeling zones are defined. In subsequent guided input steps, quantitative attributes that apply to each modeling zone, such chemical concentrations, organic carbon, and attraction factors will be entered for each of the modeling zones.

Define Site Areas Screen



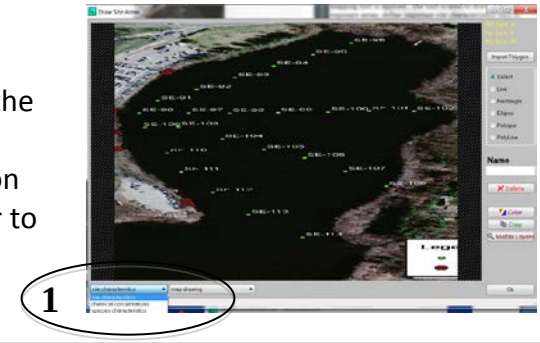
The first step is to Import the base map. Click on the *Import a Basemap* button **(1)** and select an image file to import **(2)**. There are a number of acceptable file formats including, but not limited to: .jpg, .bmp, .tif, .ico, .emf, .wmf, and .dxf.

Once a base map is imported, enter the size of the map to establish an internal coordinate system **(3)** in the model. Enter the length in meters in the North-South and East-West directions. FR-M tracks the pixel numbers and may suggest a correction to the entered measurements if warranted. If you know the size of the map, enter the lengths in meters in the data entry boxes and click *Apply Size*. To clear map work and begin again, click *Clear Basemap* **(4)**.

The next step is to define modeling zones by drawing shapes (e.g., polygons, rectangles, etc.) to define site chemistry and attraction factors. A modeling zone is defined as an area over which the particular input is the same. The size, position and shape are all user-defined based on the available data. Begin by clicking on the *Draw Site Areas* **(5)** button on the *Define Site Areas Screen*. This will open the *Draw Site Areas Tool*.

Draw Site Areas Tool

There are three pull-down menus at the bottom of the Drawing Tool screen **(1)**. The category of data to be entered is selected from the first pull down menu (on the far left hand side of the window) allowing a user to identify the type of polygon to be drawn/defined; options include: *site characteristics, chemical*



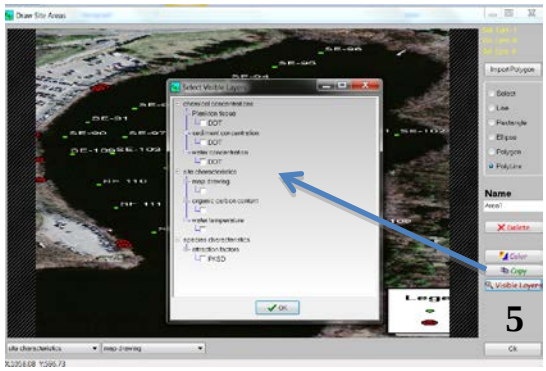
concentrations, or *species characteristics*. When a selection is made, the options in the other two pull down menus will be options specific to the first selection. For example, if a user chooses *chemical concentrations*, then the options in the second pull down menu will be *sediment concentration* or *water concentration* and the third pull down menu will include a list of all of the chemicals of concern.

Depending on which option the user selects, the second pull-down menu offers another series of choices. For *site characteristics*, a user may draw polygons representing *sediment organic carbon concentration*, *water temperature* or *map drawings*, e.g. other site features including underground structures, etc. For the *chemical characteristics* option, users select either *sediment* or *water concentration* in the second menu. For the species characteristics option, users are asked to define species-specific *attraction factors*.

Once the type of polygon is selected, then the user draws applicable modeling zones. Note: actual values associated with each modeling zone are not entered on this screen. Modeling zones are defined by polygons or other shapes, and each modeling zone/shape is assigned a unique name, either automatically or by user entry. If the site includes the entire map, then proceed to define modeling zones; background concentrations (all areas not covered by a specifically defined modeling zone) are characterized in a future step and do not require any specific name. However, if the site is smaller than the map area (e.g., there are land areas), then modeling zone drawing should begin with a polygon or other shape around the study area (e.g., waterbody). **It is very important to define the attraction factor for this zone as 1 for all species (otherwise fish will be exposed on land).** Polygon drawing continues from large to small, nesting each smaller polygon within larger polygons as applicable. Modeling zones may intersect and overlap. The value for any given location is the value of the last shape drawn over an area.

