FGETS Version 3.0.18 User's Manual

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Update: Sep.94

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Abstract

FGETS (Food and Gill Exchange of Toxic Substances) is a FORTRAN simulation program that predicts temporal dynamics of a fish's whole body concentration (g chemical / (grams live weight fish)) of non-ionic, non-metabolized, organic chemicals that are bioaccumulated from water and food. The model is based on a set of diffusion and forced convection partial differential equations, coupled to a process-based fish growth formulation. A full description of the theoretical bases and development of these equations is presented in Barber et al. (1991). FGETS also calculates the time to reach a lethal activity in the fish assuming that the chemical has a narcotic mode of action.

The model considers both biological attributes of the fish and physico-chemical properties of the chemical that determine diffusive exchange across gill membranes and intestinal mucosa. Important biological characteristics used by the model include the fish's gill morphometry, body weight, and fractional aqueous, lipid, and structural organic composition. Relevant physico-chemical properties are the chemical's aqueous diffusivity, molar volume, and n-octanol / water partition coefficient (K_{ow}). The model is parameterized for a particular fish species by means of a morphological, physiological, and trophic database that delineates the fish's gill morphometry, feeding and metabolic demands, and body composition.

Three simulation modes are provided in FGETS v3.0: "laboratory", "food_chain", and "food_web". The "laboratory" mode may be used to describe bioconcentration or bioaccumulation under controlled laboratory conditions, whereas the "food_chain" and "food_web" modes may be used to model these processes under field conditions.

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Introduction FGETS (Food and Gill Exchange of Toxic Substances) is a FORTRAN simulation program that predicts temporal dynamics of a fish's whole body concentration (g chemical / (grams live weight fish)) of non-ionic, non-metabolized, organic chemicals that are bioaccumulated from water and food. The model is based on a set of diffusion and forced convection partial differential equations, coupled to a process-based fish growth formulation. A full description of the theoretical bases and development of these equations is presented in Barber et al. (1991). FGETS also calculates the time to reach a lethal activity in the fish assuming that the chemical has a narcotic mode of action.

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The model is parameterized for a particular fish species by means of a morphological and physiological database that delineates the fish's gill morphometry, feeding and metabolic demands, and body composition. Presently, this database can be used to parameterize FGETS for salmonids, centrarchids, cyprinids, percids, and ictalurids.

Input file format The model's input file has the general structure

```
/ command1   argument(s)
/ command2   argument(s)
...          ...
/ commandn   argument(s)
/ end
```

The leading slash (/) identifies the line as a command. Blanks or tabs before or after the slash are not significant. Each slash is followed by a keyword or phrase, as indicated above, that identifies the record's data. Keywords must be spelled in full without any embedded blanks and must be separated from the record's remaining information by at least one blank or tab. One or more consecutive blanks or tabs are equivalent to one blank. The letter "c" or an exclamation symbol (!) in the first column of a line identifies the line as a comment. The exclamation symbol can also be used anywhere in the record field to start an end-of-line comment, i.e., the remainder of the line, including the exclamation symbol, will be ignored. Comments may be placed anywhere in the input file. Therefore, input files may be documented in as much detail as desired. Commands may be continued by appending an ampersand (&) to the line, e.g., the following two commands lines are equivalent:

```
/ command    arg1 arg2 arg3 &    ! a comment
             arg4 arg5  &        ! another comment
             arg6                ! yet another comment

/command  arg1 arg2 arg3 arg4 arg5 arg6
```

The letter case of the input file is not significant, because each line is transliterated to lower case before parsing. Thus, commands may be typed in upper case, lower case, or a mixture of letter case. The maximum command line length, including continuation lines, is 1024 characters.

Conventions and definitions used in this manual

The BioMagnification Factor (*BMF*) is defined as

$$BMF \quad \frac{C_f}{K_f C_w} \tag{1}$$

where:

C_f is the toxicant concentration in whole fish (g toxicant / (grams live weight fish));

$K_f = P_a + P_l K_l + P_o K_o$ is the fish's thermodynamic bioconcentration factor;

P_a, P_l, P_o are the fractions of whole fish that are aqueous, lipid, and non-lipid organic matter, respectively;

K_l is the partition coefficient between generic lipid and water; $K_l = K_{tw}$ = triolein / water partition coefficient, is calculated using the empirical regression between log(K_{tw}) and log(K_{ow}) (for data see Chiou 1985.),

$$K_l \begin{cases} 1.274\ K_{ow}, & K_{ow} \quad 10^5 \\ 212.8\ K_{ow}^{0.571}, & K_{ow} > 10^5 \end{cases} \tag{2}$$

K_o is the partition coefficient between non-lipid organic matter and water; $K_o = 0.411\ K_{ow}$ (Karickhoff 1981.);

C_w is the toxicant concentration in environmental water (g toxicant / mL);

BMF = 1 implies thermodynamic equilibrium. If the chemical is biomagnified over thermodynamic equilibrium, then *BMF* > 1. If the chemical in the organism has not yet equilibrated with water, then *BMF* < 1.

nchem - refers to the number of chemicals to be simulated; its value is set by the command "/chemicals".

<item> - angle brackets indicate an item that must be provided by the user.

<item$_1$ | item$_2$ | ... | item$_n$> - items separated with a vertical bar (|) denote a selection. Only one item may be selected.

<year_class_range> - may be either an integer or a range, e.g.,

<year_class_range> = n, or
<year_class_range> = n-m

where 1 n m Nage, Nage is the number of year classes specified for the species (see "/ maximum_age"). The <year_class_range> argument is used with fish commands that require a year class specifier. Example:

/ initial_cf 1 0
/ initial_cf 2 0
/ initial_cf 3 0

vs.

/ initial_cf 1-3 0

Both forms are valid.

Commands may be broadly classified into three categories: simulation control parameters, physico-chemical parameters, and fish characterization parameters, although there is some overlapping among classes. The simulation control parameters provide information that is applicable to the simulation as a whole, e.g., length of the simulation, units of time, mass, and concentration used in the input file, temperature of the environment [Celsius], and output options (plots and / or time series). The chemical is described by its physico-chemical properties (molecular weight, molecular volume, n-octanol / water partition coefficient (observed or calculated), etc.), and its concentration in the environment (water, plankton, benthos, and other fish). The fish is characterized by its taxonomy (i.e., genus, species, and family), its ecology (e.g., fresh water *vs.* marine, food guild), gill morphology, feeding and metabolic demands, body composition, initial weight, initial total body chemical concentration, diet, etc. The user has the option of extracting the required morphological, physiological, and ecological parameters from the program's database. Three simulation modes are provided: "laboratory", "food_chain", and "food_web".

Simulation Modes This section describes the simulation modes available in FGETS version 3.0. The "laboratory" mode may be used to describe bioconcentration or bioaccumulation under controlled laboratory conditions, whereas the "food_chain" and "food_web" modes may be used to model these processes under field conditions.

The fish's total body burden, B_f [µgram toxicant], and growth, W [grams wet weight] are modelled using the mass balance equations

$$\frac{dB_f}{dt} \quad S_g k_g (C_w \quad C_a) \quad C_p F \quad C_e E \tag{3}$$

$$\frac{dW}{dt} \quad F \quad E \quad R \quad SDA \quad EX \tag{4}$$

$$C_f \quad \frac{B_f}{W} \quad K_f C_a \tag{5}$$

where S_g is the total gill surface area [cm^2], k_g is the conductance in interlamellar water [cm / day], C_w is the concentration of toxicant in the environmental water [µgram / mL], C_a is the toxicant's concentration in the aqueous fraction of the fish [µgram / mL], C_p is the toxicant's concentration in the prey [µgram / g(w)], C_e is the toxicant's concentration in the feces [µgram / g(w) feces], *F*, *E*, *R*, *SDA*, and *EX* are the fish's daily feeding, egestion, respiration, specific dynamic action (i.e., respiration associated with digestion), and excretion, respectively [g(w) / day], C_f is the toxicant's concentration in whole fish [µgram / g(w)], and K_f is the fish's expected thermodynamic bioconcentration factor (see Eq. (1)). These equations are described in detail in Barber et al. (1991) and apply to all simulation modes.

The laboratory mode is defined as an aquarium with constant in- and out-flows of water. The volume of water in the aquarium remains constant during the simulation. The tank contains a constant number of fish of a single species. The concentration of chemical in the influx water, as well as the water's temperature, are arbitrary. Because the volume of water in the tank cannot be assumed to be infinite (relative to the fish's weight), the fish's uptake and depuration kinetics will alter the concentration of the chemical in the water. The fecal matter eliminated by the fish is thermodynamically equilibrated with the water and homogeneously distributed throughout the aquarium. The fish are feeding on non-specific organic matter (i.e., "food"). The concentration of toxicant in the food, C_p, is formulated either as a constant (i.e., C_p = constant) or as being in thermodynamic equilibrium with the tank's water. In the latter case, $C_p = C_w\, pl_{food}\, K_l\, BMF$, where pl_{food} is the lipid fraction of the food, K_l is a generic lipid-water partition coefficient, and *BMF* is the toxicant's biomagnification factor. Review the definition of *BMF* in the **Conventions** section. In this simulation mode, the concentration of the chemical in the water is modelled by

$$\begin{aligned} \frac{dW_{oc}}{dt} &= N_{fish} p_{ic} E - Q \frac{W_{oc}}{V} \\ \frac{dA_t}{dt} &= Q (C_w^{\,i} - \frac{A_t}{V}) - N_{fish} S_g k_g (C_w - C_a) - C_e E \\ C_w &= \frac{A_t}{V - K_e W_{oc}} \end{aligned} \qquad (6)$$

where W_{oc} is the amount of organic feces in the tank [grams], N_{fish} is the number of fish in the tank, p_{ic} is the fraction of organic carbon of the intestinal contents [dimensionless], Q is the tank inflow [mL / day], V is the tank volume [mL], A_t is the total amount of chemical in the tank (water and feces) [µgrams], $C_w^{\,i}$ is the toxicant's concentration in the influx water [µgram / mL], and K_e is the feces-water partition coefficient. During the simulation, the fish species will die if its internal chemical activity is greater than the lethal activity (see **Toxicological effects** section). The following commands exemplify this simulation mode.

```
/chemicals      1
/burden         laboratory  (flow = 490 mL/minute, volume = 110 Litres, nfish = 30,  &
                            cfood = constant 0)
/wtunits        grams
/cwunits        picograms / Litre                    ! 10-12 grams/Litre
/temperature    constant 10.0
```

```
/cwater        1 constant 0.35
/species       Salvelinus namaycush          ! lake trout
/initial_wt    30.0                          ! initial fish wt.
/initial_cf    1  0.0                        ! "clean" fish.
/growth        1 linear   fishpar
/fishpar       gamma (0.0, 0.0, 1.0, 10.0)   ! no growth
```

The command "/burden laboratory(...)" selects the desired mode. In this example, the tank's volume is 110 Litres, its water flow is 490 mL/minute, and its temperature is 10 C. One chemical will be simulated and its concentration in the influx water is 0.35×10^{-12} grams/Litre. The tank contains 30 lake trout. The initial weight of the trout is 30 grams. The trout will not grow during the simulation. The trout will have no initial chemical burden and will feed on food that contains no chemical ("cfood = constant 0"). Thus, this is a bioconcentration simulation.

The "food_chain" mode is described in Barber et al. (1991). This mode simulates one or two fishes. In the one-fish formulation, the fish of interest is a predator that feeds on either plankton, benthic organisms, or generic fish. See commands "/cplankton", "/cbenthos", and "/cfish". In the two-fish formulation, one fish is the prey of the other. In this formulation, the prey species feeds on either plankton, benthic organisms, or generic fish and the predator feeds on the prey species according to a specific length-length relationship. The food_chain mode requires that the concentration of chemical in the water, plankton, benthos, and generic fish as well as the water temperature be constant during the length of the simulation and only one year class per species is allowed.

The salient features of the one-fish formulation can be illustrated with the following commands:

```
/chemicals     1                                  ! simulate one chemical
/burden        food_chain (predator = "Ictalurus punctatus", prey = benthos)
/cbenthos      constant 185
/tunits        years                              ! time unit: years
/cfunits       ppm
/cwunits       ppm                                ! aq. chem. conc.: ppm == mg/Litre
/temperature   constant 10.00                     ! water temperature: 10 degree C
/cwater        1 constant 285                     ! aq. conc. chem 1: constant, 285 ppm
/species       Ictalurus punctatus                ! channel catfish
...
```

The command "/burden food_chain(...)" selects the food_chain option. In this example, Channel catfish will feed on benthic organisms whose concentration of toxicant is a constant 185 ppm. The chemical's aqueous concentration is constant and equal to 285 ppm, and the ambient water temperature is a constant 10 C.