Various drawing methods are available (e.g. ellipse, rectangle, polygon – free form) **(2).** After drawing each polygon, the program will assign a default name; for organizational and presentation purposes, user defined names may be substituted for any default name **(3)**. User-specified names should be unique identifiers and will be used to reference the polygon in future data entry steps. The user can click on *Select* **(4)** then click on a modeling zone to modify the name after the shape has been drawn and saved. *Select* is also used to delete modeling zones (*Select* and then click *Delete* (**5**)) and to move locations after a polygon has been drawn. The color of each polygon can also be modified **(5)**.

A copy function allows a user to copy previously drawn polygons to additional screens in the *Draw Site Areas* window **(5)**. For example, if chemical concentration contours are the same for all chemicals, then a user can draw one set of modeling zones and copy them for each chemical.

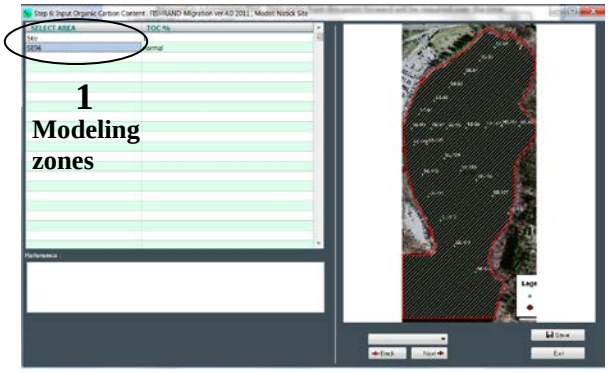


For each medium-chemical combination draw all polygons representing the different concentrations across the landscape. To guide polygon drawing a user may classify a layer as a visible layer (**5**). Visible layers appear in the background of the other drawing tool input screens. These layers are assumed to be useful guides to drawing other modeling zones and shapes. For example, a user may draw important site features under *site characteristics>map* drawing. These features may be landmarks required to draw the chemical and/or habitat polygons. The visible layer (**5**) tool provides users with the opportunity to display layers throughout the drawing tool screens.

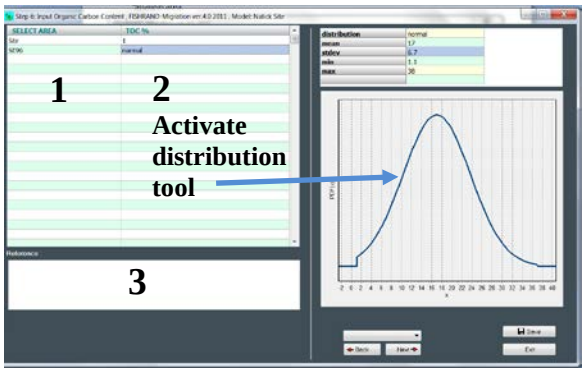
Click *Ok* when all modeling zones have been identified to return to the main screen for this step. Reminder: Quantitative values associated with modeling zones are assigned in subsequent steps.

When modeling zone drawing is complete, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file). Data entry from this point forward will be required over the time scale specified initially, and for each modeling zone.

4.10 Input Organic Carbon Content



In this step, users enter the total organic carbon (TOC) content of the sediment. The previous step defined one or more modeling zones for TOC, which may or may not be the same as the modeling zones for sediment concentrations. The modeling zone names entered previously will appear in the left-hand column *Select Area* **(1)**. Note that the modeling zone names that appear on this screen will only be the shapes defined for TOC assignment in the previous step. The area name "Site" is automatically generated and represents the entire map area. For some sites this may represent background, while for other sites this area may be outside of the analysis area.

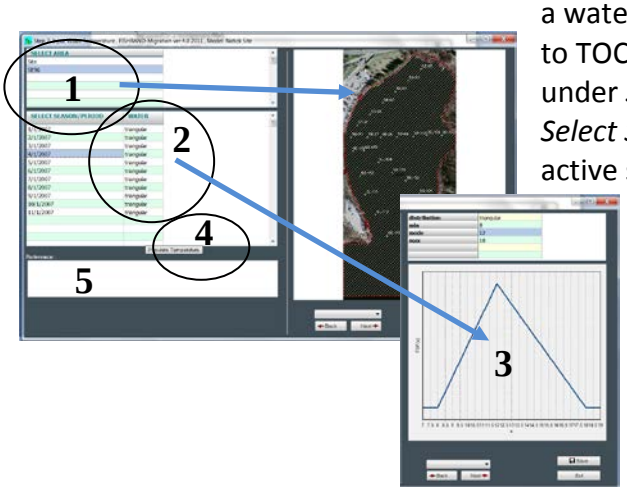


First, highlight an area **(1)**. When the name of a modeling zone is highlighted, a map will appear on the right-hand side of the screen with the selected shape highlighted (red boundary line in the figure on the previous page). Next, click on the *TOC %* value cell **(2)**. This will activate the distribution tool. Enter a point estimate TOC value or define the TOC by parameterizing a distribution. After entering TOC data, supply reference information for the data in a user-defined format **(3)**.

When finished entering inputs for this step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

4.11 Input Water Temperature

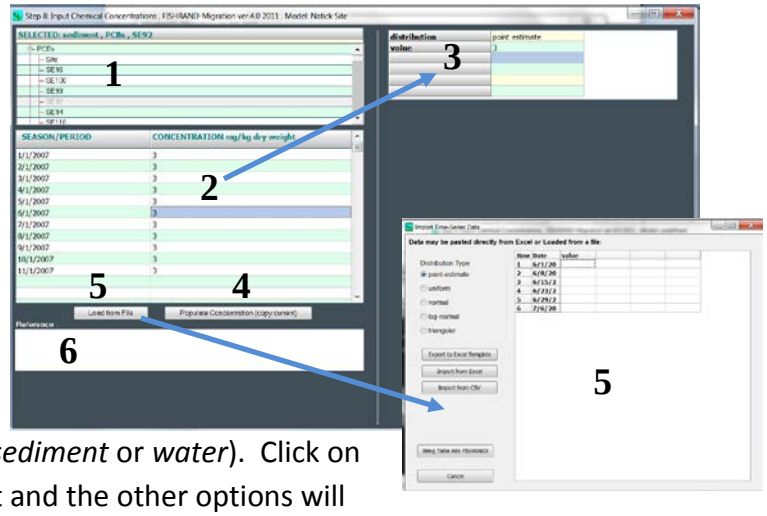
Water temperature is required for the Gobas model and is entered in this step. If modeling zones specific to water temperature were defined in previous steps, then the user should enter a water temperature for each modeling zone. Similar to TOC entry, highlight the modeling zone of interest under *Select Area* and the associated time step under *Select Season/Period* **(1)** and a map illustrating the active shape will appear on the right-hand side of the screen. Enter data by clicking on the *Water Temperature* cell (**2**). A user may enter a point estimate or, using the distribution tool (**3**), parameterize the appropriate distribution. Temperature data must be entered for each time step initially specified, and the *Populate Temperature* **(4)** button can be used to populate the data from the first cell across all time periods if water temperature does not change over time. The same temperature data will be populated whether defined as a point estimate or as a distribution. Enter user-defined references in the space provided (**5**).



When finished entering inputs for this step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