In the two-fish formulation, the simulation of the prey species is driven by the growth of the predator. At each integration step of the predator, the length of the prey that the predator is expected to ingest is calculated by the length-length relationship

$$Length_{prey} \quad a_0 \quad a_1 Length_{predator} \tag{8}$$

The prey's growth and bioaccumulation are then simulated in steps of "nstep" until the length of the prey is greater than or equal to the length calculated above. Therefore, the simulation times for the predator and prey may become asynchronous and it is for this reason that the "food_chain" mode requires constant environmental conditions. During the simulation, either the predator or the prey will die if its internal chemical activity is greater than the lethal activity (see **Toxicological effects** section). The predator also will die of starvation if no prey is available. The following commands demonstrate the salient features of this predator-prey formulation:

```
/chemicals      1                                   ! simulate one chemical
/burden         food_chain   (predator = "Oncorhynchus mykiss",   &
                              prey = "Alosa pseudoharengus", prey_food = plankton)
/cplankton      equilibrium 0.03 1.0
/tunits         years                               ! time unit: years
/cwater         ppm                                 ! aq. chem. conc.: ppm == mg/Litre
/temperature    constant 10.00                      ! water temperature: 10 C
/cwater         1 constant 285                      ! aq. conc. chem 1: constant, 285 ppm
/tstart         1
/tend           4                                   ! total time: 4-1 = 3 years
/species        Oncorhynchus mykiss                 ! rainbow trout
...
/species        Alosa pseudoharengus                ! alewife
...
```

As with the one-fish example, the command "/burden food_chain(...)" selects the desired formulation. In this case, Rainbow trout will feed on Alewife, which will feed on plankton. The plankton are assumed to be thermodynamically equilibrated with the water. That is, the concentration of toxicant in plankton will be calculated as $C_{plankton} = C_w \, pl_{plankton} \, K_l \, BMF$, where $pl_{plankton}$ is the lipid fraction of the plankton (3% in this case). Review the definition of *BMF* in the **Conventions** section. The chemical's aqueous concentration and the ambient water temperature are both constant. The predator's growth and bioaccumulation models will be run for three years; the prey models will be run to support the growth of the predator.

The simulation mode "food_web" is designed to describe more realistic predator-prey interactions. Several fish species may be simulated simultaneously, each species with an arbitrary number of year classes (see **Restrictions** section). Fish may feed on each other, plankton, or benthos, according to a user-specified diet. The exposure conditions (water temperature, and concentrations of chemical in plankton, benthos and water) are arbitrary. This mode may be illustrated by the following set of commands:

```
/chemicals      1                                   ! sample input; incomplete
/burden                 food_web
/tunits         year
/wtunits                grams
/temperature    file exposure.dat
/cwater         1 file exposure.dat
```

```
/tstart                 0
/tend                   5
!
/species                        Ontario salmonids
/maximum_age            3
/initial_wt             25.0
/initial_cf             1-3  0
/fishpar                        prey_len (1.21, 0.226)  len_wt(9.747e-03, 2.94)
!
/species                        Alosa pseudoharengus
/maximum_age            3
/initial_wt             1.0
/initial_cf             1-3  0
/fishpar                        prey_len (1.21, 0.226)  len_wt(0.024, 2.5)
!
/cplankton              constant 1.0e-5
/cbenthos               equilibrium 0.03 1
/diet
    labels (salmonid: "ontario salmonids", alewife: "alosa pseudoharengus")
    salmonid (age = 1: plankton = 0.55, benthos = 0.45)
    salmonid (age = 2: alewife = 0.75, plankton = 0.15, benthos = 0.10)
    salmonid (age = 3: alewife = 0.65, salmonid = 0.20, plankton = 0.10, benthos = 0.05)
    alewife (age = 1: plankton = 1.0)
    alewife (age = 2: plankton = 0.75, benthos = 0.25)
    alewife (age = 3: plankton = 0.75, benthos = 0.15, alewife = 0.05, salmonid = 0.05)
```

The example presents only the salient features required for the "food_web" mode. The values presented in the "/diet" command were selected to exercise the different options and they do not necessarily represent realistic values for the given system. The "food_web" model option is selected through the command "/burden food_web"; arbitrary temperature and aqueous chemical concentration are read from the file "exposure.dat".

The "/diet" command specifies the diet of each year class. In terms of the example, the diet of the alewife, year class one is 100% plankton; the diet of year class two is 75% plankton, and 25% benthos; the diet of year class three is 5% alewife, 5% salmonids, 75% plankton and 15% benthos. Similarly, the diet of the first year class of the salmonid is 55% plankton, and 45% benthos; the diet of the second year class is 75% alewife, 15% plankton, and 10% benthos; the diet of the third year class is 65% alewife, 20% salmonid, 10% plankton, and 5% benthos. The diet may be also specified in terms of weight ranges (see "/diet").

The command "/initial_wt" specifies the body weight of young-of-the-year fish. The initial body weights of the remaining age classes are generated internally by FGETS as specified by the user. See the command "/growth". In this example, young-of-the-year alewife weigh one gram. When the growth of these fish are simulated for two years (i.e., three year classes), FGETS assigns the initial body weights of two and three year old alewife to be 13.9, and 27.2 grams, respectively. The initial body lengths of these age classes are then calculated to be 4.45, 12.7, and 16.7 cm.

Similarly, the initial weights of the salmonid cohorts are 25.0, 525, and 1.41×10^3 grams; their lengths are 14.4, 40.7, and 56.9 cm, respectively. The initial chemical burden for each cohort is given by the command "/initial_cf", zero in this example for all cohorts.

After the initial weight distributions are generated for all species, the growth and bioaccumulation for all fish are simulated simultaneously. Each age class of a piscivorous species is allowed to feed only on one age class of any fish species, including its own species if the piscivore is cannibalistic. These prey age classes are determined by selecting those classes whose present body lengths are closest to that estimated by the piscivore's predator-prey function (Eq.(8)). The concentration of toxicant in the prey of the k^{th} predator, $C_{p<k>}$, is then calculated as

$$C_{p<k>} \quad \sum_i f_i C_{f<ij>} \tag{9}$$

where the index *i* runs over all fish species, plankton, and benthos, f_i is the fraction of the diet the i^{th} prey item represents, and $C_{f<ij>}$ is the whole body toxicant's concentration of the j^{th} age class of the i^{th} prey species. Note that the "food_web" mode assumes unlimited prey resources. As an example, consider year class three of the salmonids, and assume it weighs 1409 grams. The length of this specimen would be 56.9 cm, and it requires a prey 14.1 cm long (1.21 + 0.226 × 56.9). Among all alewife cohorts, year class two is closest (in length) to the prescribed length. Therefore, for the current integration step, salmonid year class three will feed on alewife year class two. Following a similar argument, the salmonid year class three will feed on salmonids year class one. The total concentration in the prey of the salmonid year class three (at the current integration step) will be

$$C_{p<s3>} \quad 0.65\,C_{f<a2>} \quad 0.20\,C_{f<s1>} \quad 0.10\,C_{<plankton>} \quad 0.05\,C_{<benthos} \tag{10}$$

where <*s3*>, <*s1*>, <*a2*> denote salmonid year classes three and one, and alewife year class two, respectively. At the end of each year, the age of each cohort is increased by one year. This may imply a change in the diet, growth, or other physiological parameters. When the age of a cohort is greater than the maximum age of the fish species (see "/maximum_age"), that cohort dies and it is replaced with a new year class one. For example, when the simulation starts its second year, year class one becomes year class two, year class two becomes year class three, year class three dies (is deleted) and it is replaced with a new year class one.

During this simulation mode, either the predator or prey (a particular age class) will die if its internal chemical activity is greater than the lethal activity (see **Toxicological effects** section); in addition, the predator (a particular age class) will die of starvation if no prey are available.

Toxicological effects The program calculates the time to reach the toxicant's lethal activity, assuming that it acts as a narcotic. The activity of a mixture of chemicals is defined as the sum of the activities of the components of the mixture. The aqueous activity of the j-th chemical is estimated from the formulae

$$C_a = \frac{C_f}{K_f}$$
$$M_a = \frac{C_a}{10^3 \, MW} \qquad (11)$$
$$X_a = {}_w M_a$$
$$A_j = {}_a X_a$$

where

C_f is the toxicant's concentration in whole fish [g / g(w)];
K_f is the thermodynamic bioconcentration factor (see Eq. (1));
C_a is the toxicant's concentration in the aqueous fraction of the fish [g / mL]
MW is the toxicant's molecular weight [grams / mole]
M_a is the molarity of the toxicant [moles / Litre]
${}_w$ is the molar volume of water (0.018 Litres / mole)
X_a is the toxicant's mole fraction [dimensionless]
${}_a$ is the toxicant's aqueous activity coefficient, ${}_a = 7.357 K_{ow}^{1.149}$, (Chiou et al. 1982.)
A_j is the toxicant's aqueous activity

The LA_{50} (chemical activity that will cause 50% mortality of the sample) may be calculated from the above formulae by substituting the observed LC_{50} value for C_f.

For 96-hour acute exposures of 30-day old fathead minnows (i.e., Veith et al. 1983) exchange kinetics appear to become limited for chemicals whose logP > 4. For 7-day acute exposures of guppies (i.e., Konemann 1981a, 1981b) exchange kinetics appear to become limited for chemicals whose logP > 5. For fathead minnows the linear least squares regression

$$\log (LC_{50}, \text{moles/Litre}) = 1.253 - 0.9408 \, clog\, P \qquad (n = 50;\ r = -0.96)$$

can be calculated (see Veith et al. 1983, Tables 1 and 2). The aqueous activity coefficient (${}_a$) of hydrophobic organics can be estimated by the linear regression (Yalkowsky et al. 1983)

$$\log ({}_a) = 1.672 - 0.944 \, clog\, P$$

Therefore

$$\log (LA_{50}) = \log ({}_a) - \log (LC_{50}) - \log ({}_w)$$
$$1.326 - 0.0032 \, clog\, P$$

which yields LA_{50} = 0.0472, approximately. For inter-species correlations see Mayer and Ellersieck 1986 and Barnthouse et al. 1986.

During a simulation, fish may die from two causes: when the internal chemical activity is greater than the lethal activity, or of starvation. All fish die when the internal activity exceeds the toxicant's lethal activity. Predators will die of starvation when all prey items of the particular predator are dead (see "food_chain" and "food_web" modes).

The commands are described alphabetically by class in the following sections. Refer to the index or the table of contents for the location of specific commands.

Simulation control commands This section describes parameters that affect the simulation globally. These commands establish the units of measurement used by other commands, length of the simulation, exchange formulation to be used in the simulation, and output options, e.g., line printer plots, time series, database parameters used in the simulation, etc.

/BURDEN <simulation_mode> (<arg_1>, ..., <arg_n>)

The command sets the simulation mode. The section **Simulation Modes** contains descriptions of all simulation modes, as well as examples. Valid forms of this command are

```
/burden    laboratory   (flow = <tank flow>,  &
                         volume = <tank volume>,  &
                         nfish = <number of fish in the tank>, cfood = <tank food item>)

/burden    food_chain   (predator = <"Predator-species-name">,  &
                         prey = <"Prey-species-name">,  &
                         prey_food = <plankton | benthos | fish>)

/burden    food_chain   (predator = <"Predator-species-name">,  &
                         prey = <plankton | benthos | fish>)

/burden    food_web
```

All keywords ("flow", "predator", etc.) may appear in any order. The form "/burden laboratory (...)" defines the characteristics of the aquarium. The keywords flow, volume, nfish, and cfood provide the values for the tank's water influx, tank volume, number of fish in the tank, and concentration of toxicant in the food, respectively. Units must be included with the fields "flow" and "volume". Note that flow = 0 is a legal value and defines a static system. The concentration of the chemical(s) in the influx water is given by the command "/cwater". The tank's temperature is provided by the command "/temperature". The field "cfood = <tank food item>" has two valid forms:

cfood = constant <$Cfood_1$> ... <$Cfood_{nchem}$>
cfood = equilibrium <pl_{cfood}> <BMF_1> ... <BMF_{nchem}>

The form "cfood = constant ..." will generate constant concentrations of toxicant in food; $Cfood_k$ (k = 1, 2, ..., *nchem*) represent the toxicant's concentration [cfunits].