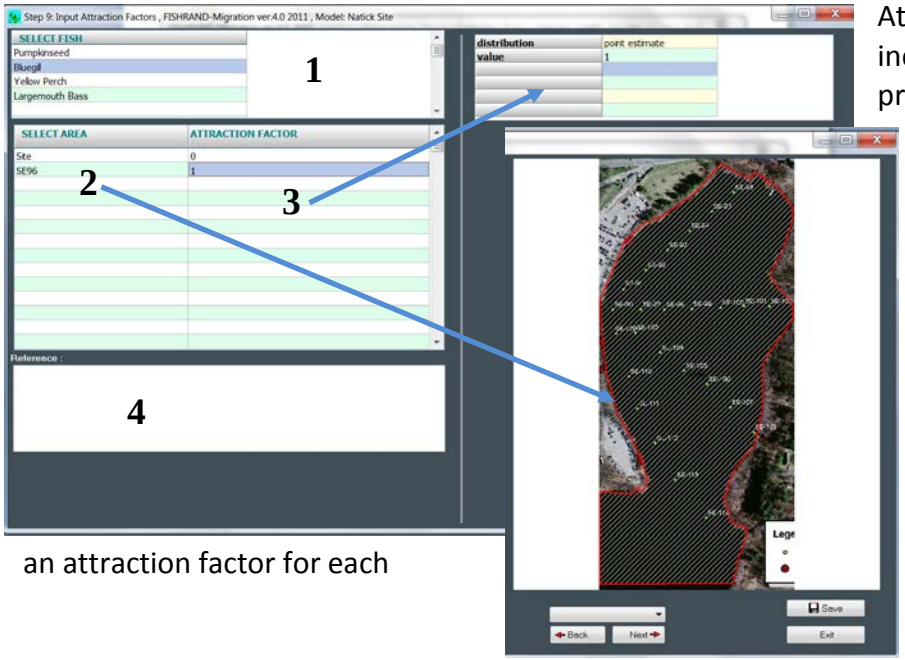
4.12 Input Chemical Concentration

Entering chemical concentration data is similar to the temperature and TOC data entry described in previous steps. Users may enter chemical concentration data for sediment, surface water, or biota (or some combination). If modeling zones specific to the media and the chemical type were defined in previous steps, then a chemical concentration will have to be entered for each modeling zone and chemical-media combination. Similar to TOC and water temperature entry, highlight the modeling zone name of interest **(1)**. In this case the display presents a tier of data entry options (**1**). The top tier is the medium (*sediment* or *water*). Click on the **+** icon next to the medium of interest and the other options will appear below. Next, click on the chemical name and click through each defined modeling zone and enter time-varying chemistry data for each period (**2**). When a modeling zone is highlighted, a map will appear in the right hand window to orient the user (not shown). Chemistry data may be entered as a point estimate or as a distribution (**3**). Click on the value entry cell to activate the distribution tool. For sites without time-varying chemical concentration data, a button is available to populate all time steps with the data entered in the first cell (**4**). Enter data for the first time step, then click *Populate Concentration* (**4**) to fill in all remaining time steps with the same entry. For biota, a user also selects whether the entered data are lipid normalized or entered on a wet weight basis. The selection window is below the data entry window. Alternatively, time-series data may be imported from an external file through the *Load from File* (5) button, which activates a dialog box with a number of options for importing data from Excel. Users can also export a template to Excel, particularly for entering distributions, which provides the exact format for the selected distribution type that FR-M requires. Finally, enter user-defined references in the space provided (**6**).



When finished entering inputs for this step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

4.13 Input Attraction Factors



Attraction factors are used to increase or decrease the probability that a species will forage in one modeling zone compared to other modeling zones. This is used to specify habitat or foraging areas within a study area that are particularly attractive to fish. If modeling zones specific to attraction factors were defined in previous steps, then enter an attraction factor for each species and each area.

Begin by highlighting the fish species of interest (**1**). Next, select the modeling zone name of interest **(2)**. A map illustrating the active polygon will appear on the right-hand side of the screen (**2**). To select the target modeling zone, click on the name in the table or click directly on the target area on the map. A user may enter a point estimate attraction factor or, using the distribution tool (**3**), parameterize the appropriate distribution for each modeling zone.

Enter user-defined references in the space provided (**4**).

When finished entering inputs for this step, click *Next* to proceed with input entry, *Save* to save the data to an external file, or *Exit* to return to the main menu (data entry up to that point will be saved in a temporary file).

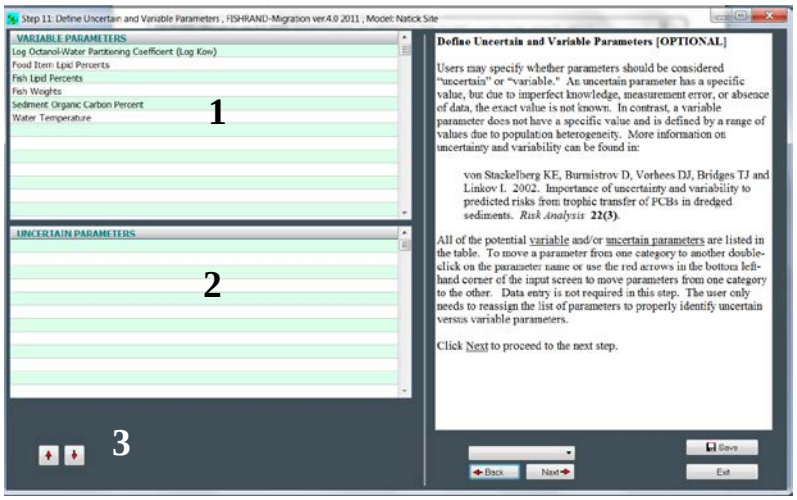
4.14 Input Site Specific Measurements (OPTIONAL)

This option is not functional in the current version of FR-M, but will be added in future releases. For some studies, the user may obtain site-specific fish tissue measurements. These data would be entered into the model for comparison to model results and model calibration/validation.

4.15 Define Uncertain and Variable Parameters (OPTIONAL)

For assessment of uncertainty and variability in the model, a user may specify which parameters are uncertain and which parameters are variable. An uncertain parameter has a

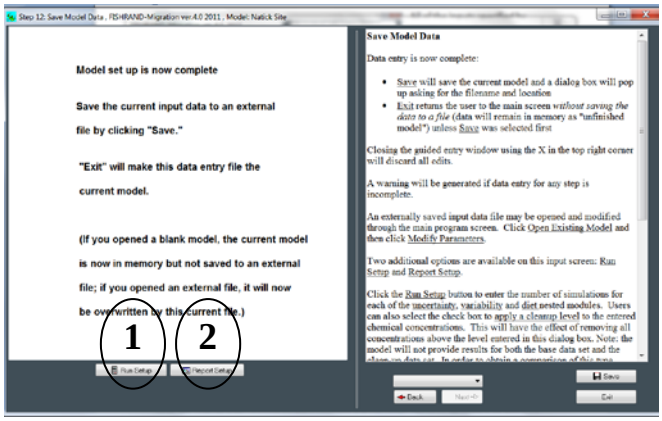
specific value, but due to a lack of knowledge, measurement error or a lack of data, the exact number is not known. In contrast, a variable parameter does not have a specific value. Variable parameters have a range of values and they vary due to the heterogeneity inherent in populations.

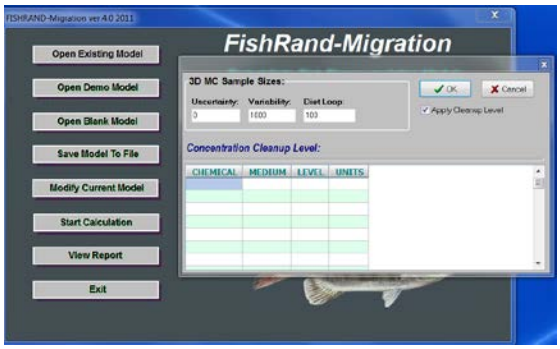


All of the inputs specified by distributions will be listed in the top table (**1**). To move a parameter from the variable **(1)** to uncertain table **(2)** or vice versa, select a parameter and click on the up or down arrow (**3**). Users may want to review von Stackelberg *et al*. (2002a) for additional background on uncertain and variable parameters and analysis of uncertainty and variability.

4.16 Running Model Simulations

The final screen of the guided setup allows users to define the number of simulations for each nested loop by clicking on *Run Setup* (**1**). This dialog box will automatically open again when clicking on *Start Calculation* on the main screen. Users may also select report output options under *Report Setup* (**2**) on this screen or *View Report* from the main screen (assuming the model has been run). Detailed information for that dialog box can be found in the next section.