The form "cfood = equilibrium ..." assumes that the food is in thermodynamic equilibrium with the water. The concentration of the toxicant in food, $C_{food}(t)$, is given by

$$K_{food} \quad pl_{food} K_l$$
$$C_{food}(t) \quad K_{food} BMF_j C_w(t)$$

where

K_{food} is the thermodynamic bioconcentration factor of the toxicant;
pl_{food} is the mean lipid fraction of the food;
K_l is a generic lipid-water partition coefficient (see Eq. (2));
BMF_j is the (observed) biomagnification factor of the toxicant (see Eq. (1));
$C_w(t)$ is the aqueous concentration of the toxicant;

The form

```
/burden    food_chain    (predator = <"Predator-species-name">,  &
                          prey = <"Prey-species-name">,  &
                          prey_food = <plankton | benthos | fish>)
```

defines a simple food chain simulation (two-fish formulation): the predator feeds on the prey, which feeds on either plankton, benthic organisms, or generic fish. The concentration of toxicant in the prey_food is set by the command "/cplankton", "/cbenthos", or "/cfish" (q.v.). The food_chain mode requires constant environmental conditions.

The form

```
/burden    food_chain    (predator = <"Predator-species-name">,  &
                          prey = <plankton | benthos | fish>)
```

defines another simple food chain simulation (one-fish formulation): the predator feeds on either plankton, benthic organisms, or generic fish. The concentration of toxicant in the prey is set by the command "/cplankton", "/cbenthos", or "/cfish" (q.v.). The food_chain mode requires constant environmental conditions.

The form

```
/burden    food_web
```

defines the food_web mode. The section **Simulation Modes** contains a description of this mode.

Examples:
Review the section **Simulation Modes** for examples. Review also "/cplankton", "/cbenthos", and "/cfish" commands.

/CFUNITS <units of concentration of chemical in fish>
The command specifies the units of "/initial_cf", i.e., the fish's initial total body chemical concentration. These are also the units used by the commands "/burden laboratory (cfood = constant ...", "/cfish constant ...", "/cplankton constant ...", "/cbenthos constant ...", and "/observations ...". The units are converted from "cfunits" to ppm (i.e., mg/Litre) for internal calculation and simulation output. Review the section **Units** for a description of the units' syntax and available units.

Example: /cfunits nanograms mL^-1
The units of concentration of chemical in fish are ng/mL.

/CWUNITS <units of concentration of chemical in water>
The command specifies the units associated with all input aqueous chemical concentrations, cwater. The given units are converted to ppm (i.e., mg/Litre) for internal calculation and model output. Review the section **Units** for a description of the units' syntax and available units.

Example: /cwunits ppm
The units of concentration of chemical in water are ppm (i.e., mg/Litre).

/END
The "/end" command terminates parameter input. This command must be the last command in the data file. Any other text/commands following it will be ignored. The program validates the input for syntactical accuracy during the initial read. After the input file is read, the parameters are checked for inconsistencies.

Example: /end
/HEADER "title"
The command specifies a title to be used on each page of the output file. The maximum length of the string is 80 characters. The command is optional.

Example: /header "Farm pond simulation, exposure with a slow hydrolysis rate constant"

/NSTEP <real_number>
The command specifies the number of steps per day used by the integration method (Euler). "Real_number" should be greater than or equal to one. Large values may increase the accuracy of the integration but will increase execution time. The command is optional; if it is not specified, a default value of 8 is assumed. If the step size is too large for proper integration, a message to that effect will be issued.

Example: /nstep 24 ! 24 steps/day, i.e., one step every hour.

/PLANKTON_STANDING_STOCK <option(s)>
The command specifies the concentration of plankton in the ambient water [grams/Litre]. The command may be used only if food_chain or food_web modes is selected. Valid forms of the command are:

/plankton_standing_stock constant *Cp*
/plankton_standing_stock file *Plankton-filename*

The form "/plankton_standing_stock constant *Cp*" will set the plankton standing stock to *Cp* grams/Litre for the duration of the simulation.

The form "/plankton_standing_stock file *Plankton-filename*" will read the standing stock from the file *Plankton-filename*. The format of this file depends on the option selected with the command "/cplankton". Review the section **General Information on Exposure files**.

If "/cplankton file *Plankton-filename*" is *not* selected, then the format of the file is

t_1 plankton_standing_stock$_1$
t_2 plankton_standing_stock$_2$
... ...
t_n plankton_standing_stock$_n$

where t_j is the simulation time [tunits], and plankton_standing_stock$_j$ has units of grams / Litre.

If "/cplankton file *Plankton-filename*" is selected, then both commands must access the same file. The format of the file is described under the command "/cplankton".

Example:

/plankton_standing_stock constant 1.40e-3

The plankton standing stock will be held constant at 1.40×10^{-3} grams / Litre (Lake Ontario nominal grazeable plankton, Scavia 1980; Flint 1986).

/PLOT <option$_1$> <option$_2$> ... <option$_n$>

The command specifies the line-printer plots or time_series data to be output. One or more options may be selected. The options may appear one per card, or all in one card, separated by one or more blanks or tabs. Valid options are:

wt (time), plot weight of fish [grams live] *vs.* time [days]

cfish (time or wt), plot whole body chemical concentration [ppm] *vs.* time [days] or *vs.* weight of fish [grams live]

total_activity (time or wt), plot activity of the mixture of chemicals in the fish [dimensionless] *vs.* time [days] or *vs.* weight of fish [grams live].

cw (time), plot chemical's water concentration [ppm] *vs.* time [days]

cf_aroclor (time or wt, arg$_1$, arg$_2$, ..., arg$_{nchem}$), plot fish's aroclor *vs.* time [days] or *vs.* weight of fish [grams live]. The aroclor (percent chlorine in a mixture) is defined by the equation

$$\text{aroclor} \quad \frac{C_i w_i}{C_i} \tag{17}$$

where C_i and w_i are the concentration and the %Cl of the i^{th} chemical, respectively. For example, assume the following concentrations [picograms / Litre] of tetra-, penta-, hexa- and hepta-PCBs (polychlorinated biphenyls) in water

PCB	concentration	% Cl
tetra	285.0	48.6
penta	356.0	54.3
hexa	130.0	58.9
hepta	29.0	62.8

The aroclor of this mixture is 53.3.

Examples:

```
/plot
  wt(time)
```
Plot weight of the fish as a function of time.

```
/chemicals      4
/toxlab         "tetra PCB"  "penta PCB"  "hexa PCB"  "hepta PCB"
/plot           cf_aroclor (wt, 48.6, 54.4, 58.9, 62.8)  cfish(time)
```

Plot the aroclor of the mixture of PCB's as a function of fish's body weight. Tetra-, penta-, hexa-, and hepta-PCB's (polychlorinated biphenyls) are 48.6%, 54.3%, 58.9%, and 62.8% chlorine respectively. Also, plot the concentration of chemical in fish as a function of time.

/PRINT <option$_1$> <option$_2$> ... <option$_n$>

The command retrieves information computed during the simulation. The command is optional; the default is to disable all options. Valid options are:

```
/print  fishpar (<reference_temperature>)
/print  update_input
/print  time_series
```

The options may appear one per card as shown, or all on one card, separated by one or more blanks, e.g.,

```
/print  fishpar(<reference_temperature>)  update_input  time_series
```

If the option "fishpar" is selected, the allometric functions used to calculate the morphological, physiological and trophic parameters will be written to the output file. These regressions will be normalized to "<reference_temperature>". See under the command "/fishpar" and the database section for more information on the allometric functions.

If the option "update_input" is selected, an updated command file will be created, which may be used for a subsequent run. The name of the file will be of the form "xxx.fcs", where "xxx" is the name of the original command file (e.g., "test.dat" will generate "test.fcs"). The file will contain the information used in the current simulation, updated as follows:

```
/tstart       <current value of "/tend">
/tend         <current value of "/tend">
/initial_wt   <weight of fish at time "/tend">
/initial_cf   <concentration of chemical in fish at time "/tend">
```

The values of "/tstart" and "/tend" must be modified as appropriate before using the file as input.

If the option "time_series" is selected, a file with time dynamics will be created; this information may be used for plotting, regressions, etc. The name of the file will be of the form "xxx.fts", where "xxx" is the name of the original command file (e.g., "test.dat" will generate "test.fts"). The command "/plot" selects the sections to be written to the file. The file "xxx.fts" may contain one or

more sections, depending on the number of options selected with the command "/plot". Each section of is of the form:

xlabel: label
ylabel: label
ztitle: label
Nsets
Nset_1
x_1 y_1
... ...
x_{Nset_1} y_{Nset_1}
...
Nset_Nsets
x_1 y_1
... ...
x_{Nset_Nsets} y_{Nset_Nsets}

where "xlabel" identifies the abscissa, "ylabel" identifies the ordinate, "ztitle" identifies the data, Nsets is the number of sets in the section, Nset_j (j = 1, 2, ..., Nsets) is the number of observations in the j-th subset. If the section contains observed data (see "/observations"), it will be the last subset. If a particular plot is not enabled (*via* "/plot"), its data will not be printed. If the option "food_web" is selected, the data will be printed at the end of each year of simulation, otherwise the data will be printed at the end of the simulation. The order of the sections is:

cwater *vs.* t - *nchem* consecutive sections
for each species:
wt *vs.* t - one section of Nage+1 sets
cf *vs.* t - *nchem* consecutive sections of Nage+1 sets
cf *vs.* wt - *nchem* consecutive sections of Nage+1 sets
aroclor *vs.* t - one section of Nage+1 sets
aroclor *vs.* wt - one section of Nage+1 sets
activity *vs.* t - one section of Nage+1 sets
activity *vs.* wt - one section of Nage+1 sets

where Nage is the number of year classes to be simulated for the particular fish species; its value is set by the command "/maximum_age".

Example:

```
/plot       cfish(time)
/print      fishpar(15)  update_input  time_series
```

Print allometric regressions at a reference temperature of 15 C. Generate an updated input file and a time series file. The time series file will contain total concentration of chemical in fish as a function of time for each species.

/TEMPERATURE <options>

The command specifies the ambient's water temperature [Celsius]. Valid forms of this command are:

/temperature	constant	p_1
/temperature	sin	$p_1\ p_2\ p_3\ p_4$
/temperature	file	*Cw-Temp-filename*

where p_1, p_2, p_3, and p_4 are numbers, and *Cw-Temp-filename* is a valid file name. To illustrate these alternative inputs let $T(t)$ denote the ambient's water temperature [Celsius] at time t [tunits]. The form "/temperature constant p_1" will generate ambient water temperatures as $T(t) = p_1$, where p_1 has units of degrees Celsius.

The form "/temperature sin $p_1\ p_2\ p_3\ p_4$" will generate ambient water temperatures dynamically as $T(t) = p_1 + p_2 \sin(p_3 t + p_4)$, where p_1 is the temperature's mean value (over one period) [Celsius], p_2 is the amplitude [Celsius], p_3 is the frequency ($p_3 = 2$ / period) and has units of 1/tunits, p_4 is the phase angle [radians].

The form "/temperature file *Cw-Temp-filename*" will read ambient water temperatures from the file "*Cw-Temp-filename*". See "/cwater file ..." for a description of this option.

Examples:

```
/tunits              years
/temperature sin 8  4  6.28  0
```

The mean water temperature (over one year) is 8.0 C, with a range of 8-4=4 C to 8+4=12 C over a period of one year; the frequency p_3 is equal to 2 /(1 year).

```
/tunits              days
/temperature sin  8.0  4.0  1.72e-02  0.0e+00
```

The period of this function is 365 days ($2 / (1.72 \times 10^{-2}$ days^{-1})); the mean temperature over that period is 8.0 C, with a range of 8-4=4 C to 8+4=12 C.

Note that the previous two examples describe the same temperature dynamics.

```
/temperature      file  dioxin.exp
```

Read environmental temperature from the file "dioxin.exp". Information on the format of this file may be found under "/cwater".

/TEND <real_number>

The command specifies the simulation's ending time. The time unit is specified by the command "/tunits". The time units will be converted into days for internal use and subsequent model output.

Example:

```
/tunits          years
/tend      2
```

Run a two-year simulation.

/TSTART <real_number>
The command specifies the simulation's beginning time. The time unit is specified by the command "/tunits". The units will be converted into days for internal use and subsequent model output. The command is optional; if it is not specified, a default value of zero is assumed.

Example:

```
/tunits      years
/tstart   1
```

The simulation will start at year one.