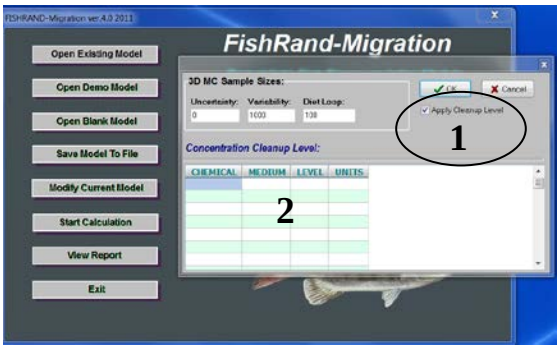




Clicking *Start Calculation* from the main screen or *Run Setup* from this screen brings up the dialog box shown to the left. If data entry is not complete, the following warning message will be generated: "Input for this model was not finished" and the user must click on *Modify Current Model* from the main menu to complete data entry. Following successful data entry, click on *Save* and then *Exit*. Then click *Start Calculation* again.

This will open the Run Model options box shown on the previous page. In this box a user may select the sample sizes for the uncertainty, variability, and diet loops. These functions will only operate if data have been entered as distributions and categorized as either uncertain or variable. As illustrated in Figure 2, FR-M employs a nested Latin Hypercube/Monte Carlo approach for sampling distributions for uncertain and variable parameters. The *Uncertainty Sample Size* refers to number of times that the uncertain parameter distributions will be sampled and, therefore, the number of simulations in the model run. The *Variability Sample Size* may also be specified by the user and refers to the number of times that the variable parameter distributions will be sampled. In general, a higher number of simulations is better, but the increase comes at a computational cost in time. Typical values for these cells range between 100 and 1000. One strategy is to run the model specifying a higher number of samples and then running it again with a lower number and comparing the results to verify that stability in the outputs have been achieved. Finally, a user may specify the diet sample size (*Diet Loop*). Forage fish are exposed to variable diet items (benthic and pelagic invertebrates and phytoplankton), therefore a distribution of diet concentrations is developed. Variability in diet may be explored by specifying the diet sample size or diet averaging time. Because fish diets are variable and the chemical concentrations of diet items are variable depending on where forage fish, invertebrates, or phytoplankton are exposed, the chemical concentrations of predator fish should also reflect diet variability. A typical value for this cell is 10 or higher.

In addition, a user may choose to modify the input dataset to assess the impact of cleanup levels on fish tissue chemical concentrations. First, check off *Apply Cleanup Level* (**1**). Next, choose the chemical, medium and cleanup level/concentration (**2**). The units in the program are fixed and will appear automatically in the units column depending on the medium selected. Any unit adjustments will have to be made externally. The cleanup tool modifies the current data set for the active model run by truncating all input distributions at the level(s) specified in this screen. The tool does not permanently modify the dataset and the model will only generate the results for the cleaned site data when this function is selected. To run the model under current conditions, deselect this function.



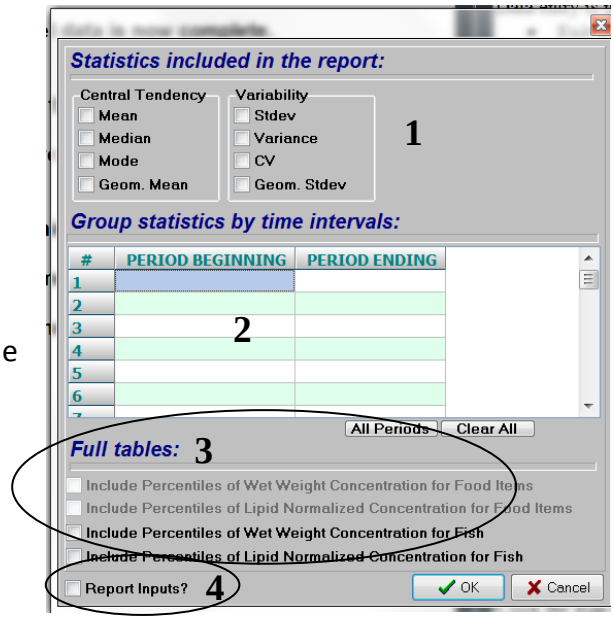
Finally, click Run to complete the calculations. FR-M will run for all chemical and species combinations.

FR-M includes a run status bar. Because some model runs can be very complex depending on the number of assessed chemicals, species and sites, model runs may require many hours. The tool provides the user with feedback on Total Time, Elapsed Time and Remaining Time. These estimates are generated after the model has run for a few minutes.

4.17 Report Viewers

FR-M employs Microsoft Excel to generate simulation reports. After completing the simulation, Click on *View Report* at the main menu.

A report may consist of multiple Excel Worksheets and Workbooks depending on the user-defined content. When a user clicks *View Report*, a statistical selector pops-up. This screen provides the user with a number of reporting options. Because FR-M output is generated in Microsoft Excel, modeling results may be readily copied and pasted into any statistical program for additional assessment.



To begin the report generation process, select the summary statistics to include in the report (**1**). Users may define specific averaging times over which to generate output statistics (**2**). The overall data table will include results across all time periods, but summary statistics can be generated over specific time-periods. For example, a user may elect to evaluate the full time period and also each season independently. The time periods are selected using pull-down menus and one time period may overlap with others. The user also selects the tables to include in the output reports (**3**); a separate output workbook is generated for each of these options. A user may select wet weight or lipid normalized tissue concentration output and view results for prey items and/or the receptor fish species. Finally, a user may elect to include the inputs in the output report using the check box (**4**). Click OK to generate the custom report; an example of a partial summary table is provided to the left.

Fish: Pumpkinseed , Chemical: PCBs

Beginning	Ending	Central Tendency: Mean (ppm)	Central Tendency: Median (ppm)	Variability: Mode (ppm)	Variability: Stdev (ppm)	Variability: Variance (ppm)	Variability: CV
10/1/07	1/1/08	2.26E+00	2.00E+00	6.41E-01	1.80E+00	3.23E+00	7.96E-01
1/1/08	4/1/08	2.42E+00	2.16E+00	5.06E-01	1.89E+00	3.56E+00	7.81E-01
4/1/08	7/1/08	2.43E+00	2.17E+00	5.26E-01	1.89E+00	3.57E+00	7.77E-01

Fish: Pumpkinseed , Chemical: PCB52

Beginning	Ending	Central Tendency: Mean (ppm)	Central Tendency: Median (ppm)	Variability: Mode (ppm)	Variability: Stdev (ppm)	Variability: Variance (p	CV
10/1/07	1/1/08	2.20E-02	2.30E-02	2.60E-03	1.70E-02	2.90E-04	7.83E-01
1/1/08	4/1/08	2.30E-02	2.40E-02	2.40E-03	1.60E-02	2.70E-04	7.23E-01
4/1/08	7/1/08	2.30E-02	2.40E-02	2.10E-03	1.60E-02	2.60E-04	7.08E-01

If the user has selected one or more of the "Include Percentiles" checkboxes shown above (**3**), several additional output files are generated. **Important: Do not work in Excel or open and close any Excel files while FR-M is generating output percentiles.** FR-M generates population distributions of predicted tissue concentrations with our without associated uncertainty depending on whether parameters

were specified as uncertain and/or variable. The predicted body burden at the 10th percentile of variability is interpreted as the concentration experienced by 10% of the population or less. If none of the user inputs were specified as "uncertain", then this would be the only distribution that FR generates. However, when there are uncertain parameters, FR fixes those parameters first, then runs variability loops. The looping is repeated a user-specified number of times with another set of uncertain parameters each time. Upon completion of the model run, there will be as many different "variability" curves representing uncertainty as were specified in *Run Setup*. Each variability percentile has an associated uncertainty distribution. The uncertainty distribution is interpreted as the percent confidence in the variability percentile.

Across the top of the table, a user will see the uncertainty percentiles with each variability percentile underneath (**1**) for each time period specified in the user-defined timescale. In the example below, the 90th percentile uncertainty distributions are shown for all the variability percentiles. We are 90% confident that 90% of the largemouth bass population will experience a predicted body burden of 6.21 mg/kg or less.