/TUNITS <time-units>
The command specifies the time units (e.g., years) associated with the commands "/tstart", "/tend", "/cwater", "/temperature", "/cplankton", "/cbenthos", and "/observations". The time units associated with these commands must be the same. The user must be careful to verify that the time units associated with these commands and any associated exposure files (see "/cwater", "/temperature", "/cplankton", "/cbenthos") are indeed the same. Review the section **Units** for a description of the units' syntax and available units.

Example: /tunits days
The time units of the input file will be days.

/UPDATE_GROWTH <option>
The command specifies the frequency at which the physiological parameters are updated. Valid forms of the command are

```
/update_growth  continuously
/update_growth  daily
```

If "continuously" is selected, the physiological parameters will be updated at every integration step (see "/nstep"); if "daily" is selected, the parameters will be updated once per simulation day. The default value is "daily".

/WTUNITS <units of mass>
The command specifies the units of the fish's live weight (e.g., kilograms). See "/initial_wt". Review the section **Units** for a description of the units' syntax and available units.

Example: /wtunits grams
The weight units of the input file are grams.

Physico-chemical parameters This section describes commands that characterize the physico-chemical properties of the chemicals whose exchange kinetics will be simulated, as well as commands that define the concentration of the chemical in the environment (water, plankton, and benthos).

/CBENTHOS <options>

The command specifies the temporal dynamics of the chemical's concentration in benthic organisms. The command may be used only if the "food_web" or "food_chain" modes were selected. Valid forms of the command are:

/cbenthos file *Benthos-filename*
/cbenthos constant Cb_1 ... Cb_{nchem}
/cbenthos equilibrium $pl_{benthos}$ BMF_1 ... BMF_{nchem}

The form "/cbenthos file *Benthos-filename*" will read the concentration of toxicant in benthic organisms from the file *Benthos-filename*. Review the section **General Information on Exposure files**. The format of the file is

t_1	$Cbenthos_{1,1}$	$Cbenthos_{1,2}$	...	$Cbenthos_{1,nchem}$
t_2	$Cbenthos_{2,1}$	$Cbenthos_{2,2}$	...	$Cbenthos_{2,nchem}$
...	...	...	...	...
t_n	$Cbenthos_{n,1}$	$Cbenthos_{n,2}$	...	$Cbenthos_{n,nchem}$

where t_j is the simulation time [tunits], and $Cbenthos_{j,k}$ represents the concentration of the k-th toxicant in benthos (k = 1, 2, ..., *nchem*), in cfunits.

The form "/cbenthos constant ..." will generate constant concentrations of toxicant in benthic organisms; Cb_k (k = 1, 2, ..., *nchem*) represent the toxicant's concentration [cfunits].

The form "/cbenthos equilibrium ..." assumes that benthic organisms are in thermodynamic equilibrium with the water. The concentration of the toxicant in benthos, $C_{benthos}(t)$, is given by

$$C_{benthos}(t) \quad K_{benthos} \; pl_{benthos} \; K_l \; BMF_j \; C_w(t)$$

where

$K_{benthos}$ is the thermodynamic bioconcentration factor of the toxicant;
$pl_{benthos}$ is the mean lipid fraction of benthic organisms;
K_l is a generic lipid-water partition coefficient of the toxicant (see Eq. (2));
BMF_j is the (observed) biomagnification factor of the toxicant (see Eq. (1));
$C_w(t)$ is the aqueous concentration of the toxicant;

Example:

/chemicals 1
/cwater ppm
/cbenthos constant 0.08

Simulate one chemical; its concentration in benthic organisms will be 0.08 ppm.

/CFISH <options>

The command specifies the temporal dynamics of the chemical's concentration in the prey-fish. The command may be used only if "food_chain" mode was selected. Review the section **Simulation Modes**. Valid forms of the command are:

/cfish	constant	Cp_1 ... Cp_{nchem}
/cfish	equilibrium	pl_{prey} BMF_1 ... BMF_{nchem}

The form "/cfish constant ..." will generate constant concentrations of toxicant in the prey; Cp_k (k = 1, 2, ..., *nchem*) represent the toxicant's concentration in the prey [cfunits].

The form "/cfish equilibrium ..." assumes that the prey is in thermodynamic equilibrium with the water. The concentration of the toxicant, C_{prey}, is determined by

$$K_{prey} \quad pl_{prey} K_l$$
$$C_{prey}(t) \quad K_{prey} BMF_j C_w(t)$$

where

K_{prey} is the thermodynamic bioconcentration factor of the toxicant;
pl_{prey} is the mean lipid fraction of prey-fish;
K_l is the partition coefficient between generic lipid and water;
BMF_j is the (observed) biomagnification factor of the toxicant (see Eq. (1));
C_w is the aqueous concentration of the toxicant;

The equilibrium value will be adjusted using the biomagnification factor (*BMF*) of the prey. If the prey is to be biomagnified above thermodynamic equilibrium, then $BMF > 1$. On the other hand, if the prey has not yet equilibrated with the water, $BMF < 1$. Based on preliminary analysis (Barber et al. 1988, 1991) typically $0 < BMF < 5$.

If the fish is a piscivore, a K_{prey} will be assigned based on MacKay's (1982) generalized fish K_{prey} regression,

$$K_{prey} \quad 0.048 K_{ow}$$

Example:

```
/chemicals      1
/burden         food_chain (predator = "Oncorhynchus mykiss", prey = cfish)
/cfish          equilibrium 0.05 1
/species        Oncorhynchus mykiss                ! rainbow trout
/ecology        fresh piscivore
```

Simulate one chemical. Rainbow trout will feed on generic prey-fish which is in thermodynamic equilibrium with water and is 5% lipid. Because the trout was identified as a piscivore ("/ecology"), MacKay's generalized K_{prey} will be used.

/CHEMICALS <number of chemicals>

The command specifies the number of chemicals to be used in the simulation. This command must precede the commands "/burden laboratory (cfood = ...", "/cbenthos", "/cfish", "/clogp", "/cplankton", "/cwater", "/logp", "/melting_point", "/molvol", "/molwt", "/plot cf_aroclor(...)", "/toxlab", and "/observations". It is suggested that "/chemicals" be the first command in the input file.

Example: /chemicals 4

/CLOGP $clogP_1$ $clogP_2$ ... $clogP_{nchem}$

The command specifies the chemical's calculated (Leo-Hansch) $\log_{10}(K_{ow})$, where K_{ow} is the n-octanol/water partition coefficient. Because Clogp generally overestimates logP for chemicals whose observed logP's > 5.0, the program adjusts clogP as

$$log\ P \begin{cases} 0.986\ cLog\ P\ 0.0276, & clog\ P\ 5.0 \quad (n\ 59;\ r\ 0.970) \\ 0.601\ clog\ P\ 1.933, & clog\ P > 5.0 \quad (n\ 90;\ r\ 0.937) \end{cases}$$

These regressions where calculated using clogP's and observed logP's for chlorobenzenes, chlorinated biphenyls, brominated biphenyls, methylated biphenyls, chlorinated dioxins, and chlorinated furans. For data see Bruggeman et al. 1982, Chiou 1985, Doucette and Andren 1987, Miller et al. 1985, Gobas et al. 1988.

Either "/logp" or "/clogp" should be specified; if both are provided, "/logp" will be used. If clogP data is to be used without the correction described above, it should be entered as "/logp" data.

Example:

/chemicals	4			
/clogp	6.88	7.59	8.31	9.02

/CPLANKTON <options>

The command specifies the temporal dynamics of the chemical's concentration in plankton. The command may be used only if the "food_web" or "food_chain" modes were selected. Valid forms of the command are:

/cplankton	file	*Plankton-filename*
/cplankton	constant	Cp_1 ... Cp_{nchem}
/cplankton	equilibrium	$pl_{plankton}$ BMF_1 ... BMF_{nchem}

The form "/cplankton file *Plankton-filename*" will read the concentration of toxicant in plankton from the file *Plankton-filename*. The format of this file depends on the option selected with the command "/plankton_standing_stock ...". Review the section **General Information on Exposure files**.

If "/plankton_standing_stock file *Plankton-filename*" is *not* selected, then the format of the file is

t_1	$Cplankton_{1,1}$	$Cplankton_{1,2}$	...	$Cplankton_{1,nchem}$
t_2	$Cplankton_{2,1}$	$Cplankton_{2,2}$	...	$Cplankton_{2,nchem}$
...	...	...	...	...
t_n	$Cplankton_{n,1}$	$Cplankton_{n,2}$	...	$Cplankton_{n,nchem}$

where t_j is the simulation time [tunits], and $Cplankton_{j,k}$ represents the concentration of the k-th toxicant in plankton (k = 1, 2, ..., *nchem*), in cfunits.

If "/plankton_standing_stock file *Plankton-filename*" is selected, then both commands must access the same file. The format of the file is

t_1 plankton_standing_stock$_1$ Cplankton$_{1,1}$ Cplankton$_{1,2}$ ... Cplankton$_{1,nchem}$
t_2 plankton_standing_stock$_2$ Cplankton$_{2,1}$ Cplankton$_{2,2}$ ... Cplankton$_{2,nchem}$
... ...
t_n plankton_standing_stock$_n$ Cplankton$_{n,1}$ Cplankton$_{n,2}$ ... Cplankton$_{n,nchem}$

where t_j is the simulation time [tunits], plankton_standing_stock$_j$ has units of grams/Litre, and Cplankton$_{j,k}$ represents the concentration of the k-th toxicant in plankton (k = 1, 2, ..., *nchem*), in cfunits.

The form "/cplankton constant Cp_1 ... Cp_{nchem}" will generate constant concentrations of toxicant in plankton; Cp_k (k = 1, 2, ..., *nchem*) represent the toxicant's concentration [cfunits].

The form "/cplankton equilibrium $pl_{plankton}$ BMF_1 ... BMF_{nchem}" assumes that plankton is in thermodynamic equilibrium with the water. The concentration of the toxicant in plankton, $C_{plankton}(t)$, is given by

$$K_{plankton} \quad pl_{plankton} K_l$$
$$C_{plankton}(t) \quad K_{plankton} BMF_j C_w(t)$$

where

$K_{plankton}$ is the thermodynamic bioconcentration factor of the toxicant;
$pl_{plankton}$ is the mean lipid fraction of plankton;
K_l is a generic lipid-water partition coefficient of the toxicant (see Eq. (2));
BMF_j is the (observed) biomagnification factor of the toxicant (see Eq. (1));
$C_w(t)$ is the aqueous concentration of the toxicant;

Example:

/chemicals 1
/cplankton equilibrium 0.05 1

Simulate one chemical. The concentration of chemical in plankton will be in thermodynamic equilibrium with the environmental water. Assume plankton in 5% lipid.

/CWATER <chemical_number> <arg$_1$> ... <arg$_n$>

The command specifies the temporal dynamics of the chemical's dissolved water concentration. See documentation and examples for "/temperature", since these commands are closely related. Valid forms of the command are:

/cwater <chemical_number> constant p_1
/cwater <chemical_number> sin p_1 p_2 p_3 p_4
/cwater <chemical_number> exp p_1 p_2 p_3
/cwater <chemical_number> file *Cw-Temp-filename*

where <chemical_number> is a number between 1 and *nchem*. Chemical_number associates the function to a particular chemical. A command must be provided for each chemical to be simulated.

To illustrate these alternative inputs let $C_w(t)$ denote the chemical's water concentration [cwunits] at time t [tunits]. The form "/cwater ... constant ..." will generate dissolved chemical water concentrations as $C_w(t) = p_1$, where p_1 has units of cwunits.

The form "/cwater ... sin ..." will generate dissolved chemical water concentrations as $C_w(t) = p_1 + p_2 \sin(p_3 t + p_4)$, where p_1 is the mean dissolved chemical water concentration (over one period) [cwunits], p_2 is the amplitude [cwunits], p_3 is the frequency ($p_3 = 2$ /period) and has units of 1/tunits, and p_4 is the phase angle [radians].

The form "/cwater ... exp ..." will generate dissolved water concentrations as $C_w(t) = p_1 + p_2 \exp(p_3 t)$, where p_1 and p_2 have units of cwunits and p_3 has units of 1/tunits.