1

PCB (total) wet weight normalized Large Mouth Bass,ppm													
Percentile unc.	90%												
Percentile var.	0%	2.50%	5%	10%	25%	50%	75%	90%	95%	97.50%	100%	Mean	Stdev
Time,years													
2/15/77	7.69E-01	7.76E-01	8.19E-01	8.50E-01	8.70E-01	9.21E-01	9.71E-01	1.02E+00	1.09E+00	1.11E+00	1.45E+00	9.32E-01	9.06E-02
3/15/77	2.19E+00	2.27E+00	2.36E+00	2.43E+00	2.58E+00	2.75E+00	2.93E+00	3.18E+00	3.32E+00	3.44E+00	6.11E+00	2.81E+00	4.28E-01
4/15/77	4.07E+00	4.12E+00	4.27E+00	4.32E+00	4.61E+00	5.03E+00	5.45E+00	6.21E+00	6.71E+00	7.18E+00	1.54E+01	5.26E+00	1.23E+00
5/15/77	6.27E+00	6.39E+00	6.66E+00	6.81E+00	7.48E+00	7.99E+00	8.59E+00	9.64E+00	1.02E+01	1.07E+01	2.21E+01	8.27E+00	1.69E+00
6/15/77	8.88E+00	8.94E+00	9.10E+00	9.43E+00	1.02E+01	1.10E+01	1.17E+01	1.27E+01	1.34E+01	2.10E+01	2.38E+01	1.13E+01	2.31E+00
7/15/77	1.20E+01	1.22E+01	1.28E+01	1.31E+01	1.40E+01	1.52E+01	1.65E+01	1.77E+01	1.86E+01	2.33E+01	3.41E+01	1.56E+01	2.80E+00
8/15/77	2.48E+01	2.49E+01	2.55E+01	2.61E+01	2.71E+01	3.00E+01	3.16E+01	3.37E+01	3.54E+01	3.61E+01	4.59E+01	2.99E+01	3.30E+00
9/15/77	3.38E+01	3.44E+01	3.47E+01	3.61E+01	3.77E+01	3.98E+01	4.25E+01	4.50E+01	4.57E+01	5.05E+01	5.61E+01	4.04E+01	3.86E+00
10/15/77	3.34E+01	3.37E+01	3.44E+01	3.52E+01	3.66E+01	3.84E+01	4.02E+01	4.26E+01	4.44E+01	4.54E+01	5.07E+01	3.87E+01	3.04E+00
11/15/77	2.62E+01	2.67E+01	2.69E+01	2.75E+01	2.89E+01	3.04E+01	3.22E+01	3.44E+01	3.71E+01	3.81E+01	9.11E+01	3.15E+01	6.35E+00
12/15/77	2.50E+01	2.50E+01	2.55E+01	2.61E+01	2.72E+01	2.86E+01	3.08E+01	3.29E+01	3.52E+01	3.59E+01	9.21E+01	2.99E+01	6.53E+00
1/15/78	2.34E+01	2.37E+01	2.43E+01	2.46E+01	2.57E+01	2.71E+01	2.90E+01	3.16E+01	3.28E+01	3.43E+01	8.58E+01	2.83E+01	6.08E+00
2/15/78	2.22E+01	2.24E+01	2.30E+01	2.35E+01	2.46E+01	2.56E+01	2.75E+01	2.98E+01	3.07E+01	3.28E+01	8.10E+01	2.68E+01	5.73E+00
3/15/78	2.15E+01	2.16E+01	2.21E+01	2.28E+01	2.36E+01	2.46E+01	2.64E+01	2.82E+01	2.91E+01	3.28E+01	7.68E+01	2.58E+01	5.46E+00
4/15/78	2.09E+01	2.10E+01	2.14E+01	2.19E+01	2.26E+01	2.37E+01	2.54E+01	2.70E+01	2.80E+01	3.11E+01	7.16E+01	2.47E+01	5.02E+00
5/15/78	2.07E+01	2.07E+01	2.11E+01	2.18E+01	2.26E+01	2.35E+01	2.51E+01	2.63E+01	2.74E+01	3.09E+01	6.64E+01	2.44E+01	4.56E+00

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