The form "/cwater file *Cw-Temp-filename*" will read time series of chemical concentrations from the file *Cw-Temp-filename*. Review the section **General Information on Exposure Files**. The format of the exposure file is

time_1 temperature_1 $\text{Cwater}_{1,1}$ Cwater$_{1,2}$ ... $\text{Cwater}_{1,nchem}$
time_2 temperature_2 $\text{Cwater}_{2,1}$ Cwater$_{2,2}$ ... $\text{Cwater}_{2,nchem}$
... ...
time_n temperature_n $\text{Cwater}_{n,1}$ Cwater$_{n,2}$ ... $\text{Cwater}_{n,nchem}$

where time_j (j = 1, 2, ..., n) is the time associated with the observation [tunits]; temperature_j is the environmental water temperature [Celsius]; $\text{Cwater}_{j,k}$ (k = 1, 2, ..., *nchem*) is the water concentration of the k-th chemical [cwunits]. If the "file" option was selected for either the temperature or one of the chemicals, the exposure file should still contain information for all chemicals and temperature, regardless of the options selected for the other variables. If the "file" option is selected for both "/temperature" and "/cwater", *only one* exposure file may be used. The following fragment shows an *improper* sequence:

```
/cwunits       ppm                ! this example shows an improper sequence !
/temperature   file temp.exp
/chemicals         2
/cwater        1 file chem1.exp   ! incorrect.
/cwater        2 constant 0.5
```

i.e., the same file name should appear on both "/temperature file" and "/cwater file" options.

Function options (i.e., sin, exp, constant) overrides the "file" option, both for "/temperature" and "/cwater". For example, given the fragment

```
/cwunits       ppm
/temperature   file cw.exp
/chemicals         2
```

```
/cwater      1 file cw.exp
/cwater      2 constant 0.5
```

The program will simulate both the water concentration of chemical 1 and the ambient temperature using data obtained from the exposure file; water concentration for chemical 2 will be simulated as a constant (5 ppm), regardless of the data present in the exposure file.

Examples:

```
/cwunits  ppm
/chemicals    1
/cwater   1 constant   10
```

Simulate uptake of one chemical; dissolved water concentration shall be 10 ppm.

```
/tunits          years          ! time units: years
/tstart      1                  ! start simulation at year 1
/tend        2                  ! end simulation at year 2
/temperature sin 8 4 6.28 0     ! temperature: sin function;
/cwunits     ppm                ! dissolved chemical in water units: ppm
/chemicals       3              ! simulate 3 chemicals
/cwater      1 constant 10      ! concentration of chemical 1: 10 ppm
/cwater      2 file ex1.exp     ! read concentration from file
/cwater      3 file ex1.exp     ! read concentration from file
```

format of the file "ex1.exp":

```
1.0 10  1.1 2.1 3.1 ! first line
1.2 10  1.2 2.2 3.2
2.0 10  1.3 2.3 3.3 ! last line
```

The temperature will be simulated using the given sine function (for a full description, see examples for the "/temperature" command). The concentration of chemical 1 will be held constant at 10 ppm during the simulation. Chemicals 2 and 3 will be simulated using the data in the file, linearly interpolating between consecutive points as needed.

/LOGP $logP_1\ logP_2 \ldots logP_{nchem}$

The command specifies the chemical's experimental $\log_{10}(K_{ow})$, where K_{ow} is the n-octanol/water partition coefficient. Either "/logp" or "/clogp" should be specified; if both are provided, "/logp" will be used. (See also "/clogp".)

Example:

```
/chemicals       4
/logp        5.91    6.34    6.75    7.19
```

Four chemicals will be simulated; their partition coefficients are as stated.

/MELTING_POINT $MP_1\ MP_2 \ldots MP_{nchem}$

The command specifies the chemical's melting point [Celsius]. These data, together with the chemical's logP, are used to calculate the toxicant's chemical activity.

Example:

```
/chemicals      4
/melting_point  92  100  100  100
```

Four chemicals will be simulated; their melting points are as stated.

/MOLVOL $MV_1\ MV_2 \ldots MV_{nchem}$

The command specifies the chemical's molecular volume [cm^3]. These data are used to calculate the toxicant's aqueous diffusivity:

$$D_w \quad \frac{2.10\,1\times10^{-7}}{1.4\quad M\,V^{0.589}} \tag{23}$$

where D_w is the toxicant's aqueous diffusivity [cm^2/sec], is the viscosity of water [poise], and MV is the molecular volume of the chemical [cm^3] (Hayduk and Laudie 1974). The viscosity of water over its entire liquid range is represented with less than 1% error by

$$\mathrm{Log}_{10}\left(\frac{20}{T}\right) \quad \frac{1.370\,23(T\ \ 20) \quad 8.36\times10^{-4}(T\ \ 20)^2}{10\,9\ \ T} \tag{24}$$

where $_T$ is the viscosity [centipoise] at temperature T [Celsius], and $_{20}$ is the viscosity of water at 20 C (1.002 cp) (Atkins 1978.).

Example:

```
/chemicals      4
/molvol     210     228     245     263
```

Four chemicals will be simulated; their molecular volumes are as stated.

/MOLWT $MW_1\ MW_2 \ldots MW_{nchem}$

The command specifies the chemical's molecular weight [grams/mole].

Example:

```
/chemicals   4
/molwt      292     326     361     395
```

Four chemicals will be simulated; their molecular weights are as stated.

/TOXLAB $<Tlab_1>\ <Tlab_2>\ \ldots\ <Tlab_{nchem}>$

The command simply specifies the name of the chemicals whose exchange kinetics will be simulated and is used for output purposes only. Each label must be delimited with double quotes (").

Example:

```
/chemicals      4
/toxlab         "tetra PCB"  "penta PCB"  "hexa PCB"  "hepta PCB"
```

Four chemicals will be simulated; their labels are as stated.

Fish Characterization Parameters This section describes commands that identify the fish in terms of its taxonomy, physiological characteristics, feeding habits, initial chemical burden, etc.

/ ACTIVE_GILL <fraction>

The command specifies the fraction of the fish's anatomical gill surface area [cm^2] which is physiologically active. Permissible values are such that 0 < fraction 1, although typical values for the variable range between and 1 (Booth 1978, Piiper et al. 1986, Duthie and Hughes 1987). This value is used to adjust the predicted kinetic exchange rates (Barber et al. 1988). It is assumed that the physiologically active fraction of the gill is constant across all year classes for a particular species.

Example: / active_gill 0.5

The fish's physiologically active surface area is 50% of the total gill surface area.

/ DIET

The command describes the diet of all the fish to be simulated, thereby specifying the contribution of each prey item to the predator's total body burden. This command may be used only if the "food_web" mode is selected. The command should appear after all fish species have been defined. The general form of the command is

/ diet
labels (lab_1: "species_name$_1$", lab_2: "species_name$_2$", ..., lab_n: "species_name$_n$")
lab_1 (<range_type> = <range_value>: $lab_1 = f_1$, $lab_2 = f_2$, ... $lab_n = f_n$)
lab_2 (<range_type> = <range_value>: $lab_1 = f_1$, $lab_2 = f_2$, ... $lab_n = f_n$)
...
lab_n (<range_type> = <range_value>: $lab_1 = f_1$, $lab_2 = f_2$, ... $lab_n = f_n$)

The "labels" function defines abbreviations for the species' scientific name (see example below). The first character of a label must be a letter, followed by zero or more letters or digits. Labels must be provided for all species to be simulated. The labels "plankton", "benthos", and "fish" are predefined and may be used only as prey items. These labels should not be redefined.

The "lab_j(...)" function defines the diet of a weight, age, or length class range of a species. These labels are defined by the "labels" function. Diets must be provided for all ranges of all species. The first argument of the function, <range_type> = <range_value>, specifies the type of range to be used for the species, as well as its value. Valid forms are

age = *integer*
age = *integer* - *integer*
weight = *real_number* - *real_number*
length = *real_number* - *real_number*

The form "age = ..." identifies the datum as an age class range (in years), whereas the form "weight = ..." identifies a weight range (in wtunits). The form "length = ..." identifies a length range (in cm). All range types (weight, age, or length) must be the same for a given species. The range type may be different between species. The rest of the arguments of the function specify the prey items (lab_k) and the fraction of the diet they represents (f_k, see example below). "Lab_k" (inside the parenthesis) represents either "plankton", "benthos","fish" or any of the abbreviations defined by the "labels"

function. For each "lab_j(...)", 0 f_k 1, and $_k f_k$ = 1. The section **Simulation Modes** describes how this information is used.

Example:

```
/burden          food_web
/wtunits         grams
/species         Lepomis macrochirus                    ! bluegill
/maximum_age     3
...
/species         Micropterus salmoides                  ! largemouth bass
/maximum_age     6
/initial_wt                                             17.4
...
/species         Ictalurus punctatus
                                                        ! channel catfish
/maximum_age     8
...
/diet
   labels (bluegill: "Lepomis macrochirus", bass: "Micropterus salmoides", &
           catfish: "Ictalurus punctatus")
   bluegill (age = 1-3: benthos = 0.5, plankton = 0.5)
   bass (weight = 17.4 - 41.8: benthos = 0.50, plankton = 0.50)
   bass (weight = 41.8 - 72.2: benthos = 0.50, bluegill = 0.50)
   bass (weight = 72.2 - 300.: benthos = 0.10, bluegill = 0.90)
   catfish (length = 1 - 15: benthos =  1.00)
   catfish (length = 15 - 100: benthos = 0.50, bluegill = 0.50)
/end
```

The diet of the bluegill is 50% plankton, 50% benthos for all year classes. The diet of largemouth bass with weights between 17.4 and 41.8 grams is 50% benthos, 50% plankton; bass with weights between 41.8 and 72.2 grams will feed on 50% benthos, 50% bluegill. The diet of bass with weight larger than 72.2 grams is 10% benthos, 90% bluegill. The diet of catfish in the range of 1 to 15 cm is 100% benthos, and for catfish in the range of 15-100 cm, 50% benthos, 50% bluegill. Note that the last weight range is extended automatically, e.g., the diet of a 350 gram bass is the same as the diet of a 300 gram bass.

/ECOLOGY <fish's aquatic environment>

The command specifies the life form of the fish to be modelled. Presently, the only recognized environments are "fresh" or "marine". This information is used to parameterize the allometric functions that describe gill surface area, lamellar length, and lamellar density. In addition, the keyword "piscivore" may be used to denote a predator-prey relationship (see "/cfish", and the simulation mode "food_chain"). Review "/cfish" for an example on "/ecology piscivore" usage.

Example:

```
/species    Oncorhynchus mykiss          ! rainbow trout
/ecology    fresh
```

/FAMILY <fish's family name>
The command specifies the family of the fish to be modelled. The fish's taxonomy is used to extract appropriate gill morphometric, physiological and trophic parameters from its database file.

Example:

```
/species   Oncorhynchus mykiss          ! rainbow trout
/family    salmonidae
```

/FISHPAR <option$_1$> ... <option$_n$>
The command specifies the species' morphometric, physiological, and trophic parameters to be used in the simulation. Each <option> is of the form "option_name(arg$_1$, ..., arg$_n$)". Valid options (Barber et al. 1988, 1991) are:

assim_eff($_f$). The fish's food assimilation efficiency is approximated by $_f$.

cvol(p_1, p_2, Q_{10}, T_{ref}). The maximum daily clearance volume (Litre / day) = $e^{(T \ T_{ref}) \ln(Q_{10})/10} p_1 W^{\ p_2}$

gamma(p_1, p_2, Q_{10}, T_{ref}). The fish's specific growth rate (day^{-1}) = $e^{(T \ T_{ref}) \ln(Q_{10})/10} p_1 W^{\ p_2}$

gastric_evac(p_1, p_2, p_3, Q_{10}, T_{ref}). The stomach evacuation (grams / day) = $e^{(T \ T_{ref}) \ln(Q_{10})/10} p_1 W^{\ p_2} \ I^{p_3}$ where I is the mass of food resident in the intestine [grams wet]. In general, p_3 = ½ , , or 1 (Jobling 1981).

gill_area(p_1, p_2). The fish's total gill surface area (cm^2) = $p_1 W^{\ p_2}$

lamellar_den(p_1, p_2). The number of lamellae per mm gill filament (mm^{-1}) = $p_1 W^{\ p_2}$

lamellar_len(p_1, p_2). The fish's lamellar length (cm) = $p_1 W^{\ p_2}$

len_wt(p_1, p_2). The fish's body length (L, cm) is approximated by: $W \quad p_1 L^{p_2}$

max_ingestion(p_1, p_2, Q_{10}, T_{ref}). The fish's maximum observed ingestion (grams / day), is $e^{(T \ T_{ref}) \ln(Q_{10})/10} p_1 W^{\ p_2}$

o2_consumption(p_1, p_2, Q_{10}, T_{ref}). The fish's routine respiration (mg O_2 consumed hr^{-1}) is $e^{(T \ T_{ref}) \ln(Q_{10})/10} p_1 W^{\ p_2}$

pafish(p_1, p_2). The fish's aqueous fraction (p_a) = $p_1 \quad p_2 p_l$ where p_l is fish's lipid fraction, and $p_2 < 0$ (Barber et al. 1991).

plfish(p_1, p_2). The fish's lipid fraction (p_l) = $p_1 W^{\ p_2}$

prey_len(p_1, p_2). The prey's body length (L_{prey}, cm) is approximated as a function of the predator's body length ($L_{predator}$, cm) by $L_{prey} \quad p_1 \quad p_2 L_{predator}$

resp_quotient(rq). The fish's respiratory quotient [Litres CO_2 respired / Litres O_2 consumed] is approximated by rq.

satiation_meal(p_1, p_2, Q_{10}, T_{ref}). The size of the satiation meal (F_{sat}, grams) consumed during the interval (0, T_{sat}), is $e^{(T \ T_{ref}) \ln(Q_{10})/10} p_1 W^{\ p_2}$

satiation_time(p_1, p_2, Q_{10}, T_{ref}). The time to satiation when feeding with an initially empty stomach (T_{sat}, minutes), $e^{(T \ T_{ref}) \ln(Q_{10})/10} p_1 W^{\ p_2}$

where W is the live weight of the fish in grams, Q_{10} is the increase/decrease for 10 C rise in temperature, and T_{ref} is the physiological reference temperature [C]. Missing values are denoted by -999. If the option (function) is not provided or has missing values, the missing parameters will be obtained from the database. If the required parameters cannot be obtained, the program will terminate with an appropriate message.

Example:

```
/species   Ontario salmonids
/fishpar   gill_area(2.40, 1.03)  gastric_evac(1.47, 0.000e+00, 0.500, 1.84, 10.0)
/fishpar   resp_quotient(1.00)  o2_consumption(0.234, 0.790, 2.34, 10.0)
/fishpar   pafish(0.80, -1.25)
```

/GROWTH <year_class_range> <option> <arg_1> ... <arg_n>

The command specifies how the fish's growth model will be parameterized (for a particular year class range). Valid forms of this command are:

```
/growth <year_class_range> linear       database
/growth <year_class_range> linear       fishpar
/growth <year_class_range> allometric   <functional_response>
/growth <year_class_range> holling      <functional_response>
/growth <year_class_range> clearance    fishpar <functional_response>
/growth <year_class_range> clearance    database <functional_response>
```

The fish's growth, W[grams wt weight], will be modelled using the mass balance equation

$$\frac{dW}{dt} \quad F \quad E \quad R \quad SDA \quad EX \tag{39}$$

where F, E, R, SDA, and EX are the fish's daily feeding, egestion, respiration, specific dynamic action (i.e., respiration associated with digestion), and excretion, respectively. If the option "linear" is selected, then equation (39) is assumed to be equivalent to the linear differential equation

$$\frac{dW}{dt} \qquad W \tag{40}$$

where , the fish's specific growth rate, is defined as $(dW/dt)/W$ [gram gram^{-1} day^{-1}], and is computed using the function

$$e^{(T \quad T_{ref}) \ln(Q_{10})/10} \quad {}_1W \quad {}^2 \tag{41}$$

where Q_{10} is the change in the growth rate associated with a 10 C rise in temperature; T is the environmental temperature [Celsius] at time t; the parameters $_1$ and $_2$ describe the fish's specific growth rate as a function of its body weight W[grams] at the reference temperature T_{ref} [Celsius]. F, E, SDA, and EX are back-calculated using the fish's respiration, R, and assimilation efficiency. If the modifier "database" is selected, the parameters $_1$, $_2$, Q_{10}, and T_{ref} will be acquired from the database. If "fishpar" is selected, the parameters will be presented in the input file through the command "/fishpar gamma (...)". Any missing parameters will be retrieved from the database.

If the option "allometric" is selected, then feeding is modelled by

$$\begin{aligned} F &= f(\ )F_{max} \\ F_{max} &= e^{(T - T_{ref})\ln(Q_{10})/10} f_1 W^{f_2} \end{aligned} \tag{42}$$

where *f( )* (functional_response) is the ratio of the fish's realized consumption to its *ad libitum* consumption, F_{max}. The program does not attempt to model the fish's functional response. Rather, it may be used to calibrate the fish's predicted growth rate to field or observed growth rates. If the parameters f_1, f_2, Q_{10}, and T_{ref} are not presented in the input file through the use of "/fishpar max_ingestion(...)", the database will be used to determine values appropriate for the particular species and/or family.

If the option "holling" is selected, then feeding is modelled by a Holling-Rashevsky type formulation,

$$\begin{aligned} F &= f(\ )F_{max} \\ F_{max} &= (I_{max} - I) \end{aligned} \tag{43}$$

where *f( )* (functional_response) is again the ratio of the fish's realized consumption to its *ad libitum* consumption, F_{max}, is the fish's *ad libitum* feeding rate [days^{-1}]; I_{max} is maximum amount of food present in the intestinal track, I is the amount of food presently resident in the intestinal track. The fish's stomach contents is itself modelled by

$$\begin{aligned} \frac{dI}{dt} &= F - D \\ D &= e^{(T - T_{ref})\ln(Q_{10})/10} d_1 W^{d_2} \end{aligned} \tag{44}$$

where D represent intestinal evacuation (Holling 1966, Ware 1972, Jobling 1987). If the parameters d_1, d_2, Q_{10}, and T_{ref} are not presented in the input file through the use of "/fishpar gastric_evac(...)", the database will be used to determine values appropriate for the particular species and/or family.

If the option "clearance" is selected, then the particular fish year class (or range) is assumed to be planktivorous and its feeding is modelled by

$$\begin{aligned} F &= f(\ )F_{max} \\ F_{max} &= C_{vol} \\ C_{vol} &= e^{(T - T_{ref})\ln(Q_{10})/10} c_{vol_1} W^{c_{vol_2}} \end{aligned} \tag{45}$$

where *f( )* (functional_response) is the ratio of the fish's realized consumption to its *ad libitum* consumption, F_{max}, is plankton standing stock [grams/Litre], and C_{vol} is the clearance volume of the planktivorous fish [Litre/day]. The program does not attempt to model the fish's functional response. Rather, it may be used to calibrate the fish's predicted growth rate to field or observed growth rates. If the parameters c_{vol1}, c_{vol2}, Q_{10}, and T_{ref} are not presented (see "/fishpar cvol(...)"), the database will be used to determine values appropriate for the particular species and/or family.

In all cases, the required physiological parameters will be retrieved from the database file, based on either the fish's family or species. If any required function cannot be fully parameterized, the program terminates with an appropriate message.

Example:

```
/growth    1 allometric 1.00
/fishpar   max_ingestion (0.03, 1.0, 1, 10.0)
```

The fish will feed at a constant ration, 3% of its body weight; since $Q_{10} = 1$, there is no temperature effect; the value of T_{ref} is completely arbitrary (for this example).

/INITIAL_CF <year_class_range> <cf_1> <cf_2> ... <cf_{nchem}>

The command specifies the fish's initial chemical whole body concentration on a live weight basis for the specified year class (or range of year classes). The units of concentration are specified by "/cfunits". The command "/chemicals" must precede this command.

Example:

```
/cfunits          nanograms / mL
/chemicals        2
/toxlab                              "tetra PCB"   "penta PCB"
/species          Oncorhynchus kisutch
! coho salmon
/maximum_age      2
/initial_cf       1 310 110
/initial_cf       2 320 120
```

Simulate uptake kinetics of tetra- and penta-PCB in coho salmon, using two year classes. The initial total body chemical concentration of tetra- and penta-PCB for year class one will be 310 and 110 nanograms/mL; for year class two will be 320 and 120 nanograms/mL.

/INITIAL_WT <arguments>

The command specifies the initial live weight of the species' young of the year or of all age classes. Valid forms of this command are:

```
/initial_wt       W1
/initial_wt       W1 W2 ... WNage
```

where W is the weight of the particular age class, its units specified by the command "/wtunits", and "Nage" is the number of age classes, defined with the command "/maximum_age". If either "/burden laboratory ..." or "/burden food_chain ..." is selected, only the first form of the command (providing only one fish weight) is valid, because these modes allow only one age class. If "/burden food_web" is selected, either form of the command may be used. If only one weight is provided, and Nage > 1, then FGETS will generate the species' initial weight distribution using the growth model selected by the user, otherwise the values presented by the user define the distribution. In all cases, the initial weight will be converted from "wtunits" into live grams for internal usage and subsequent model output.

Example:

```
/wtunits        grams
/species        Alosa pseudoharengus    ! alewife
/maximum_age    2
/initial_wt         0.5
```

Simulate two year classes for alewife; the initial weight of year class one is 0.5 grams. FGETS will generate the weight of year class two.

/LC50 <chemical number> <option> <arg_1> ... <arg_n>

The command specifies the formulation to be used to determine the toxicant's lethal activity. The command is optional. Valid forms of this command are:

/lc50 <chemical number> log/log_fathead p_0 p_1
/lc50 <chemical number> observed p_0 <units>

where <chemical number> is an integer between one and *nchem*. The form "/lc50 <chemical number> log/log_fathead p_0 p_1" will determine the toxicant's lethal activity as

$$\log(LA_{toxicant}) \quad p_0 \quad p_1 \log(LA_{fathead})$$

where $LA_{fathead}$ (i.e., lethal activity in fathead minnows) is 0.0472 (see **Toxicological effects** section).

The form "/lc50 <chemical number> observed p_0 <units>" will set the LC_{50} for the given chemical to p_0 <units>; <units> will be converted to ppm and the lethal activity will be computed using Eq.(11). If the command is not provided for a particular chemical and species, the lethal activity will be determined from the generalized inter-species correlation from Barnthouse at al. 1986.

$$\log(LA_{toxicant}) \quad 0.501 \quad 1.01 \log(LA_{fathead})$$

The lethal activity that will be used in the simulation will be the geometric mean of the LA_{50}'s of the *nchem* chemicals.

Example:

```
    /chemicals      1
    /toxlab         "Fenvalerate"
    /molvol     382
    /molwt      419.9
    /logp       5.2
!
! channel catfish LC50 from: Smith, S., T.E. Reagan, J.L. Flynn, and G.H. Willis. 1983.
!   Azinphosmethyl and Fenvalerate runoff loss from a sugarcane-insect
!   IPM system. J.Environ.Qual. 12: 534-537.
!
    /species    Ictalurus punctatus                 ! channel catfish
    /lc50       1 observed 1.83 microgramme / Litre  ! 24-hour LC50
```

The observed 24-hour LC_{50} (1.83 µg/Litre) will be used to determine the lethal activity of Fenvalerate in catfish. The lethal activity (Eq.(11)) is 5.44×10^{-4}.

/LENWT allometric <option>
The command describes the allometric function relating the length of the fish [cm] to its body weight [grams]. This command is required only if a predator-prey formulation is requested (see "/burden food_chain or food_web"). Valid forms are:

/lenwt allometric fishpar
/lenwt allometric database

If the form "/lenwt allometric fishpar" is used, the parameters will be presented through the command "/fishpar len_wt (<a_0>, <a_1>)" such that

$$W \quad a_0 L^{a_1}$$

where W is the weight of the fish [grams wet weight], and L is the fish's length [cm]. The form "/lenwt allometric database" implies that Eq. (48) will be parameterized using the database.

Examples:

```
/species    Alosa pseudoharengus    ! alewife
/lenwt      1  allometric fishpar
/fishpar    len_wt (7.76e-03, 3.01)
```

The length-weight regression to be used is weight_alewife [grams] = 7.76×10^{-3} length_alewife$^{3.01}$[cm].

```
/species    Alosa pseudoharengus
/lenwt      1  allometric database
```

Use the length-weight allometric regression present in the database for alewife.

/MAXIMUM_AGE <Nage>
The command is used to specify the maximum age of the fish (Nage). The command must be provided if the "food_web" mode is selected; in this case, "Nage" year classes of the given fish species will be simulated. When the age of a cohort (year class) is greater that "Nage", that cohort dies and is replaced with a new one year old cohort. The command is ignored if either "laboratory" or "food_chain" modes are selected. Review the "food_web" mode in the **Simulation** section.

Example:

```
/burden         food_web
/species        Alosa pseudoharengus    ! alewife
/maximum_age    2
```

Maximum age of the alewife is two years.

/ OBSERVATIONS $<arg_1>$ ... $<arg_n>$

Observed data may be plotted along with the model predictions. This command specifies which type of observations and the order in which they are presented in the input file line. Valid arguments are:

"time" (simulation time, units given by "/tunits"),
"cfish" (fish total body toxicant concentration, units given by "/cfunits"),
"wt" (weight of the fish, units given by "/wtunits")

Two or more arguments must be present. If more than one chemical is present in the simulation (see "/chemicals") and "cfish" is specified, then all the fish toxicant concentrations must be in consecutive columns. Example: to compare observed data for a simultaneous exposure to three chemicals against the model predictions, the input file may look like:

/chemicals 3
/plot cfish(wt)
/species Species name
/observations time wt cfish
$time_1$ wt_1 $cfish_{1,1}$ $cfish_{1,2}$ $cfish_{1,3}$
$time_2$ wt_2 $cfish_{2,1}$ $cfish_{2,2}$ $cfish_{2,3}$
... ...
$time_n$ wt_n $cfish_{n,1}$ $cfish_{n,2}$ $cfish_{n,3}$
/end

Example:

```
/chemicals      4
/plot           cfish(wt)
/species        Ontario salmonids
/observations wt cfish
        1186.     217.3    398.5    274.3    142.3    ! oncorhynchus mykiss/ vineland
        1000.     39.7     153.6    177.7    111.9    ! oncorhynchus mykiss/ vineland
        1410.     363.2    790.0    599.2    275.6    ! oncorhynchus kisutch/ vineland
```

Simulate four chemicals. Plot the toxicant's concentration in whole fish (cfish) *vs.* weight of fish(wt); the observed data will be included in the plot.

/plfish <year_class_range> <option> $<arg_1>$ ... $<arg_n>$

The command specifies the fraction of the fish's live weight that is lipid (*pl*), for the specified year class (or year class range). Valid forms for this command are:

/plfish <year_class_range> allometric database
/plfish <year_class_range> allometric fishpar
/plfish <year_class_range> allometric pl_1 pl_2
/plfish <year_class_range> constant pl_1
/plfish <year_class_range> linear pl_1 pl_2

All forms "/plfish ... allometric ..." will estimate the fish's lipid fraction using the allometric function, $pl \quad pl_1 W^{pl_2}$. The form "... allometric database" will retrieve the parameters (pl_1, pl_2) from

the FGETS database. The form "... allometric fishpar" will retrieve the parameters from the command "/fishpar plfish (pl_1, pl_2)". The form "... allometric pl_1 pl_2" provides the parameters directly; this form is particularly useful when the fish's lipid fraction is a function of the age class.

The form "/plfish ... constant pl_1" will estimate the fish's lipid fraction by $pl \quad pl_1$. The form "/plfish ... linear pl_1 pl_2" will estimate the fish's lipid fraction by $pl \quad pl_1 \quad pl_2 W$. In all cases, W has units of wtunits.

Example: /plfish 1-3 constant 0.03
The fish's lipid fraction (for age classes one through three) will be 3% for the duration of the simulation.

/SPECIES <fish's scientific name>
The command specifies the scientific name of the fish to be modelled, e.g., rainbow trout must be specified as *Oncorhynchus mykiss*. The fish's taxonomy is used to extract appropriate gill morphometric, physiological and trophic parameters from the database file.

Example: /species Oncorhynchus mykiss ! rainbow trout
The commands following the "/species" command will apply to Rainbow trout.

Files used by FGETS:

FGETS3.DB, database file containing gill morphometric, physiological and trophic parameters. The database file is provided with the program. Review the **FGETS Database** section for a description of the file, its parameters, and format.

command file, containing the commands describing the simulation. Extra input files containing exposure information may be required, depending on the options selected by the user.

chemical aqueous concentration and temperature file: this file is required if either "/cwater ... file" or "/temperature file" options were selected.

concentration of chemical in benthos file: this file is required if "/cbenthos file" was selected.

concentration of chemical in plankton file: this file is required if "/cplankton file" was selected; if both "/cplankton file" and "/plankton_standing_stock file" options were selected, the information must be contained in the same file.

plankton standing stock: this file is required if "/plankton_standing_stock file" was selected; if both "/cplankton file" and "/plankton_standing_stock file" options were selected, the information must be contained in the same file.

output file, containing the results of the simulation and any error conditions detected by the program. The file will have the name of the input file, with extension ".fgz"; e.g., "test.dat" will generate "test.fgz". If the file already exists, it will be silently overwritten.

updated command file, containing an updated input file. This file is created only by request; see "/print update_input" for more information. The file will have the name of the input file, with extension ".fcs"; e.g., "test.dat" will generate "test.fcs".

time series file, containing time series information. This file is created only by request; see "/print time_series" for more information. The file will have the name of the input file, with extension ".fts"; e.g., "test.dat" will generate "test.fts".

General Information on Exposure Files This section contains information that is common for all exposure files. Files are free format and may contain end-of-line comments. The general format of the files is

t_1 $v_{1,1}$ $v_{1,2}$ ... $v_{1,M}$! comment
t_2 $v_{2,1}$ $v_{2,2}$ ... $v_{2,M}$! comment
... ...
t_n $v_{n,1}$ $v_{n,2}$ ... $v_{n,M}$! comment

where n is the number of lines in the file, and M is the number of dependent variables. The first column of the file is simulation time, in units of tunits. The time sequence must be nondecreasing (i.e., t_i t_{i+1}, i = 1, 2, ..., n-1), and, t_1 tstart < tend t_n. The increment between consecutive time points is completely arbitrary. The time sequences for each file are completely arbitrary. Linear interpolation will be utilized as required during the simulation to approximate the dependent variable at simulation-generated times.

FGETS Database The database file (FGETS3.DB) provides the morphological, physiological, and trophic parameters required to parameterize the growth, gill geometry, and predator-prey size dependent feeding relationships.

Parameter Description The database file contains the following allometric functions and parameters:

Total gill surface area [cm^2] = $sa_1 W^{sa_2}$

Number of lamellae / mm gill filament ( ) = $_1 W^{\ 2}$

Lamellar length [cm] = $lam\ l_1 W^{lam\ l_2}$

Fish's lipid fraction (p_l) = $pl_1 W^{pl_2}$

Fish's aqueous fraction = pa_1 $pa_2\ p_l$ where $pa_2 < 0$, see Barber et al. 1991)

Fish weight [grams wet] = $lw_1 L^{lw_2}$ where L is the fish's body length [cm].

Predator feeds on prey according to: L_{prey} $pred_1$ $pred_2\ L_{predator}$ where L_{prey} is the prey's body length [cm], and $L_{predator}$ is the predator's body length [cm].

Maximum observed ingestion (F_{max}, grams / day) = $e^{(T\ T_{ref,cmax}) \ln(Q_{10,cmax})/10}\ cmax_1 W^{cmax_2}$

Maximum daily clearance volume (C_{vol}, Litre / day) = $e^{(T\ T_{ref,cvol}) \ln(Q_{10,cvol})/10}\ cvol_1 W^{cvol_2}$

Size of the satiation meal (F_{sat}, grams) consumed in the interval (0, T_{sat}) = $e^{(T\ T_{ref,fsat}) \ln(Q_{10,fsat})/10}\ fsat_1 W^{fsat_2}$

Time to satiation when feeding with an initially empty stomach (T_{sat}, min.) = $e^{(T\ T_{ref,tsat}) \ln(Q_{10,tsat})/10}\ tsat_1 W^{tsat_2}$

Stomach evacuation (*Evac*, grams / day) = $e^{(T\ T_{ref,evac})\ln(Q_{10,evac})/10}\ evac_1 W^{\ evac_2}\ I^{evac_3}$ where *I* is the mass of food resident in the intestine [grams wet]. In general, $evac_3$ = ½ , , or 1 (Jobling 1981).

Routine respiration (O_2, mg O_2 consumed hr^{-1}) = $e^{(T\ T_{ref,ox})\ln(Q_{10,ox})/10}\ ox_1 W^{\ ox_2}$

Specific growth rate (, day^{-1}) = $e^{(T\ T_{ref,})\ln(Q_{10,})/10}\ {}_1W^{\ 2}$

Food assimilation efficiency: $_f$

Respiratory quotient [Litres CO_2 respired / Litres O_2 consumed]: *rq*

Average weight [grams wet] of the species' young of the year: $W_{year\ one}$

Q_{10} = increase / decrease for 10 C rise in temperature (for each process)

T_{ref} = physiological reference temperature [C]

Database Organization The database is partitioned in sets of 13 records, each set representing data for one species. The XXX-th data set contains the following information:

XXX.01	species / family / habitat / ecological_function					
XXX.02	Reference					
XXX.03	sa_1	sa_2	$_1$	$_2$	$laml_1$	$laml_2$
XXX.04	pl_1	pl_2	pa_1	pa_2		
XXX.05	lw_1	lw_2	$pred_1$	$pred_2$		
XXX.06	*cmax1*	$cmax_2$	$Q_{10,cmax}$	$T_{ref,cmax}$		
XXX.07	$cvol_1$	$cvol_2$	$Q_{10,cvol}$	$T_{ref,cvol}$		
XXX.08	$fsat_1$	$fsat_2$	$Q_{10,fsat}$	$T_{ref,fsat}$		
XXX.09	$tsat_1$	$tsat_2$	$Q_{10,tsat}$	$T_{ref,tsat}$		
XXX.10	$_f$	$evac_1$	$evac_2$	$evac_3$	$Q_{10,evac}$	$T_{ref,evac}$
XXX.11	*rq*	ox_1	ox_2	$Q_{10,ox}$	$T_{ref,ox}$	
XXX.12	$_1$	$_2$	$Q_{10,}$	$T_{ref,}$		
XXX.13	$W_{year\ one}$					

A value of -999 designates a parameter which was not reported. A list of the fishes represented in the database can be found in Table 3.

Restrictions and Limitations The program will issue appropriate error messages if any of the following conditions are violated. In general, entries should be defined before they can be used, e.g., define the number of chemicals to be simulated (*nchem*) before providing chemical information.

Commands may be presented in any order with the exceptions noted below.

- the "/chemicals" command must precede any other command that is chemical-specific (e.g., /melting_point, /clogp, "/plot cf_aroclor ...", etc.) because it defines the number of entries that will be present in these commands. This permits more robust error checking.
- the "/species" command must precede the commands for the particular fish, since this command essentially defines a (new) fish.
- the "/maximum_age" command must precede commands that require year class identifiers. The command is required when the food_web simulation mode is enabled.
- the "/diet" command, if present, should be the penultimate command in the input file.
- the "/end" command must be the last command. Any other text or commands following it will be ignored.

A maximum of ten chemicals may be simulated simultaneously.

The maximum number of species is five.

The maximum number of observations per species is 50.

The maximum number of age classes per species is 15.

Units recognized by FGETS The commands "/cfunits", "/cwunits", "laboratory (flow = ..., volume = ...)", /tunits", "/wtunits", and "/lc50 ... observed ..." require units (or combination of units) as arguments. This section describes the syntax of units and the units and prefixes recognized by the program.

All units are referenced to the MKS system (i.e., metre, kilogramme, second). Table 1 presents the prefixes available; Table 2 presents the units, the conversion factor to the MKS system, and their dimensionality.

Units and prefixes may be presented in upper or lower case. If prefixes are used, no embedded blanks may occur between the prefix and the unit name, e.g., "milligrams" is correct, "milli grams" is incorrect. Only those units presented in Table 2 are valid, with the exception of simple translation of plural to singular form, i.e., remove the trailing "s" and search the table, "inches" translated to "inch" being the most notable exception to the rule. The circumflex (^) is used to denote exponentiation (e.g., cm^{-2} is presented as cm^-2). The slash (/) is used to denote division, with the proviso that it may be used only *once* per expression. For example, both "mg/Litre", and "mg Litre^-1" are correct; the form "mg/g/day" is incorrect; it may be presented as "mg g^-1 day^-1" or "mg/g day", although the first form is preferred. The unit conversion factor (Table 2) converts from the given unit to the MKS system, e.g., 1 electron volt $\times$ 6.24×10^{18} $1\ metre^2\ kilogram\ second^{-2}$.

Table 1. Valid Unit Prefixes

Prefix Name	Conversion Factor
atto	10^{-18}
centi	10^{-02}
deca	10^{+01}
deci	10^{-01}
exa	10^{+18}
femto	10^{-15}
giga	10^{+09}
hecto	10^{+02}
kilo	10^{+03}
mega	10^{+06}
micro	10^{-06}
milli	10^{-03}
myria	10^{+04}
nano	10^{-09}
peta	10^{+15}
pico	10^{-12}
tera	10^{+12}

Table 2. Valid Unit Names

	Conversion	Dimensions			
Unit Name	Factor	Metre	Kg	Second	Description
acre	2.471×10^{-04}	2	0	0	4840 yards^2
amu	$6.022 \times 10^{+26}$	0	1	0	atomic mass unit
angstrom	$1.000 \times 10^{+10}$	1	0	0	
are	1.000×10^{-02}	2	0	0	100 metre^2
atm	9.869×10^{-06}	-1	1	-2	atmosphere
atmosphere	9.869×10^{-06}	-1	1	-2	
au	6.684×10^{-12}	1	0	0	astronomical unit
bar	1.000×10^{-05}	-1	1	-2	10^5 pascal
barn	$1.000 \times 10^{+28}$	2	0	0	10^{-24} cm^2
barrel	$8.386 \times 10^{+00}$	3	0	0	31.5 gallons
btu	9.479×10^{-04}	2	1	-2	
bushel	$2.838 \times 10^{+01}$	3	0	0	2150.42 inches^3
calorie	2.388×10^{-01}	2	1	-2	
carat	$5.000 \times 10^{+03}$	0	1	0	0.2 grams
cc	$1.000 \times 10^{+06}$	3	0	0	cm^3
century	3.169×10^{-10}	0	0	1	100 years
chain	4.971×10^{-02}	1	0	0	66 feet
chaldron	9.173×10^{-01}	3	0	0	288 gallons
circularmill	$1.974 \times 10^{+09}$	2	0	0	
cm	$1.000 \times 10^{+02}$	1	0	0	
cup	$4.227 \times 10^{+03}$	3	0	0	8 fluidounces
day	1.157×10^{-05}	0	0	1	
decade	3.169×10^{-09}	0	0	1	10 years
dyne	$1.000 \times 10^{+05}$	1	1	-2	
electronvolt	$6.242 \times 10^{+18}$	2	1	-2	
eon	3.169×10^{-17}	0	0	1	10^9 years
erg	$1.000 \times 10^{+07}$	2	1	-2	
fathom	5.468×10^{-01}	1	0	0	6 feet
feet	$3.281 \times 10^{+00}$	1	0	0	
firkin	$3.355 \times 10^{+01}$	3	0	0	4 firkin 1 barrel
fluidounce	$3.381 \times 10^{+04}$	3	0	0	16 fluidounces 1 pint
foot	$3.281 \times 10^{+00}$	1	0	0	
fortnight	8.267×10^{-07}	0	0	1	2 weeks
ft	$3.281 \times 10^{+00}$	1	0	0	feet, foot
furlong	4.971×10^{-03}	1	0	0	660 feet
g	$1.000 \times 10^{+03}$	0	1	0	grams
galileo	$1.000 \times 10^{+02}$	1	0	-2	
gallon	$2.642 \times 10^{+02}$	3	0	0	3.785 Litre
gm	$1.000 \times 10^{+03}$	0	1	0	grams
grain	$1.543 \times 10^{+04}$	0	1	0	7000 grains 1 pound
gram	$1.000 \times 10^{+03}$	0	1	0	

Table 2: Valid Unit Names (Continuation)

	Conversion	Dimensions			
Unit Name	Factor	Metre	Kg	Second	Description
gramforce	$1.020 \times 10^{+02}$	1	1	-2	
gramme	$1.000 \times 10^{+03}$	0	1	0	
hand	$9.843 \times 10^{+00}$	1	0	0	4 inches
hectare	1.000×10^{-04}	2	0	0	100 are
hertz	$1.000 \times 10^{+00}$	0	0	-1	
hogshead	$4.193 \times 10^{+00}$	3	0	0	14553 inches^3
horsepower	1.340×10^{-03}	2	1	-3	746 watts
hour	2.778×10^{-04}	0	0	1	
hr	2.778×10^{-04}	0	0	1	hour
hz	$1.000 \times 10^{+00}$	0	0	-1	hertz
imperialgallon	$2.200 \times 10^{+02}$	3	0	0	4.54 Litre
inch	$3.937 \times 10^{+01}$	1	0	0	
jeroboam	$3.251 \times 10^{+02}$	3	0	0	104 fluidounces
joule	$1.000 \times 10^{+00}$	2	1	-2	
kg	$1.000 \times 10^{+00}$	0	1	0	kilograms
km	1.000×10^{-03}	1	0	0	kilometre
knot	$1.944 \times 10^{+00}$	1	0	-1	1 nauticalmile / hour
l	$1.000 \times 10^{+03}$	3	0	0	Litre
lb	$2.205 \times 10^{+00}$	0	1	0	pound
league	2.071×10^{-04}	1	0	0	3 miles
lightyear	1.057×10^{-16}	1	0	0	
link	$4.971 \times 10^{+00}$	1	0	0	0.66 feet
liter	$1.000 \times 10^{+03}$	3	0	0	
litre	$1.000 \times 10^{+03}$	3	0	0	
lunation	3.919×10^{-07}	0	0	1	29.53 days
m	$1.000 \times 10^{+00}$	1	0	0	metre
magnum	$6.763 \times 10^{+02}$	3	0	0	50 fluidounces
meter	$1.000 \times 10^{+00}$	1	0	0	
metre	$1.000 \times 10^{+00}$	1	0	0	
metricton	1.000×10^{-03}	0	1	0	1 tonne
mg	$1.000 \times 10^{+06}$	0	1	0	milligrams
micron	$1.000 \times 10^{+06}$	1	0	0	10^{-6} metre
mil	$3.937 \times 10^{+04}$	1	0	0	0.001 inch
mile	6.214×10^{-04}	1	0	0	5280 feet
millennium	3.169×10^{-11}	0	0	1	1000 years
min	1.667×10^{-02}	0	0	1	minute
minim	$2.029 \times 10^{+07}$	3	0	0	600 minim 1 fluidounce
minute	1.667×10^{-02}	0	0	1	
ml	$1.000 \times 10^{+06}$	3	0	0	
mm	$1.000 \times 10^{+03}$	1	0	0	
mmhg	7.501×10^{-03}	-1	1	-2	mm Mercury 1 torr
month	3.858×10^{-07}	0	0	1	

Table 2: Valid Unit Names (Continuation)

	Conversion	Dimensions			
Unit Name	Factor	Metre	Kg	Second	Description
nauticalmile	5.400×10^{-04}	1	0	0	1852 metre
nebuchadnezzar	$6.604 \times 10^{+01}$	3	0	0	4 gallons
newton	$1.000 \times 10^{+00}$	1	1	-2	
ng	$1.000 \times 10^{+12}$	0	1	0	nanograms
ounce	$3.527 \times 10^{+01}$	0	1	0	
oz	$3.527 \times 10^{+01}$	0	1	0	ounce
parsec	3.241×10^{-17}	1	0	0	
pascal	$1.000 \times 10^{+00}$	-1	1	-2	101325 pascal 1 atm
peck	$1.135 \times 10^{+02}$	3	0	0	4 peck 1 bushel
petroleumbarrel	$6.290 \times 10^{+00}$	3	0	0	42 gallons
pint	$2.113 \times 10^{+03}$	3	0	0	8 pint 1 gallon
poise	$1.000 \times 10^{+01}$	-1	1	-1	
pound	$2.205 \times 10^{+00}$	0	1	0	
poundal	$7.233 \times 10^{+00}$	1	1	-2	
poundforce	2.248×10^{-01}	1	1	-2	
ppb	$1.000 \times 10^{+06}$	-3	1	0	nanograms / mL
ppm	$1.000 \times 10^{+03}$	-3	1	0	µgrams / mL
ppq	$1.000 \times 10^{+12}$	-3	1	0	femtograms / mL
ppt	$1.000 \times 10^{+09}$	-3	1	0	parts per trillion, picogram / mL
quart	$1.057 \times 10^{+03}$	3	0	0	4 quarts 1 gallon
quintal	1.000×10^{-02}	0	1	0	100 Kilograms
rod	1.988×10^{-01}	1	0	0	16.5 feet
s	$1.000 \times 10^{+00}$	0	0	1	second
sec	$1.000 \times 10^{+00}$	0	0	1	second
second	$1.000 \times 10^{+00}$	0	0	1	
slug	6.854×10^{-02}	0	1	0	14.59 Kilograms
span	$4.374 \times 10^{+00}$	1	0	0	9 inches
stere	$1.000 \times 10^{+00}$	3	0	0	
stoke	$1.000 \times 10^{+04}$	2	0	-1	
stone	1.575×10^{-01}	0	1	0	6.35 Kilograms
tablespoon	$6.763 \times 10^{+04}$	3	0	0	0.5 fluidounces
teaspoon	$2.029 \times 10^{+05}$	3	0	0	3 teaspoon 1 tablespoon
ton	1.102×10^{-03}	0	1	0	2000 pounds
tonne	1.000×10^{-03}	0	1	0	1000 Kilograms
torr	7.501×10^{-03}	-1	1	-2	760 torr 1 atm
troyounce	$3.215 \times 10^{+01}$	0	1	0	31.10 grams
watt	$1.000 \times 10^{+00}$	2	1	-3	
week	1.653×10^{-06}	0	0	1	
yard	$1.094 \times 10^{+00}$	1	0	0	
year	3.169×10^{-08}	0	0	1	

Fishes of the FGETS model. The FGETS database contains physiological, morphological, and trophic allometric functions for the fishes listed in Table 3. The parameters of the database are used to predict characteristics of fishes (growth, lipid content, oxygen consumption, etc.) needed for predicting bioaccumulation of organic chemicals. The database itself contains references to the original work from which the parameters were derived.

Table 3. Species in the FGETS database.

Species	Family	Common name
Alosa pseudoharengus	Clupeidae	alewife
Anabas testudineus	Anabantidae	oriental climbing perch
Blennius pholis	Blenniidae	mudskipper, shanny
Boleophthalmus boddarti	Blenniidae	mudskipper
Botia dario	Cobitidae	
Botia lohachata	Cobitidae	loach
Catostomus commersoni	Catostomidae	white sucker
Channa punctata	Channidae	Indian air-breathing catfish
Cirrhinus mrigala	Cyprinidae	freshwater major carp
Clarias batrachus	Clariidae	walking catfish
Clarias mossambicus	Clariidae	African air-breathing catfish
Cobitis taenia	Cobitidae	spined loach
Coregonus clupeaformis	Salmonidae	lake whitefish
Coryphaena hippurus	Coryphaenidae	dolphin
Cyprinus carpio	Cyprinidae	common carp
Gambusia affinis	Poeciliidae	mosquitofish
Glossogobius giuris		freshwater goby
Ictalurus nebulosus	Ictaluridae	brown bullhead
Katsuwonus pelamis	Scombridae	skipjack tuna, oceanic bonito
Lampetra fluviatilis	Petromyzontidae	river lamprey (parasitic)
Lampetra planeri	Petromyzontidae	brook lamprey (nonparasitic)
Leiopotherapon unicolor	Teraponidae	spangled perch
Lepidocephalichthys guntea	Cobitidae	snakeheaded loach
Lepisosteus oculatus	Lepisosteidae	spotted gar

Species	Family	Common name
Lepisosteus osseus	Lepisosteidae	longnose gar
Lepisosteus platostomus	Lepisosteidae	shortnose gar
Micropterus dolomieui	Centrarchidae	smallmouth bass
Micropterus salmoides	Centrarchidae	largemouth bass
Mystus cavasius		Indian freshwater catfish
Noemacheilus barbatulus	Cobitidae	stone loach
Oncorhynchus kisutch	Salmonidae	coho salmon
Oncorhynchus mykiss	Salmonidae	rainbow trout
Oncorhynchus tshawytscha	Salmonidae	chinook salmon
Opsanus tau	Batrachoididae	toadfish
Oryzias latipes	Oryziidae	medaka
Platichthys flesus	Pleuronectidae	sole, flounder
Raja clavata	Rajidae	thornback ray
Saccobranchus fossilis	Saccobranchidae	Asian airsack catfish
Salmo trutta	Salmonidae	brown trout
Salvelinus alpinus	Salmonidae	arctic char
Salvelinus namaycush	Salmonidae	lake trout
Scomber scombrus	Scombridae	Atlantic mackerel
Scyliorhinus canicula	Scyliorhinidae	lesser spotted dogfish
Scyliorhinus stellaris	Scyliorhinidae	large spotted dogfish
Seriola quinqueradiata	Carangidae	yellowtail
Stizostedion canadense	Percidae	sauger
Stizostedion vitreum	Percidae	walleye
Thunnus thynnus	Scombridae	bluefin tuna
Tinca	Cyprinidae	tench

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